

Supplementary Information

Regioselective N- versus P-deprotonation of aminophosphane tungsten(0) complexes

Tatjana Terschüren,^a Philip Junker,^a Alexander Schmer,^a Arturo Espinosa Ferao^{*b} and Rainer Streubel^{*a}

^a Prof. Dr. R. Streubel, M. Sc. Tatjana Terschüren, Dr. P. Junker, Dr. A. Schmer Institute of Inorganic Chemistry, University of Bonn, Gerhard-Domagk-Str. 1 53115 Bonn, Germany. Email: r.streubel@uni-bonn.de
<https://www.chemie.uni-bonn.de/akstreubel>

^b Prof. Dr. A. Espinosa Ferao, Departamento de Química Orgánica, Facultad de Química, Universidad de Murcia, Campus de Espinardo, 30100 Murcia, Spain. Email: artuesp@um.es
<https://www.um.es/funcmolecma/artuesp>

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1. NMR spectra of compounds 3-7

1.1 Complex 3a

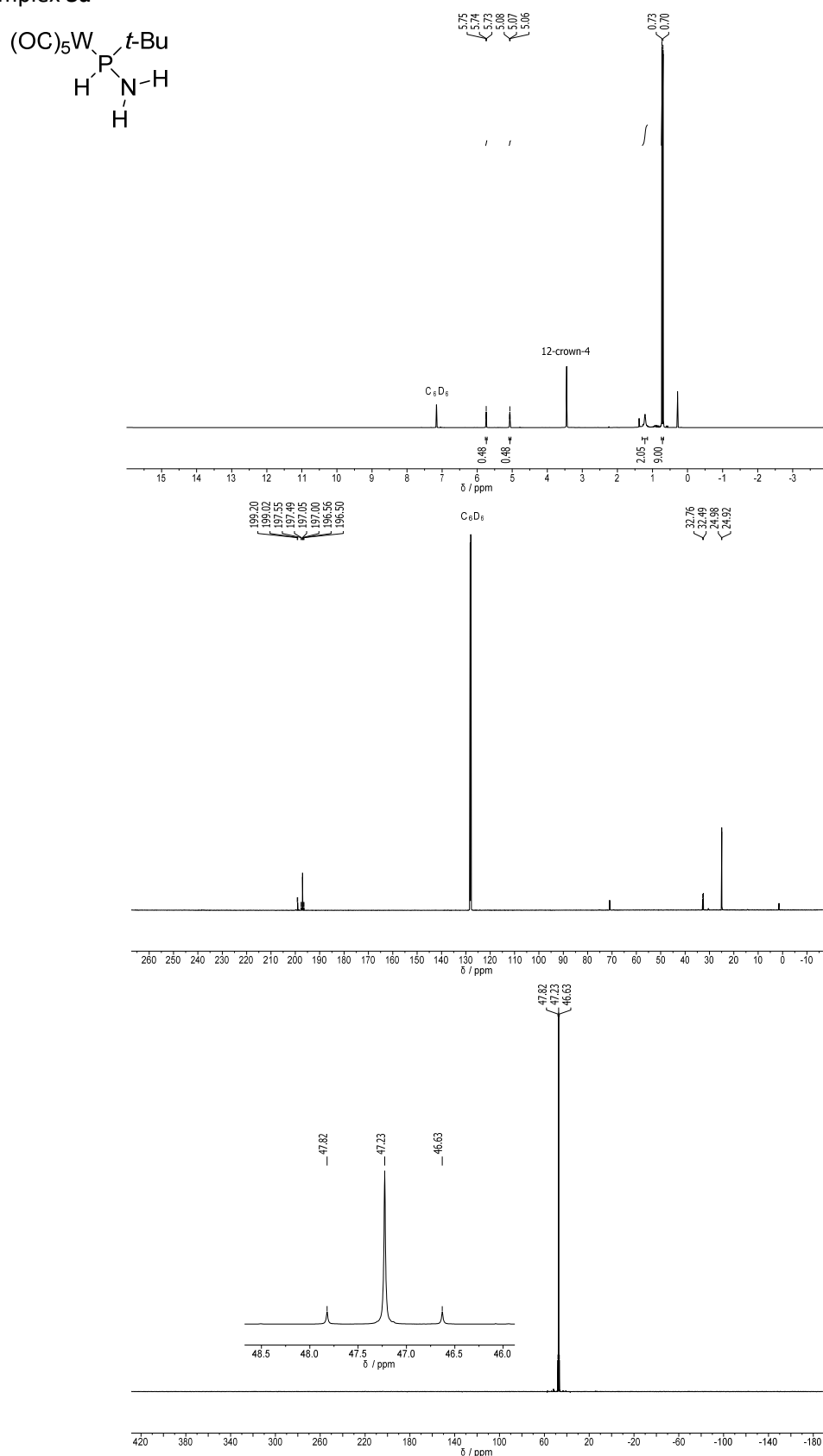


Figure S1. 1H NMR (top), $^{13}C\{^1H\}$ NMR (mid) and $^{31}P\{^1H\}$ NMR (bottom) spectra of complex 3a in C_6D_6 .

1.2 Complex **3b**

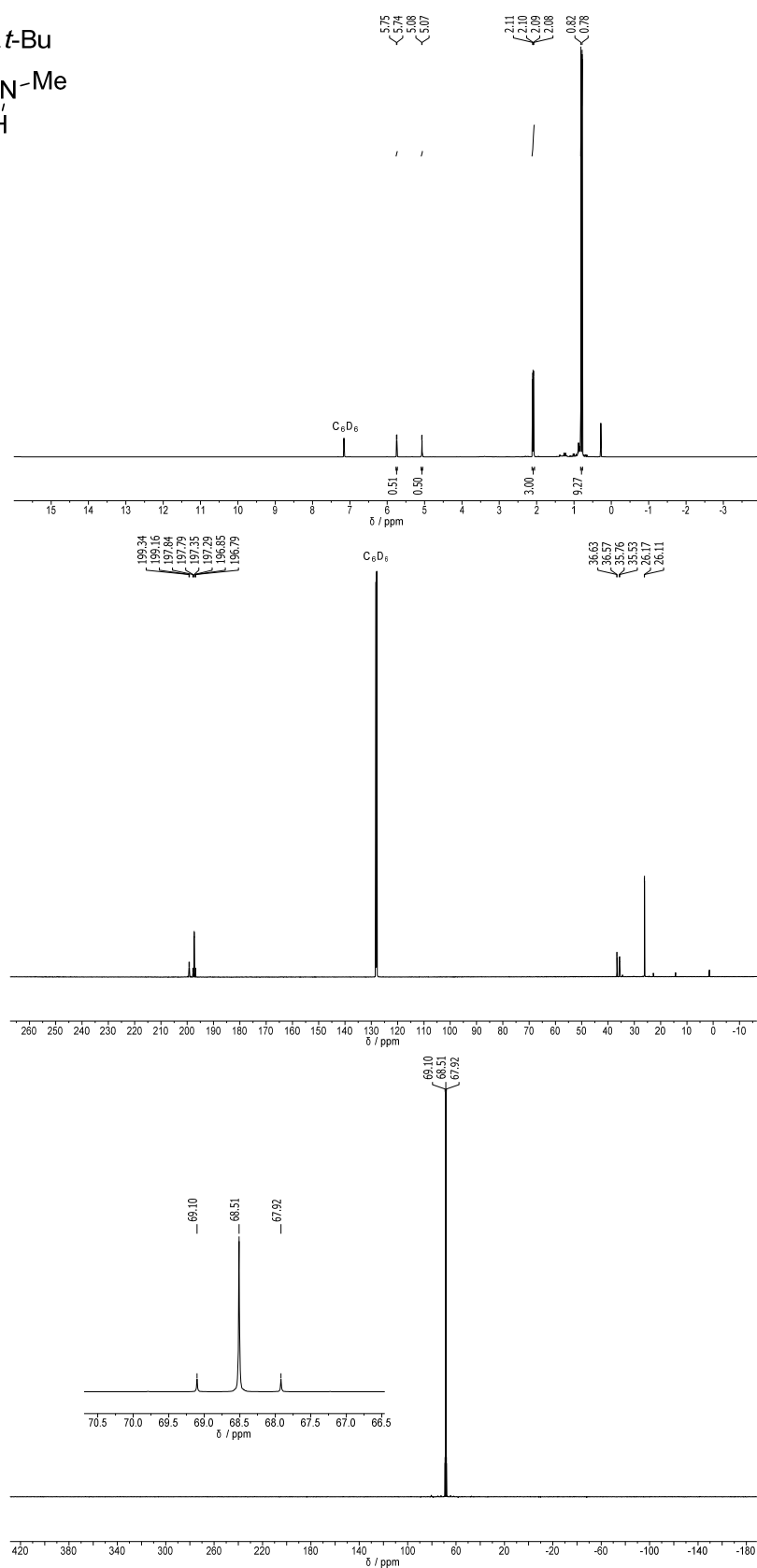
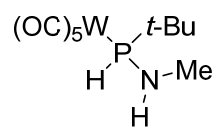


Figure S2. ^1H NMR (top), $^{13}\text{C}\{^1\text{H}\}$ NMR (mid) and $^{31}\text{P}\{^1\text{H}\}$ NMR (bottom) spectra of complex **3b** in C_6D_6 .

1.3 Complex **3c**

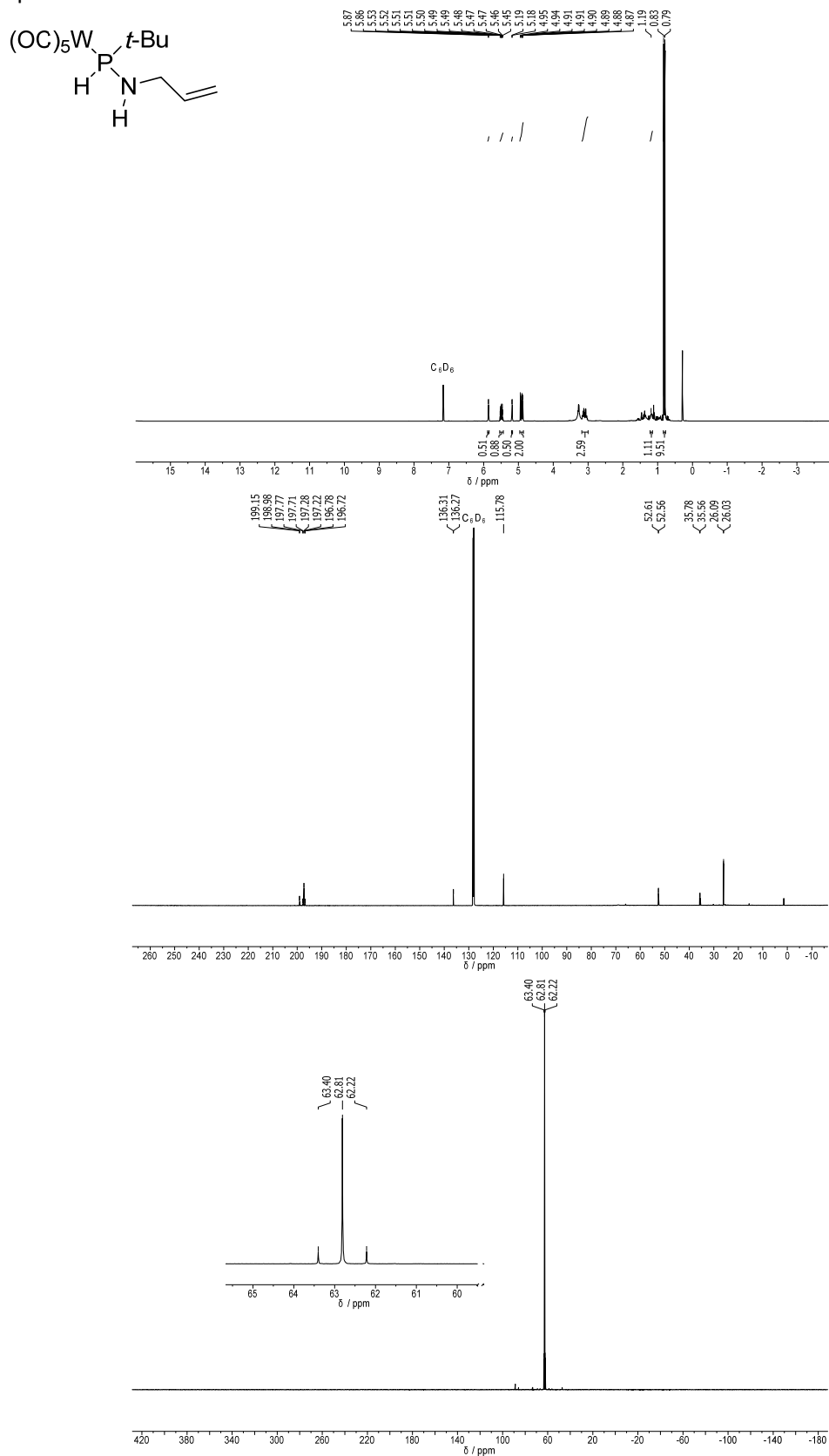


Figure S3. 1H NMR (top), $^{13}C\{^1H\}$ NMR (mid) and $^{31}P\{^1H\}$ NMR (bottom) spectra of complex **3c** in C_6D_6 .

1.4 Complex **3d**

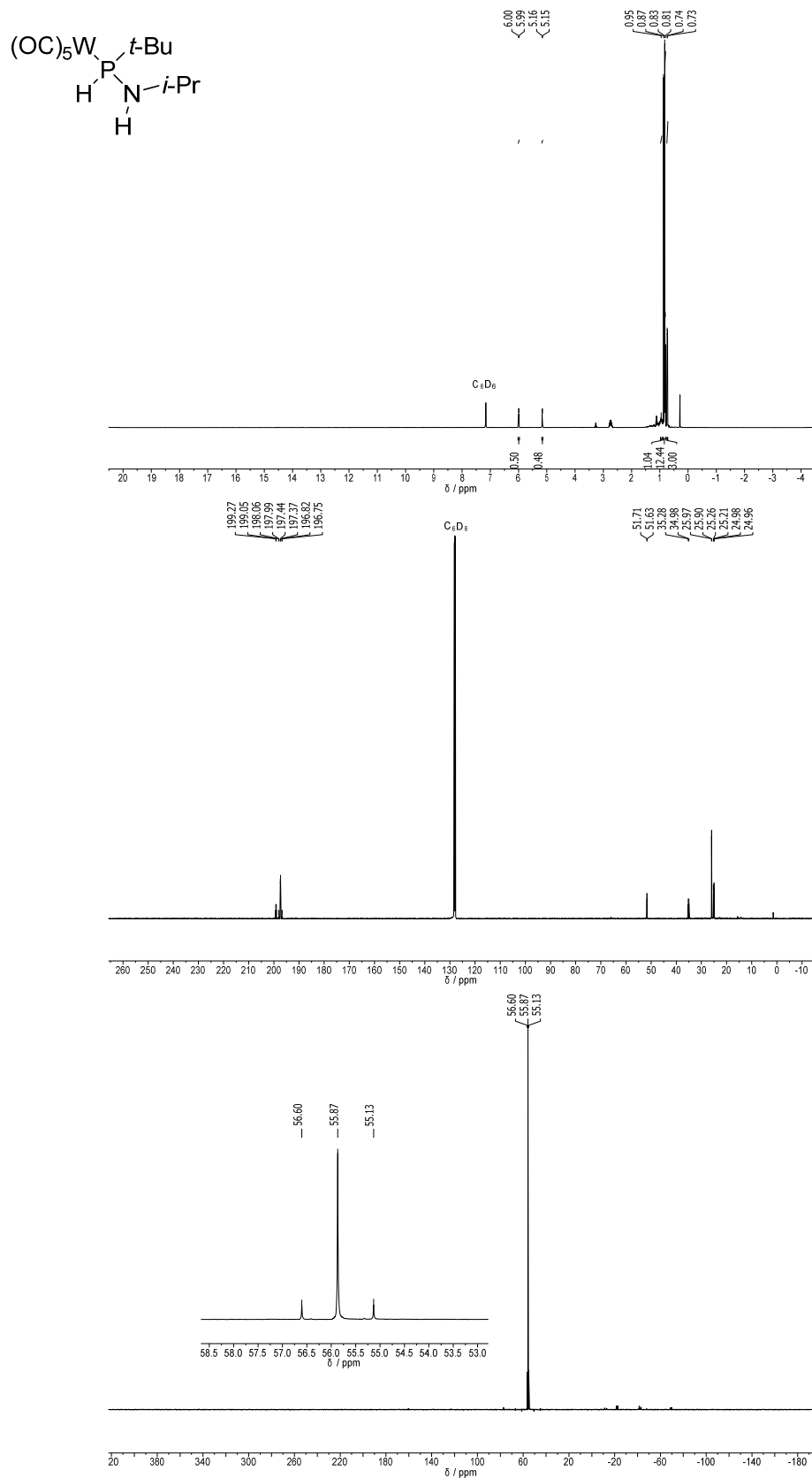


Figure S4. ^1H NMR (top), $^{13}\text{C}\{^1\text{H}\}$ NMR (mid) and $^{31}\text{P}\{^1\text{H}\}$ NMR (bottom) spectra of complex **3d** in C_6D_6 .

1.5 Complex **3e**

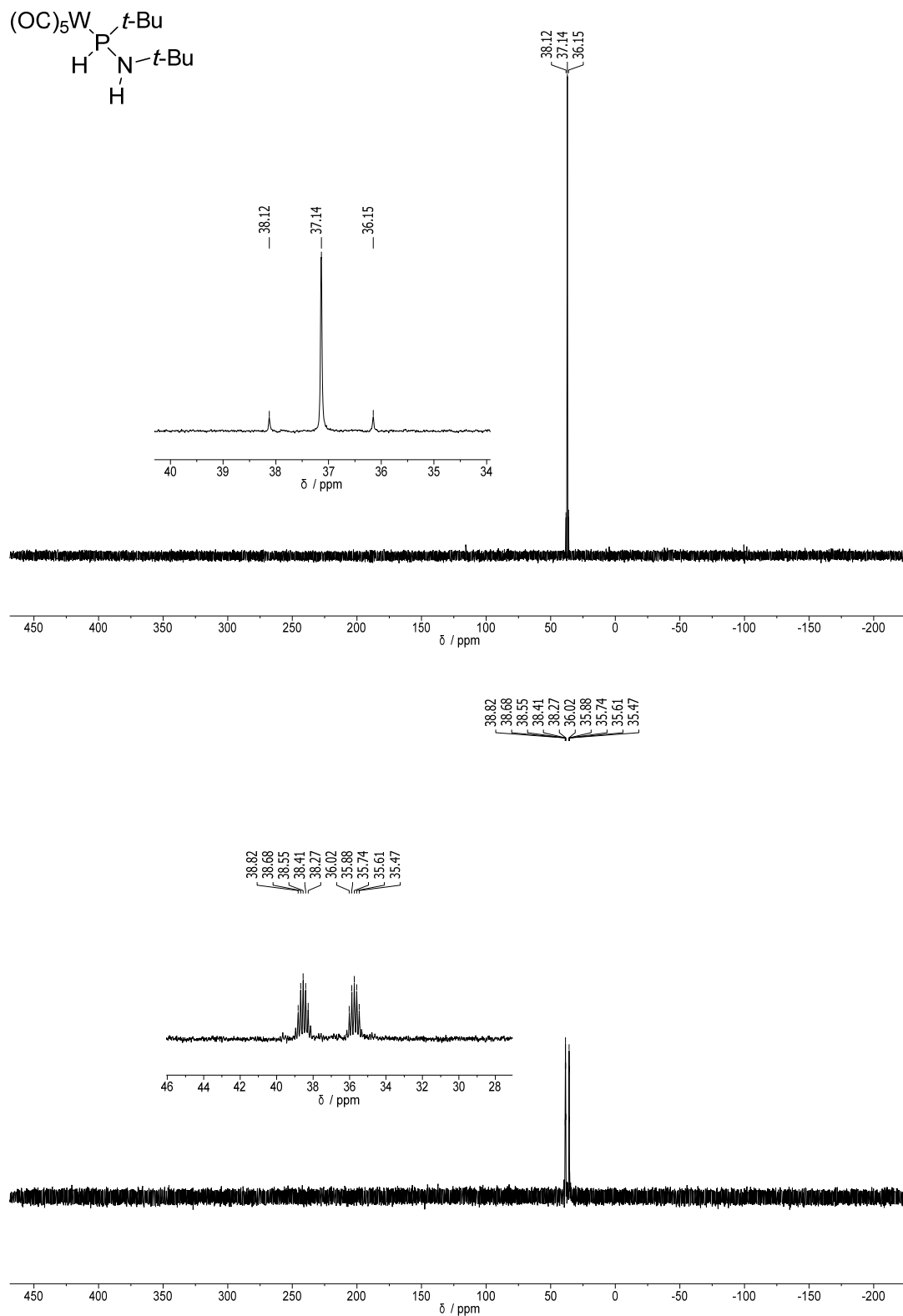


Figure S5. $^{31}\text{P}\{^1\text{H}\}$ NMR (top) and ^{31}P NMR (bottom) spectra of complex **3e** in THF.

1.6 Complex **3f**

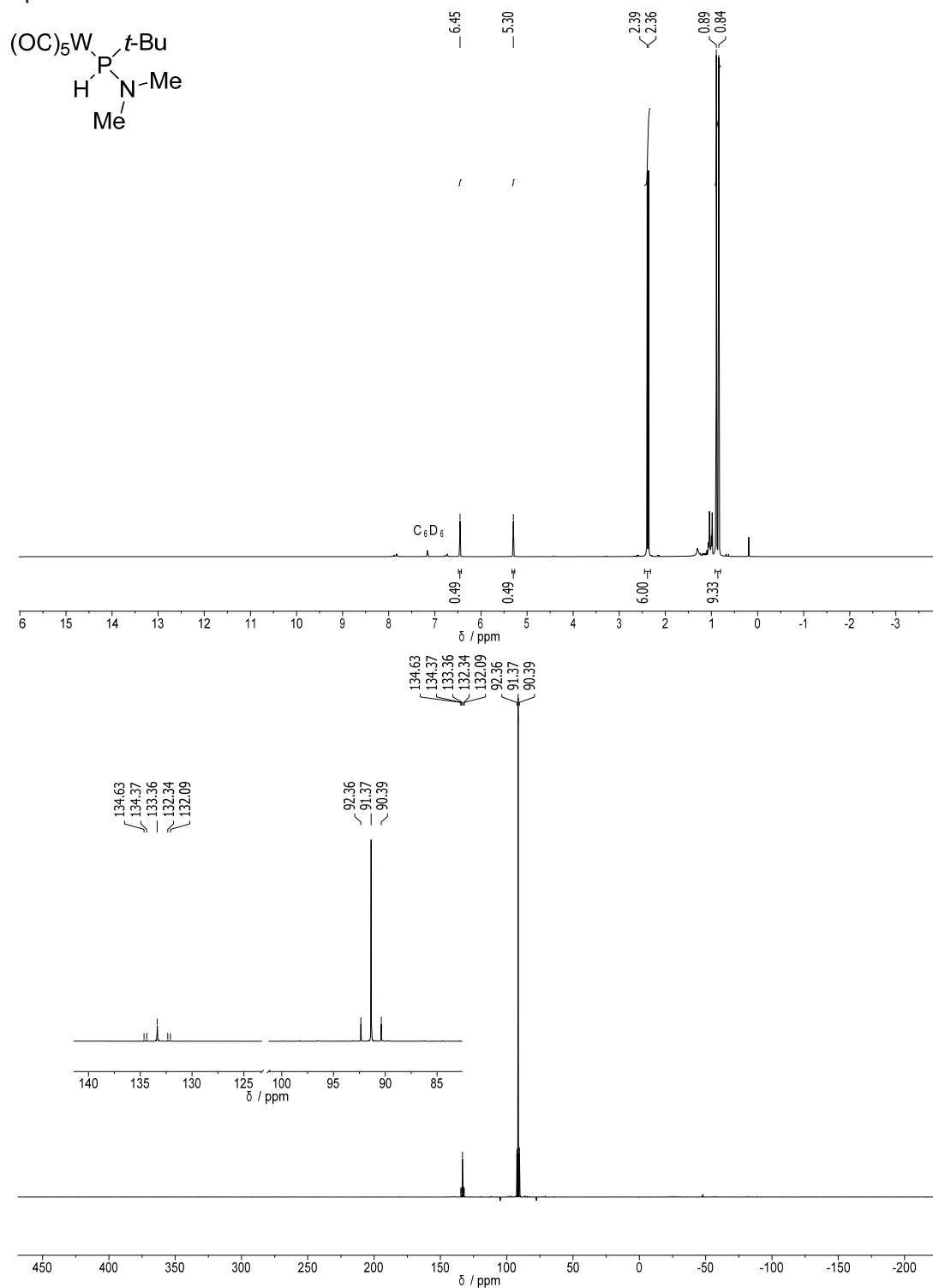


Figure S6. ¹H NMR (top) and ³¹P{¹H} NMR (bottom) spectra of complex **3f** in product mixture in C₆D₆.

1.7 Compound Li-4b

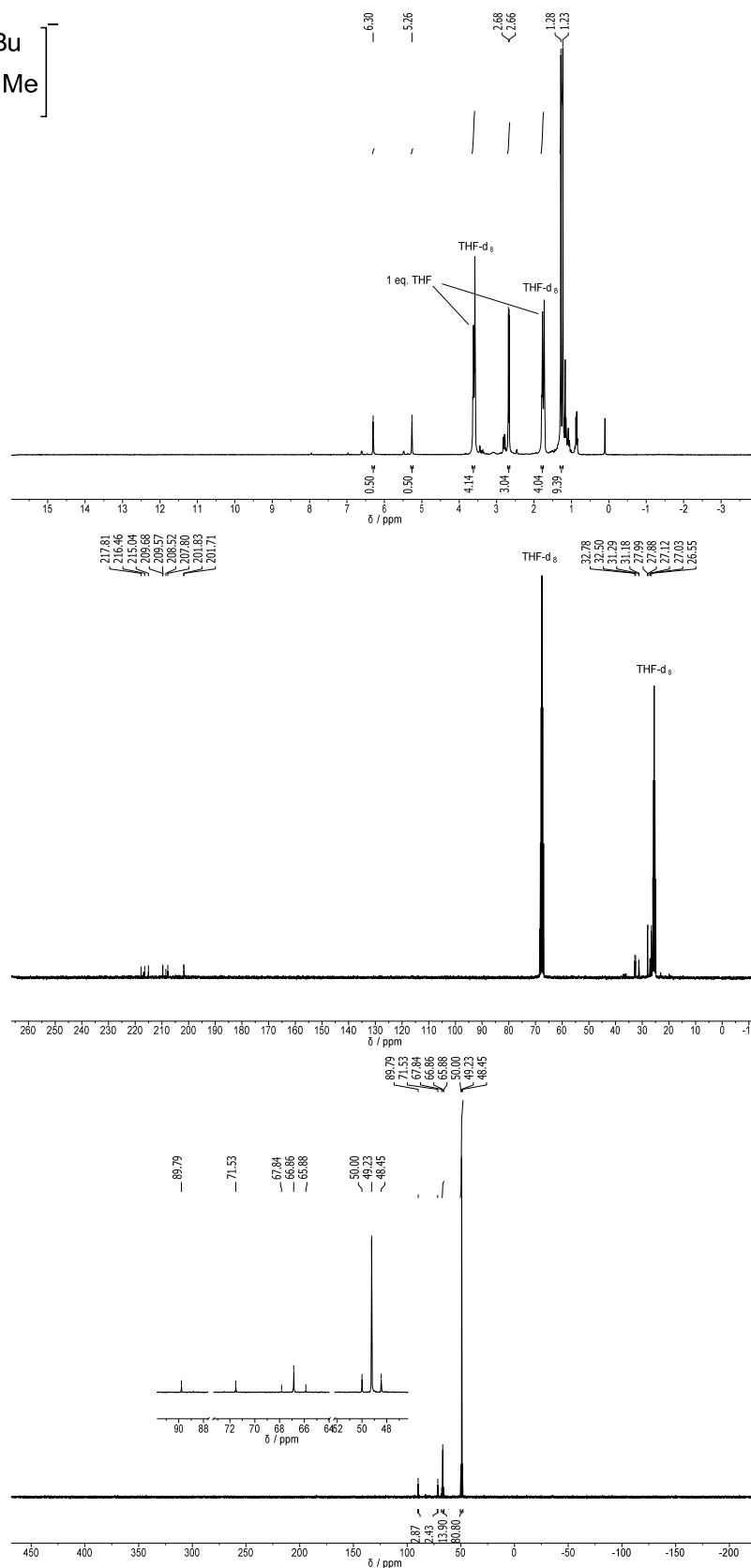
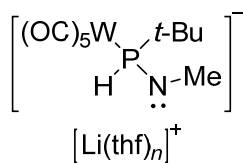


Figure S7. ¹H NMR (top), ¹³C{¹H} NMR (mid) and ³¹P{¹H} NMR (bottom) spectra of compound Li-4b in product mixture in THF-d₈.

1.8 Compound Li-5b

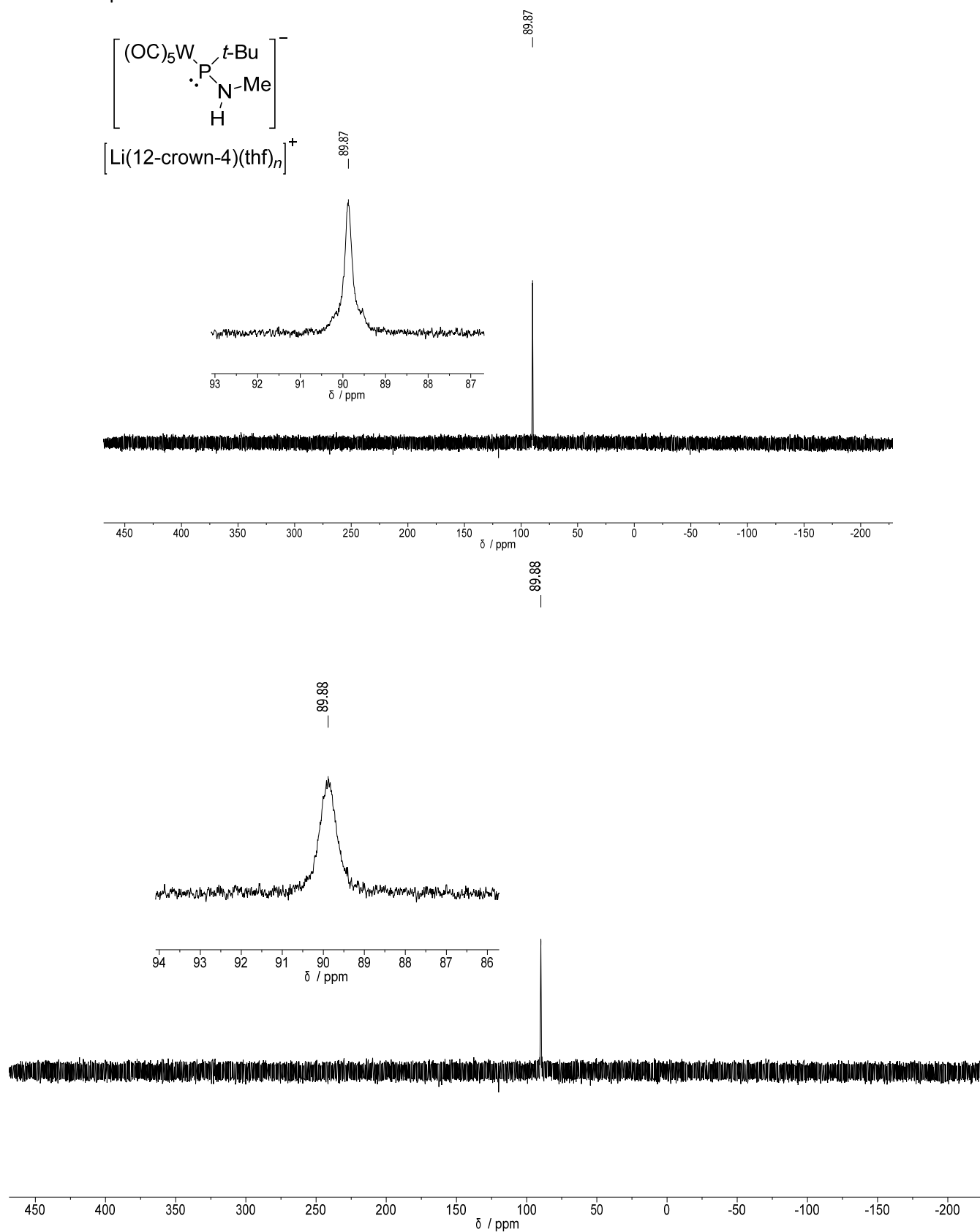


Figure S8. $^{31}\text{P}\{^1\text{H}\}$ NMR (top) and ^{31}P NMR (bottom) spectra of compound Li-5b in reaction mixture in THF.

1.9 Compound K-5b

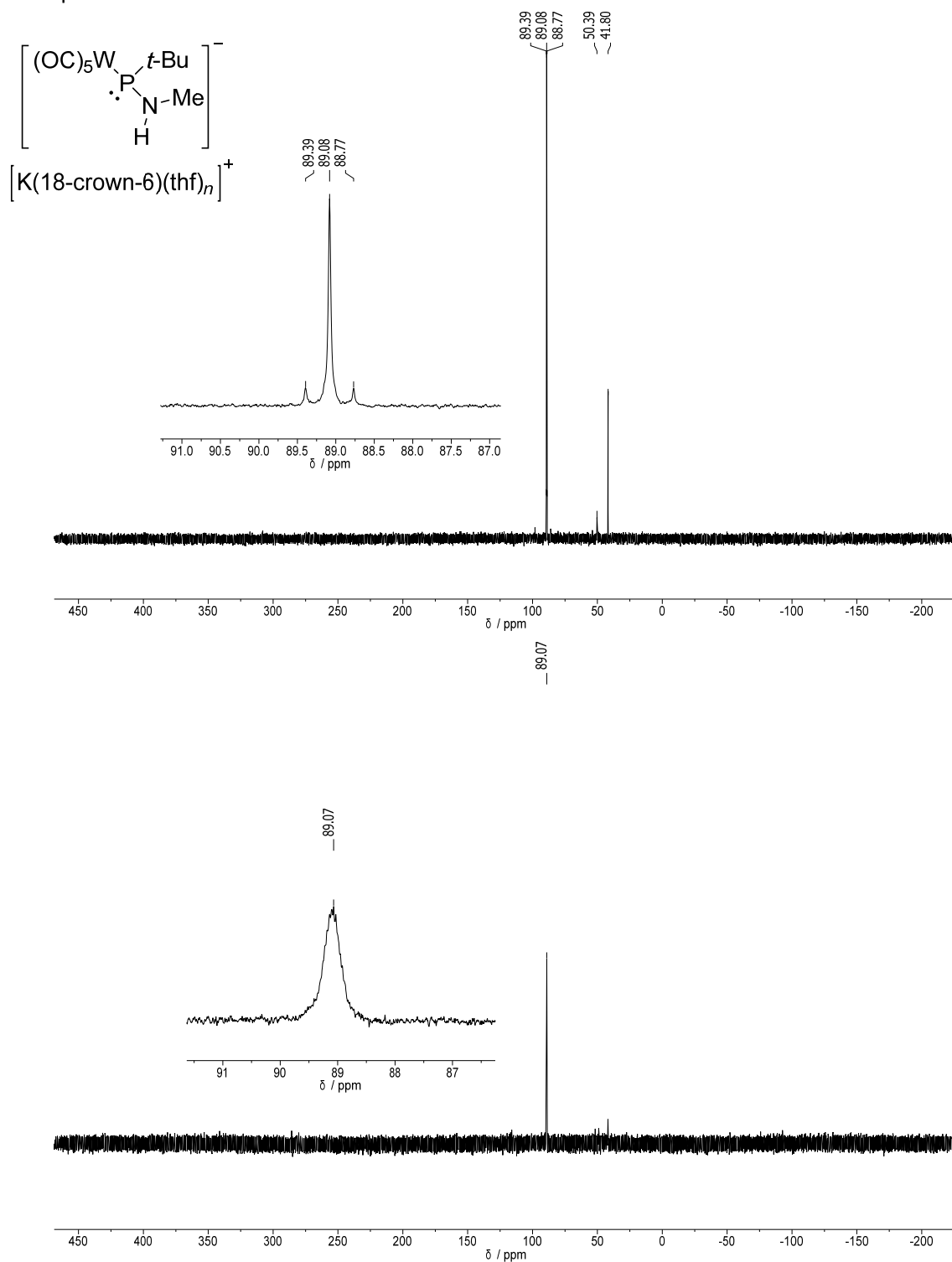


Figure S9. $^{31}\text{P}\{^1\text{H}\}$ NMR (top) and ^{31}P NMR (bottom) spectra of compound K-5b in reaction mixture in THF.

1.10 Complex **7b**

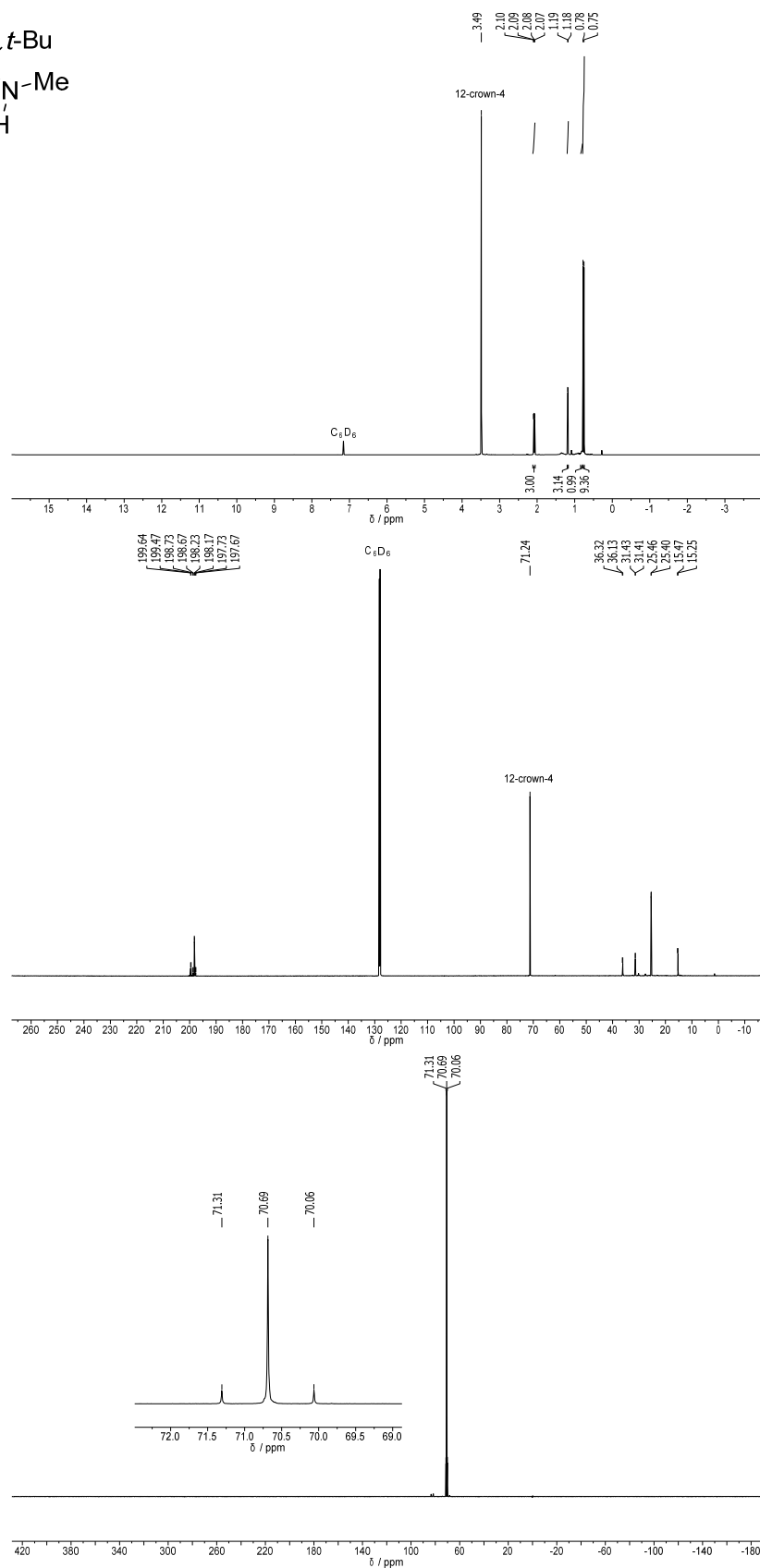
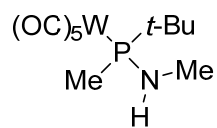


Figure S10. ^1H NMR (top), ^{13}C NMR (mid) and $^{31}\text{P}\{^1\text{H}\}$ NMR (bottom) spectra of compound **7** in product mixture in C_6D_6 .

2. Stacked NMR spectra of reaction monitoring

2.1 Decomposition of Li-5b

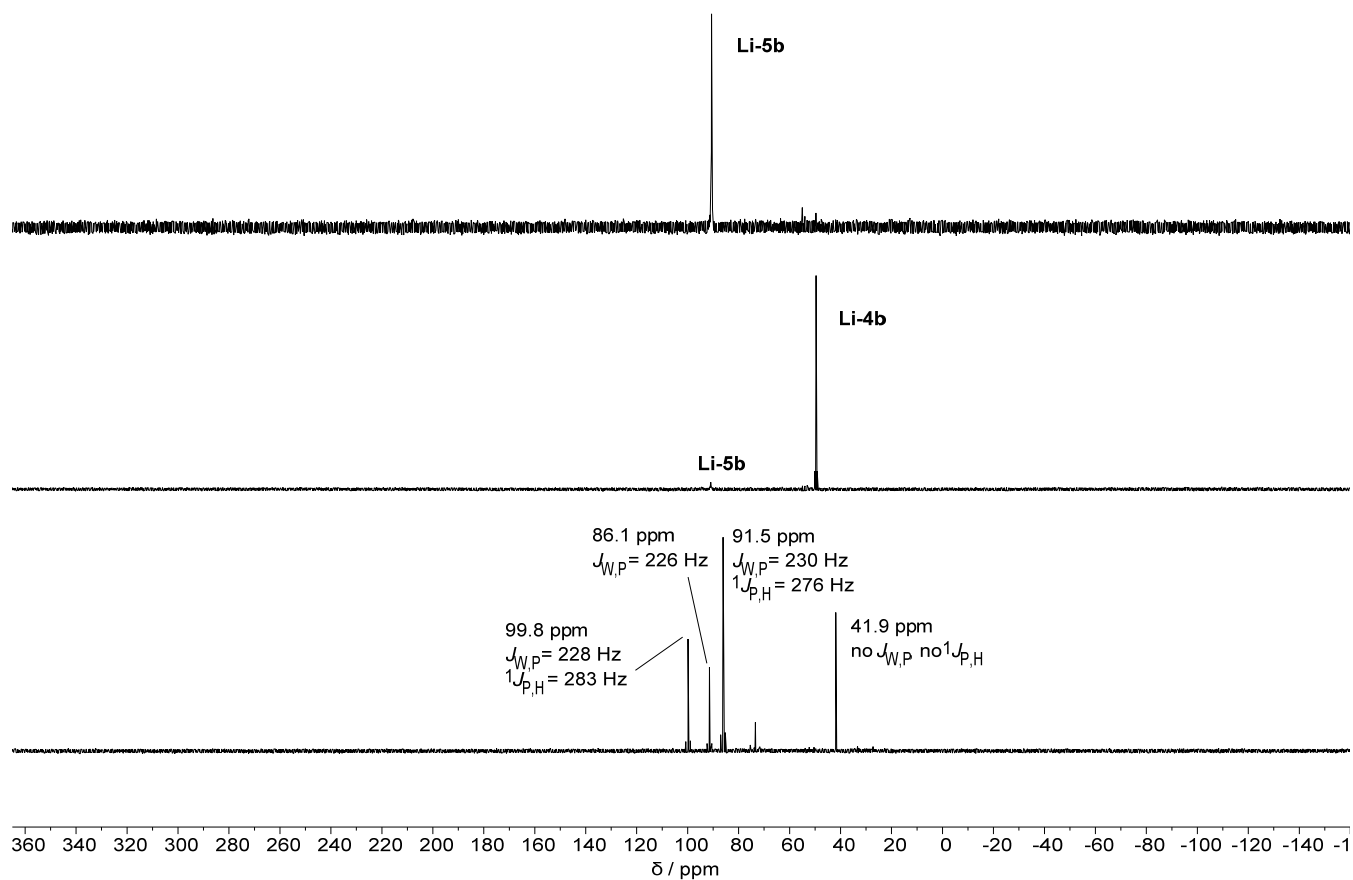


Figure S11. Decomposition of **Li-5b** in THF solution while warming up from -80 °C.

2.2 Reaction of **Li-5b** with MeI

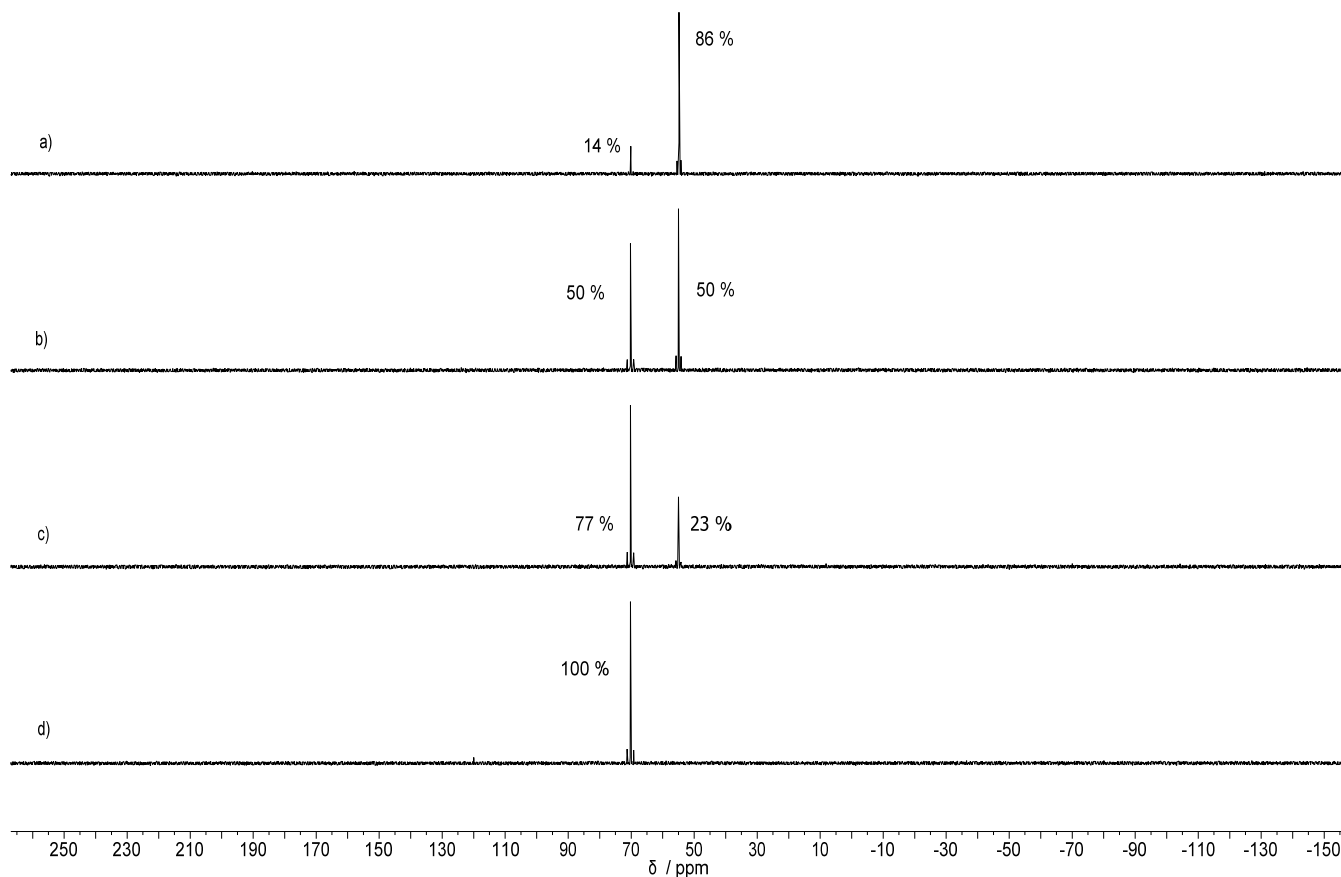
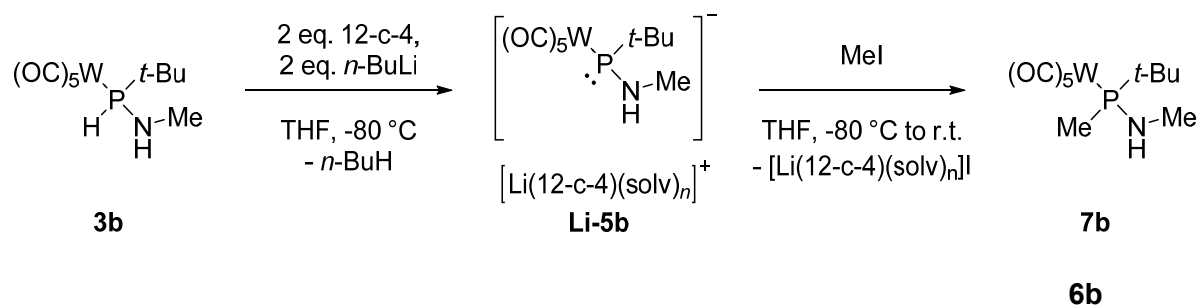


Figure S12. Reaction of **3b** with MeLi in presence of 12-crown-4 and *n*-BuLi, followed by treatment with MeI after a) 2 h, b) 3.5 h, c) 4.5 h, d) after removal of the THF; NMR spectra were measured at 298 K.

3. Computational Part

Computed structures.

The TPSS-D3/def2-TZVP + CPCM optimized atomic Cartesian coordinates (in Å) with electronic energies (hartrees) at the PW6B95-D3/def2-QZVP + CPCM level, unless otherwise stated, in THF solution. Gibbs energy correction and zero point energy (hartrees) are given at the optimization level.

MeI

Energy = -337.877442400231

ZPE = 0.03604972

G_{corr} = 0.01131705

C	-2.19860185618582	0.79951920591875	-0.00005077924849
H	-1.81086493743841	1.26556178331201	0.90208991778410
H	-1.81088258765711	1.26572535207774	-0.90212062145789
H	-3.28416115012322	0.74491460685609	0.00001744883588
I	-1.47688946859543	-1.24172094816460	0.00006403408641

MeLi

Energy = -47.525044632700

ZPE = 0.0313387

G_{corr} = 0.00973460

C	-2.16609844279837	0.70589307792485	-0.00069991632543
H	-1.83621144123252	1.29474255513530	0.87771025198534
H	-1.83696517959732	1.29689923136529	-0.87786334719108
H	-3.27054378266101	0.79081748934174	-0.00006927364667
Li	-1.47158115371078	-1.25435235376717	0.00092228517783

MeH

Energy = -40.585271166429

ZPE = 0.04405286

G_{corr} = 0.02541858

C	-2.11628830770084	0.56678908750223	-0.00000648401542
H	-1.75209648672109	1.08242026470679	0.89247696397568
H	-1.75198611751084	1.08212378903304	-0.89261385165813
H	-3.20946312085268	0.56642140759829	-0.00008606185686
H	-1.75156596721456	-0.46375454884033	0.00022943355475

THF

Energy = -232.847274153018

ZPE = 0.11451906

G_{corr} = 0.08768055

O	-0.35846877242579	-1.45439597242257	-0.55921119328542
C	-0.53276952425428	-0.69347131259984	-1.78442256307928
C	-1.63374123105372	-1.40272356313895	-2.57339010555809
C	-2.49737397105338	-1.99246283726605	-1.44800557088542
C	-1.43431748815173	-2.42081055724627	-0.43861564759112
H	-0.82636534656677	0.33176731661497	-1.52071654066627
H	0.42806263899053	-0.66445268528296	-2.30822756744036
H	-2.18282927598127	-0.71937823664880	-3.22674023895395
H	-1.20937882303094	-2.20604313027904	-3.18564044471993
H	-3.14286973649645	-1.21868279876499	-1.01785457189181
H	-3.12246058659162	-2.82743288597772	-1.77598675910722
H	-1.78288435819143	-2.40936018436984	0.59868724122909
H	-1.04348163525938	-3.42110504488082	-0.67325831737847

3b [W(CO)₅P^tBu(H)NHMe]

Energy = -1230.724438825169

ZPE = 0.22484892

G_{corr} = 0.17542362

P	-1.56297966593033	-0.36583870722497	0.42935206082393
H	-1.50353932963800	0.25664868089089	-0.83455084327756
W	-0.68912651119695	1.10314076543470	2.32052188060560
C	-0.06100677528319	2.38100298724488	0.83332883534148
O	0.30083479984720	3.07894364616094	-0.01479389415493
C	-2.55308032826987	1.98604557767230	2.32394811083713
O	-3.58789024950780	2.50059081353832	2.34148169253075
C	-0.10850037281078	2.40566769060072	3.75410555399943
O	0.21098472667454	3.16521302288431	4.57276016755150
C	1.19678805899805	0.28624832806248	2.38757432671109
O	2.27233239681412	-0.13365251859182	2.47796828940210
C	-1.25651115500320	-0.26984639802808	3.74503351925131
O	-1.54187602405635	-1.04635455454609	4.55494267787472
C	-0.64941762998425	-1.94020462312472	-0.01324298088172
C	0.69111183718518	-1.51499530959290	-0.63571844170795
H	0.53543208368371	-0.95001797458833	-1.56127005810026
H	1.28051498084383	-0.89859607855875	0.04912825157901
H	1.27973517220036	-2.40847527499708	-0.87520405882193
C	-0.42269618209160	-2.78233343055821	1.25118490640191
H	0.17272100673282	-2.23823401903593	1.99034527890249
H	-1.37109052196270	-3.06800621955077	1.71829959302640
H	0.11497262615534	-3.70110906560711	0.98855676579656
C	-1.47658222028166	-2.72964526920906	-1.04049391507242
H	-1.69106413741327	-2.12662771603818	-1.93027547284152
H	-0.91084132549309	-3.61358934639386	-1.35855508978217
H	-2.42447650369795	-3.07347977324247	-0.61403331668390
C	-3.91139338145810	-1.14629127841142	1.67656320444226
H	-4.98524404464910	-0.97227398681793	1.57038850018661
H	-3.74098108944048	-2.21610087190633	1.85262941895970
H	-3.55859840172520	-0.59018810132088	2.54725946166442
N	-3.23300665890992	-0.63598908131838	0.47793189482024
H	-3.61292518033136	-1.02615191382626	-0.38136631938428

3f [W(CO)₅P^tBu(H)NMe₂]

Energy = -1270.093546820719

ZPE = 0.25192135

G_{corr} = 0.20051301

P	-1.66044959797431	-0.25663359161204	0.38656493521973
H	-1.60917916101313	0.33220587715092	-0.89347696454714
W	-0.65797228873910	1.33894509647060	2.11469183204155
C	0.47224630652450	2.02539409635904	0.53676946131052
O	1.11569401509413	2.40441368133005	-0.34677070422995
C	-2.23166346786943	2.55876136428698	1.58879464481492
O	-3.12122264774493	3.24168238577934	1.30433250682731
C	0.08814908288851	2.80357484817565	3.28923844057997
O	0.51452264886820	3.66245745665076	3.94541596673276
C	0.88515400775400	0.11368989752912	2.70929432510882
O	1.75898249037960	-0.54286691593253	3.09176864292101
C	-1.71921120173373	0.61371596317223	3.72264358418037
O	-2.26929876699293	0.22663947631351	4.66491163038934
C	-0.80431229932799	-1.86859815840444	-0.01218713020712
C	0.63805324473456	-1.53006736684264	-0.41965057618628
H	0.65943669881217	-0.88308010317031	-1.30387111730596
H	1.18256001099196	-1.03029216223498	0.38623395501873
H	1.17096575915788	-2.45664773844800	-0.66323352090803
C	-0.83441065301438	-2.76344175532275	1.23579341877245
H	-0.35597824797158	-2.27587348977722	2.09108663293483

H	-1.86384212849020	-3.01625492331308	1.51150091784562
H	-0.29886908231326	-3.69775817120669	1.03066515166622
C	-1.53950577961657	-2.54998288677639	-1.17628295232468
H	-1.51380910176222	-1.93000089747029	-2.07931470391581
H	-1.05150912250585	-3.50544253937538	-1.40389768125830
H	-2.58358441613017	-2.74824094080185	-0.91656986805849
C	-4.20702077523612	-0.17594972177316	-0.63304072681939
H	-5.03766546740733	-0.88651730108772	-0.71332459735846
H	-4.62241920999894	0.82740272637173	-0.45537911391684
H	-3.66239169648104	-0.17058777782103	-1.57865779293395
N	-3.31875635818766	-0.59792164466316	0.45488772114200
C	-3.98006897535929	-0.69489535763939	1.75653883105766
H	-3.31001050871815	-1.15088217436727	2.48619147135065
H	-4.30591686159982	0.28601584469634	2.13497195532211
H	-4.86019644901744	-1.33886309624596	1.65486142473385

4b⁻ [W(CO)₅P^tBu(H)NMe)]

Energy = -1230.205104243794

ZPE = 0.20977607

G_{corr} = 0.16125875

P	-1.73074995712985	-0.32088654234966	0.46015182291067
H	-1.64035780894529	0.31076199603551	-0.83524967366870
W	-0.64726768718720	1.15753469773759	2.27245027359190
C	0.26633328201587	2.16196878543680	0.74039545803197
O	0.77593072775117	2.68676003538421	-0.16298052644912
C	-2.38187120690281	2.23871274326141	1.98765866571828
O	-3.34372565674915	2.86655339253573	1.84393489899152
C	-0.06486115218999	2.46086073752443	3.69128666745612
O	0.25736675704429	3.22904847698517	4.51223393900891
C	1.08422788622555	0.11671449634605	2.60493654635025
O	2.08462687306245	-0.43083087516436	2.83695282293249
C	-1.62092032367671	-0.11381852746218	3.56578630622467
O	-2.15534072037358	-0.85656637645094	4.27761313840892
C	-0.71975549640728	-1.84080711942418	-0.05557507855745
C	0.63102385491733	-1.36022300189710	-0.59839857532298
H	0.49410069365509	-0.71750944409814	-1.47654478563470
H	1.18610639625366	-0.79173082030309	0.15423768305606
H	1.24624695095015	-2.21919720985373	-0.89931550420510
C	-0.53546748182697	-2.74940968061563	1.16542518747488
H	0.03655971083519	-2.24627681219683	1.95129551693636
H	-1.50767198050533	-3.03445155930287	1.58359968599680
H	0.00095203495657	-3.66552060254507	0.88373131262476
C	-1.48083898420607	-2.59737392696512	-1.15606739733138
H	-1.69806385160593	-1.94530151799118	-2.01030615085714
H	-0.87546352464410	-3.44096042406345	-1.51685797675306
H	-2.42680148310032	-2.99521948451107	-0.77812020079562
N	-3.28499456011247	-0.56895217110345	0.80748488367917
C	-4.21697452184365	-0.89233087638537	-0.26770965588436
H	-5.21206446835089	-0.48714789303988	-0.02653067403422
H	-3.92316742876513	-0.46607356286886	-1.24797283034811
H	-4.35361687314460	-1.97652693265471	-0.43094577955179

Li(thf)-4b [Li(thf)]⁺ [W(CO)₅P^tBu(H)NMe)]⁻

Energy = -1470.58893575999

ZPE = 0.32989544

G_{corr} = 0.27186468

P	-2.35627995984294	-1.27940283339952	0.29818993473244
H	-2.72622898305398	0.07432922824869	0.10428719570885
W	-1.42175779953301	-1.58658036585914	2.70297212496117

C	-1.50788197060827	0.46104324909788	2.75442250083363
O	-1.54393646623093	1.62124294599877	2.73995913789644
C	-3.39544227749865	-1.74913964124273	3.26313892940252
O	-4.49696089356120	-1.84267097979633	3.61097852611841
C	-0.90559279584120	-1.73063474272308	4.64362388782760
O	-0.62059035651227	-1.80284981155906	5.77188046234018
C	0.57879630222894	-1.47434868856984	2.25305792999548
O	1.72422783441827	-1.43298515587053	2.07127931401602
C	-1.27096581817571	-3.61751173560439	2.40822363565197
O	-1.13188518408108	-4.75631498649691	2.23616946006925
C	-1.08739673299597	-1.31656246503146	-1.09763646024552
C	-0.12871955217961	-0.13492678910175	-0.90180125075364
H	-0.66531631636642	0.81944900300352	-0.96052640383901
H	0.37880271463863	-0.18035818675113	0.06582354387955
H	0.63837732916459	-0.14147431316785	-1.68653151672999
C	-0.33256074509316	-2.65236104187042	-1.06958880697703
H	0.19642980910685	-2.78829771472454	-0.12102360803161
H	-1.01887489927640	-3.49618768529647	-1.20039352954899
H	0.40531704349964	-2.68549333164630	-1.88128140282629
C	-1.84181094907984	-1.16029261503863	-2.42637948368041
H	-2.37964813899739	-0.20482289242278	-2.46359997287557
H	-1.13121412927033	-1.18209533647805	-3.26285422908049
H	-2.56989041567819	-1.96592201294105	-2.55957134653999
C	-3.90870283609192	-3.44659059739523	0.29186385835243
H	-4.96743203903794	-3.72571731169720	0.20948059078616
H	-3.33868884214935	-4.15149485399259	-0.33537860220777
H	-3.60556362115988	-3.63205602279473	1.33610795953796
N	-3.74420842443578	-2.04952970558274	-0.10068525260250
Li	-5.20520519283181	-0.96278615134453	-0.62175991167899
O	-5.36136608175200	0.86017596236138	-0.06840170897723
C	-5.20964918035335	1.14248264474509	1.36208200447469
C	-4.84541929446560	1.98691064078842	-0.84603087806420
C	-4.83125703629084	2.61652890847725	1.44906725080783
H	-6.15525711769095	0.89439902083389	1.84956950284606
H	-4.41745895686054	0.49201193138391	1.74918751447845
C	-4.05045483130743	2.83045463931546	0.14317537896460
H	-4.24628642194478	1.57927814133802	-1.66474234733801
H	-5.70011732821341	2.53584490941529	-1.25733207258377
H	-4.23790261736514	2.83226497297583	2.34033544696526
H	-5.72929707640149	3.24263173854294	1.46370598920705
H	-3.03048599574499	2.44516952003673	0.24217153052941
H	-4.00034375508315	3.87919051183593	-0.15923482580248

Li(thf)₂-4b [Li(thf)₂]⁺ [W(CO)₅P^tBu(H)NMe)]⁻

Energy = -1703.45228371707

ZPE = 0.44680840

G_{corr} = 0.38072176

P	0.05906036772475	-0.00018802469810	-0.07263127366907
H	1.48940816168955	0.04347659129143	-0.10465782899764
W	-0.90432439023276	2.38987880502197	-0.04863948328969
C	0.11239227987261	2.51987771738889	-1.83352864704726
O	0.72579548947782	2.62464464730792	-2.80997643352551
C	-2.54077635875854	1.47246067663059	-0.84863163474311
O	-3.44269553708238	0.86999058252649	-1.27708788249777
C	-1.59442439638241	4.26715222393648	-0.32758548869299
O	-1.99180986759137	5.34540849652764	-0.52058503165052
C	0.82454674901957	2.98336925147624	0.89696417639515
O	1.80417834532679	3.27219740055818	1.44338920427224
C	-1.83706340341195	2.37934753510877	1.78210844349549

O	-2.36537209540301	2.44297346073736	2.81329120860461
C	-0.06625909836761	-0.94594530451173	1.55516979255396
C	0.63900536185912	-0.12458049470742	2.64198169922569
H	1.69317610727935	0.04326025386920	2.39162886557260
H	0.16055129361787	0.85004542276900	2.78005836951357
H	0.59893465868541	-0.66036420918878	3.59906653261929
C	-1.54694082717427	-1.14815567930284	1.89867084271847
H	-2.05491351110806	-0.19183026154018	2.05135044271467
H	-2.06297728352259	-1.68154694709417	1.09420192344873
H	-1.64528330706758	-1.73863979305381	2.81841642479749
C	0.62443156898344	-2.31034128656681	1.39872509414174
H	1.66962215796659	-2.19707917763471	1.08928539690226
H	0.60839715631902	-2.84550174148545	2.35751492741862
H	0.11091830597567	-2.92930039049271	0.65737856561003
C	0.49544019355055	-1.87649991900570	-1.91426980032108
H	0.40628775357100	-1.92262743984541	-3.00953249610557
H	1.55442133164302	-1.67397548794475	-1.68121959277581
H	0.27341306114090	-2.88704758649736	-1.53342781594050
N	-0.40321192364111	-0.83825102525119	-1.39182610299684
Li	-2.11531647915499	-0.98139738173738	-2.25592481356971
O	-2.38014342627081	-0.33843993439008	-4.05032332184891
C	-3.68040067808189	-0.01810227318545	-4.61594114592637
H	-3.79542274727883	-0.57450531574810	-5.55360876709528
H	-4.43234558080732	-0.35498147461484	-3.90022169714248
C	-3.67763803041017	1.50626783931475	-4.85542327460709
H	-4.34989671438928	2.01854937975351	-4.16383954423049
H	-4.00138008720503	1.73164687720710	-5.87443344560451
C	-2.20568517128159	1.93275494208327	-4.61915024033832
H	-1.83963946785818	2.62069926886798	-5.38497383311694
H	-2.10119650624361	2.41725385130890	-3.64509558919030
C	-1.44526950113335	0.60897078063847	-4.62713948198677
H	-0.55146472134173	0.58788354638930	-4.00294531964624
H	-1.19913223421172	0.28698325507787	-5.64771167063894
O	-3.08727377016280	-2.64562241928359	-2.15094166464264
C	-3.24801795765751	-3.48878800006745	-3.33319841107374
H	-4.31765693049423	-3.56293481178318	-3.56488486019338
H	-2.72849804873532	-2.99524928364515	-4.15672226063278
C	-2.66288422084287	-4.83599755789769	-2.93433326300601
H	-1.57144509809923	-4.81679638078296	-3.02464600724974
H	-3.05245335109778	-5.65463814960186	-3.54459611297745
C	-3.08290306893628	-4.93347121976651	-1.45954271020310
H	-2.47110109579842	-5.63172724452863	-0.88343997510765
H	-4.13022052091519	-5.24361773041224	-1.38495411858326
C	-2.91456991127680	-3.49540175977026	-0.97080194752188
H	-1.91034215038552	-3.30643199703000	-0.57822891259487
H	-3.65813244388872	-3.19561792272472	-0.22772250902219

5b⁻ [W(CO)₅P^tBuNHMe]]

Energy = -1230.218241498138

ZPE = 0.21335403

G_{corr} = 0.16403998

P	-1.69236334515294	-0.37430088878824	-0.03038400205173
W	-0.84610100521498	1.23756659205170	1.97347611881966
C	0.31102997630618	1.98761180078993	0.46358522025174
O	0.94177059284803	2.34362868051977	-0.44811286089964
C	-2.39169597826358	2.47427404194880	1.42145593300034
O	-3.23286787536354	3.22670986429404	1.13941646646696
C	-0.38328616626413	2.57905501190813	3.38192468838432
O	-0.12471842837275	3.35904151855640	4.21937416690488

C	0.75627304116904	0.14861010208165	2.64282057877405
O	1.67890363365390	-0.41029786813207	3.08280408918605
C	-2.09540691332115	0.03829164876810	3.04711977930053
O	-2.81968731180515	-0.72187198044493	3.55573447947479
C	-0.58779687796759	-1.91114552711556	-0.14928442034732
C	0.83146503586434	-1.43328221530398	-0.48589558866424
H	0.83208968959609	-0.81777259458773	-1.39353206589373
H	1.25747718047547	-0.83873997570380	0.32694610399596
H	1.48594901772509	-2.29826038825694	-0.65821998847830
C	-0.57602930406787	-2.75277604332427	1.13347470772077
H	-0.24472459038109	-2.15969825846234	1.99042265898575
H	-1.57171443503704	-3.15313216176739	1.35586220881315
H	0.10522737609199	-3.60847709055314	1.02025627699938
C	-1.11548890162278	-2.76739968510015	-1.31686152860338
H	-1.08792871997382	-2.20513199192193	-2.25709091333966
H	-0.49298953648799	-3.66598082667116	-1.43331163550821
H	-2.14796628782526	-3.07909242796371	-1.13218490879199
C	-4.37913213389084	-0.32221710077473	0.36649786466739
H	-5.27763372988729	-0.93498844282315	0.50282059075296
H	-4.37680166506137	0.46207445571930	1.14080974299333
H	-4.43391678294874	0.17045776874778	-0.60994287910904
N	-3.18912298747755	-1.17912405474988	0.40064229315855
H	-3.14751256734269	-1.65823196294051	1.30087682303664

⁶Li(thf)₂-5b [Li(thf)₂]⁺ [W(CO)₅P^tBuN(H)Me]⁻

Energy = -1703.44799381023

ZPE = 0.44930819

G_{corr} = 0.38488838

P	0.68917863174184	0.21431913576777	-0.00551754242327
H	-0.21026304658251	0.73000599092965	-2.02697119532280
W	-0.64073330534535	2.42720903137695	0.62119986968514
C	0.00732011039259	3.15362776485300	-1.18549702514702
O	0.35844087241452	3.59851683017026	-2.19981479957508
C	-2.17047350845349	1.43674697783923	-0.24825960456940
O	-2.97785156795729	0.76215644922139	-0.77120955458748
C	-1.57540905436025	4.18517169271473	0.90578479801245
O	-2.14290712048253	5.19662591890377	1.04333642033210
C	1.15885401448874	2.94448125765176	1.48597890306413
O	2.19253362466724	3.15592308355671	1.96303379545646
C	-1.32502647549924	1.87987167044558	2.48226096995990
O	-1.74241790450403	1.64082587034633	3.53836625636594
C	0.14666057010868	-1.24041231005751	1.08682565266332
C	0.80649346054396	-0.95570371754301	2.44785310439290
H	1.89379544887659	-0.86232017271873	2.34525357886778
H	0.42567964988388	-0.03106779893690	2.89215584103430
H	0.59575202306572	-1.78011357128213	3.14123504968757
C	-1.36221939639264	-1.42740549895672	1.26255885295972
H	-1.82920039797053	-0.54280860620745	1.70130485027170
H	-1.84731254735547	-1.63773832894184	0.30477256227314
H	-1.56115460445597	-2.28432638668891	1.92189786080132
C	0.74334117206590	-2.54009967479575	0.51504370415218
H	1.81959930000443	-2.44195917449780	0.33688457673883
H	0.58188044975037	-3.36456483321313	1.22312146524785
H	0.26052990218304	-2.81618825038348	-0.42758225285984
C	0.88766007742106	-0.89256342695589	-2.54449237440325
H	0.42706544241731	-0.95822505214524	-3.53697351669545
H	1.85122322540708	-0.37385700142277	-2.62765187024582
H	1.07268528497026	-1.90405760493008	-2.18045627523963
N	-0.04760543257500	-0.19479264403426	-1.62077499764107

Li	-1.99352051238763	-0.72456124268530	-1.97628314032573
O	-2.33223602903023	-0.00658407705375	-3.72713681021353
C	-3.05626947138665	-0.71106541772068	-4.78230699623635
H	-2.62332126954265	-1.71019691024220	-4.87028687467257
H	-4.10698348731992	-0.79259525534921	-4.48075965040313
C	-2.88580693785035	0.15131907497118	-6.02766951808841
H	-3.70620344310851	0.01515009107392	-6.73641581784760
H	-1.94283418001888	-0.08763388190417	-6.53061789709121
C	-2.83197726724148	1.56745066102134	-5.43370014669876
H	-2.36553578190695	2.29604283506088	-6.10085020124497
H	-3.83946817694378	1.91438453746092	-5.18197511645806
C	-2.01505338684641	1.35011791035979	-4.16480859031087
H	-2.27445804280324	2.03327240782886	-3.35208989820143
H	-0.93730974083437	1.40324306978182	-4.36113746111030
O	-2.85103150158511	-2.41179674503069	-1.84402280244302
C	-2.24814020717881	-3.70356440910855	-2.14950710924652
H	-2.39087275826627	-3.91263201563635	-3.21681119706274
H	-1.18042766044481	-3.62631231169264	-1.93302745183255
C	-2.99680387834722	-4.69685557066940	-1.27341223525335
H	-2.59294012494624	-4.68404181218891	-0.25561069542300
H	-2.94122443725381	-5.71609666846069	-1.66295000790806
C	-4.42195387291465	-4.12107431884647	-1.29885029118734
H	-5.03469867191055	-4.45813522391178	-0.45968019367847
H	-4.92377068189362	-4.39729077592164	-2.23173436365266
C	-4.17536205318802	-2.61389952424054	-1.25080879690416
H	-4.13862460962749	-2.23261938812951	-0.22507615320499
H	-4.89579228368912	-2.03180547883085	-1.83128018655496

TS(4b⁻→5b⁻)

Energy = -1230.1170130699

ZPE = 0.20727689

G_{corr} = 0.15795785

Imf = -1425.61 cm⁻¹

P	-1.62199534003794	-0.16242527678598	0.28417017688118
H	-2.83932183875783	0.50247534798897	-0.25374351931267
W	-0.57571598069852	1.23685208691059	2.19622856915836
C	0.49046995617497	2.26001877790566	0.77568188918146
O	1.09749267896493	2.80001147879721	-0.05514652491572
C	-2.24826691326720	2.40051076234833	1.87642597556434
O	-3.17243097487748	3.08387556696080	1.72399009389658
C	-0.02979449473439	2.45244466806110	3.69766933611024
O	0.26616540105647	3.15866051550749	4.58336632933849
C	1.07573622715683	0.09466669248535	2.58848819094211
O	2.02009429378371	-0.52709505627355	2.86665103408945
C	-1.65659854649658	-0.02904972195162	3.40902248340811
O	-2.23141228574815	-0.78085982009443	4.07672315925731
C	-0.70818210919174	-1.77702935509568	-0.16321296197394
C	0.73137429748896	-1.40980554373586	-0.54300493382893
H	0.74536571963975	-0.75419115192257	-1.42207956577834
H	1.24519410334071	-0.89438609603048	0.27216988392488
H	1.29692373341481	-2.31919939625910	-0.78815190469007
C	-0.76157991777481	-2.67674406596464	1.07823394507414
H	-0.14630337761317	-2.27067083732732	1.88638406703746
H	-1.79107657755163	-2.76572419088271	1.44702712717223
H	-0.39635752506660	-3.68484119600425	0.83734036710330
C	-1.36785612737642	-2.47998246107243	-1.36163284474358
H	-1.45821372851788	-1.80140592010432	-2.21690039003481
H	-0.74732497497933	-3.33493822316960	-1.66580116274515
H	-2.36260819677822	-2.85725546298414	-1.11584125838189

N	-3.28006169914366	-0.44328171200093	0.83935177059358
C	-4.14266098793943	-1.21652294680488	-0.06399347831888
H	-5.18971852384090	-0.93043386432769	0.11250607870682
H	-3.93017588698474	-1.06067240261199	-1.14205279855685
H	-4.06766040364406	-2.30120119556104	0.11673086584048

TS(Li(thf)₂-4b→^NLi(thf)₂-5b)

Energy = -1703.36133323089

ZPE = 0.44386542

G_{corr} = 0.37752200

Imf = -1474.33 cm⁻¹

P	0.22930583945769	0.06681833124028	-0.17750851407203
H	0.80047188907339	0.11476213743389	-1.56499052962310
W	-1.26806385486095	2.14400640508688	0.21134542314038
C	-0.28272158099215	2.86474457816210	-1.42064279164414
O	0.28032125352811	3.26152982117714	-2.34885075997094
C	-2.64210743234238	1.30770585276440	-0.97313961198975
O	-3.40247945931195	0.76437285620695	-1.67552182215387
C	-2.30554698095706	3.84232884922229	0.37054064567784
O	-2.92326844283976	4.82358485242445	0.44642945067267
C	0.22779541236812	2.85394413160424	1.42869689009711
O	1.07014881065455	3.25318779651485	2.10757137827385
C	-2.26918840524218	1.39785844102101	1.81767692370471
O	-2.88711714302905	1.00382609299936	2.71401038474687
C	0.41616128701945	-1.16218100893223	1.27188581193455
C	0.68293250986016	-0.36481046651899	2.53974777339332
H	1.58705397681954	0.23585655520096	2.44639851489560
H	-0.13757752080682	0.29944991696207	2.79048450023803
H	0.82614073983345	-1.04751479911668	3.37955356533968
C	-0.88755689253687	-1.93812856900385	1.36400204100055
H	-1.72273576756997	-1.29268918095897	1.62375687885568
H	-1.12206161342904	-2.42555967102183	0.41902256954493
H	-0.81351889057472	-2.71360406157241	2.12937179280780
C	1.59175897233158	-2.10681345795629	1.03664539088653
H	2.51370411183000	-1.55452212622171	0.86483632124712
H	1.73582374966124	-2.73342935545252	1.92010542969211
H	1.43123955338611	-2.76663733328211	0.19105795237640
C	0.44955263515586	-1.92204755603343	-2.09446870346364
H	0.30845877816958	-2.06215442812556	-3.17000028080982
H	1.53025313385622	-1.80244253015910	-1.92577768335135
H	0.16217439665791	-2.86029573206152	-1.60928231422910
N	-0.34785245732266	-0.78300885352375	-1.65165887458053
Li	-2.10001463441209	-0.82169188827594	-2.52926874884756
O	-2.01305716829375	-0.36141482606492	-4.43278865512614
C	-3.21925609412865	-0.12925254229309	-5.18447419608431
H	-3.08662887567965	-0.53209017649620	-6.19135017845707
H	-4.01881300352200	-0.67401737106727	-4.69047179795774
C	-3.41067238833689	1.38764870976640	-5.20899692899674
H	-4.16451150668055	1.69687729329894	-4.49015890088448
H	-3.73389622276431	1.72034435017893	-6.19243016518931
C	-2.02814196791631	1.95240741708254	-4.82778614077281
H	-1.66079151571408	2.68483860822541	-5.54210720021396
H	-2.06790488778090	2.43345811950295	-3.85457785263449
C	-1.13082129573402	0.72609671549476	-4.77372010844791
H	-0.35848889489073	0.76222429740101	-4.01138317282133
H	-0.67262123997614	0.51857003948860	-5.74415799966915
O	-3.35050630197520	-2.32907021429395	-2.32307001373313
C	-2.96699541534345	-3.62424386282541	-2.82988479066026
H	-3.76551620743377	-4.01311938835640	-3.46681369544084

H	-2.07153022286579	-3.49244307131166	-3.43278386589121
C	-2.77201819492434	-4.48090318079980	-1.59992959517638
H	-1.79480662503728	-4.28660145078021	-1.15978449815835
H	-2.84380571208305	-5.54405935748694	-1.81655620734959
C	-3.88849449893558	-3.98064748326369	-0.68812059085632
H	-3.67969862115307	-4.14410189015518	0.36600978955895
H	-4.82336798571653	-4.48496203107023	-0.92769759816186
C	-3.98123612599923	-2.49731470100962	-1.02468010435491
H	-3.43780697573165	-1.87762139515623	-0.31383137897414
H	-5.00659959481635	-2.13755102781176	-1.08562565733455

TS(Li(thf)₂-4b→^NLi(thf)₂-5b)-THF

Energy = -1936.21632924166

ZPE = 0.55879111

G_{corr} = 0.4860187

Imf = -1443.75 cm⁻¹

P	-0.20311386396571	0.16957885526325	0.11321555512377
H	-0.12620236285712	-0.41541638119942	1.49187635740617
W	2.11164107994530	0.16144792828982	-1.08724418916302
C	2.98843093364526	-0.43268583607005	0.67472591002997
O	3.56743658347158	-0.78266737408740	1.61619008017148
C	1.69960065556237	-1.78307981014192	-1.47994408194313
O	1.39194752839735	-2.90212766429948	-1.61215137036048
C	3.96112589745457	0.12691845800182	-1.88051258246267
O	5.03179863393759	0.08051417198463	-2.34116480085656
C	2.21428217628347	2.14259124399235	-0.51197924465839
O	2.23355112524349	3.24715064012892	-0.16732715175141
C	1.45202665302648	0.67951982738214	-2.96443026785631
O	1.16346551042013	0.93684426325924	-4.05834286894984
C	-1.64365982624686	0.89535539690858	-0.89429450026796
C	-1.20057222284392	2.26357285759380	-1.43010816393211
H	-0.96777820926410	2.94824960391539	-0.60629657620212
H	-0.31804507634513	2.18715203994602	-2.06916304329833
H	-2.01380639509801	2.70653259243008	-2.01944898449207
C	-1.93625055291328	-0.09518115358127	-2.02876873409006
H	-1.10002239973413	-0.15384619446664	-2.73119424470828
H	-2.11432982090576	-1.10062909489754	-1.62901038536908
H	-2.83196989577874	0.21623560147775	-2.58244414196088
C	-2.89752194412599	1.10637304325345	-0.02656599938248
H	-2.66470765687434	1.69587142438378	0.86637840014639
H	-3.64804459658306	1.65364189575819	-0.61300355021109
H	-3.34396586706918	0.16207842013005	0.28905551068106
C	-1.85707103947734	-1.67530542970984	1.35689095355603
H	-1.77113614529518	-2.53817453866973	2.03191915856275
H	-2.12771402739021	-0.79776391986510	1.97142587043403
H	-2.70231846699305	-1.86843239827600	0.68066792444792
N	-0.59106087517351	-1.50391329160382	0.62657015396923
Li	0.36838231633955	-3.16889703219909	0.38191146025031
O	1.61311105425145	-3.58638486550880	1.75883623267001
C	2.75712729947208	-4.48625918677501	1.69911499630653
H	2.45828715764131	-5.36196234830681	1.11711226439403
H	3.57732237404899	-3.96877910780219	1.18706409904236
C	3.10034454175836	-4.79003472840501	3.15286573420749
H	4.14877752674517	-5.07181083186217	3.27793416960624
H	2.46998206212150	-5.60219507681473	3.53074913724778
C	2.74519271682791	-3.46528281128369	3.84690638142048
H	2.57062876083653	-3.57606245736977	4.91966400159061
H	3.54218506475404	-2.73114877973905	3.69571377656872
C	1.48271923468634	-3.03525387959345	3.10720291643079

H	1.36933386426294	-1.95461626026775	3.02082770598832
H	0.57880625254434	-3.46143678412186	3.55852955970295
O	-0.66367377050918	-4.73187558242972	-0.07508355655631
C	-1.15196126684478	-5.64924309727992	0.94698332702285
H	-0.71808763173011	-6.63993713977447	0.76330367127153
H	-0.80605362925388	-5.27663596442810	1.91416255076486
C	-2.66551044833475	-5.65620386237448	0.77913392958145
H	-3.10724976825262	-4.78862651373474	1.28014782044542
H	-3.12283806637740	-6.56439213958870	1.17958559933007
C	-2.81162434957084	-5.53326628787745	-0.74621474670777
H	-3.78758231392157	-5.14969908427810	-1.05312384516496
H	-2.65559591262419	-6.50790324168385	-1.21986457543200
C	-1.68115729524205	-4.57291016391828	-1.11635435559194
H	-2.00199266323207	-3.52562809427116	-1.10223130787019
H	-1.21422748386218	-4.79576946388175	-2.07902632803961
O	1.14120294739001	0.01306788547128	4.91283519467442
C	2.17419438842395	0.92512517972426	4.45294265889091
H	2.50573864739482	1.53518449720419	5.30447735669300
H	3.01689978749448	0.32778887884211	4.09266149356291
C	1.52963385697650	1.78485197376093	3.36728433100106
H	1.58595893859241	1.28835763023520	2.39300506517246
H	1.99567657866086	2.77023078026578	3.28305537020628
C	0.06533559205703	1.84008244172994	3.82492543766840
H	-0.62137362842772	2.05972788132279	3.00251926866288
H	-0.06841225897170	2.58695120402423	4.61518609193369
C	-0.13784231889928	0.43075356382394	4.37615233058853
H	-0.42967321274703	-0.26546287154218	3.57519960491708
H	-0.87987525693236	0.37127079347821	5.17869845493450

6b⁻ [W(CO)₅P^tBu(Me)NMe]

Energy = -1269.599366224397

ZPE = 0.23890678

G_{corr} = 0.18846502

P	-1.73922054368885	-0.20171685626386	0.24464519149940
W	-0.64221500180049	1.34385563082045	2.09982460340954
C	0.34303950905334	2.25404859549302	0.55153870392613
O	0.93542181900303	2.75164294776591	-0.31678348744114
C	-2.34219703269231	2.45631728886088	1.76017849132920
O	-3.28879176847240	3.09990971897383	1.57535663832634
C	-0.00479916287256	2.70802044845769	3.41962773817683
O	0.36057459957071	3.51894314918744	4.18063619304865
C	1.05079834115380	0.25173733851483	2.47057092846489
O	2.02508033434948	-0.32647020294529	2.73624026572917
C	-1.53114152142144	0.23815590671255	3.59028139733187
O	-1.94543755443198	-0.40116787336339	4.46887979872146
C	-0.80698965180090	-1.84925338057620	0.02670469417418
C	0.64499242840793	-1.62407581214997	-0.41306059216718
H	0.69748939690574	-1.28256707816211	-1.45190544491001
H	1.14346648352073	-0.87900650135651	0.21484700425997
H	1.21251896980191	-2.56195256524246	-0.33793218650531
C	-0.85100773329966	-2.57349608724438	1.38050400184117
H	-0.33439714237420	-1.99887880532220	2.15547830420810
H	-1.88475702621562	-2.73003879641385	1.70696686541025
H	-0.36455278389227	-3.55495109791305	1.29796888460923
C	-1.54976329952556	-2.69593083366785	-1.01932017884045
H	-1.48811479657271	-2.24678298311607	-2.01659607168733
H	-1.10345107775916	-3.69846395452635	-1.07314093480979
H	-2.60666061970632	-2.79137204880176	-0.75090446684374
N	-3.33739587399200	-0.43895923965140	0.31114181244522

C	-4.01518000005330	-0.59793778594986	1.58107311588626
H	-3.90018778960148	-1.59715665354569	2.04324238897056
H	-3.68072087029290	0.13199506337902	2.34314483743230
H	-5.09537920535932	-0.43868498442280	1.44363749935774
C	-1.52637468727306	0.55805074877044	-1.41603305154173
H	-0.47567057448615	0.61409436169731	-1.71178906675676
H	-2.08584596139556	-0.02658537406278	-2.15367859943466
H	-1.93903020278647	1.57017771606446	-1.38224527762034

[Li(thf)₂I]7b [Li(thf)₂I] [W(CO)₅P^tBu(Me)NHMe]

Energy = -2041.42494939422

ZPE = 0.49001675

G_{corr} = 0.41988973

P	-0.13278352533495	1.13895455065824	-0.00082195578096
H	0.18440321977780	1.22867762455225	-2.23167991202331
W	1.90947261503318	2.42464905325153	0.85938502483051
C	3.08420453252867	0.73355583186548	0.89674708957114
O	3.77643064564016	-0.19269304579417	0.95028025340165
C	2.34902362096294	2.75604755950618	-1.11993562812435
O	2.57740646633785	2.94545681642271	-2.23968578052452
C	3.51771547924087	3.52311328959204	1.40500656234634
O	4.44177449364548	4.15826077375665	1.70730091697285
C	1.45648502242538	2.12905503105171	2.84753963414000
O	1.23526583347092	1.99395141218263	3.97513651075158
C	0.75588393206325	4.12864841088973	0.89094174436575
O	0.12531130041165	5.09756140339529	0.92296342338306
C	-0.85253429747526	-0.24265791326404	1.03795468409652
C	-1.67676741079320	0.43176777153270	2.15325661241720
H	-1.10532374198613	1.20888391867760	2.67141591667907
H	-2.59403274406881	0.87783627487438	1.76010753426622
H	-1.95411082660847	-0.32856730488734	2.89178429832880
C	-1.75896095411601	-1.15451215375170	0.19898456341455
H	-2.53483698951732	-0.59676243740747	-0.33533204255445
H	-1.18115558823467	-1.72853659882716	-0.53055646346252
H	-2.25563899148566	-1.86747441424900	0.86770269332821
C	0.27878373425115	-1.06730040238168	1.67574098124682
H	0.90665845850976	-0.45025324549545	2.32373270800125
H	-0.16708851401242	-1.86001211009244	2.28746457104270
H	0.91946409171032	-1.53987314209810	0.92610046086596
C	1.20694396531237	-0.48774296233473	-1.77893088224461
H	1.28307825719806	-0.72863479836206	-2.84129185637240
H	2.15529624786993	-0.05318874108677	-1.44302851976349
H	1.02659392480660	-1.41136854969577	-1.22737585973276
N	0.06276201412587	0.43638487672272	-1.58959505518942
Li	-1.54619193011268	0.06191303893414	-2.97930156359081
O	-0.85316661652261	1.60380492417622	-4.05078857191096
C	0.02759761923788	1.44092688800087	-5.20169870114121
H	0.91873629977402	2.05813345211325	-5.04011202090027
H	0.31255648256142	0.38858219337773	-5.23490311162766
C	-0.78267226394497	1.92056239032005	-6.42315079675353
H	-1.06175422993752	1.08605445010376	-7.07019938498140
H	-0.19418509270450	2.62617756133781	-7.01437477552833
C	-2.03623352078104	2.59850597150683	-5.81077434475385
H	-2.27603204834411	3.54922230922614	-6.29286414101783
H	-2.90667515645687	1.94027975694426	-5.88602773203115
C	-1.66457549382436	2.77613626892235	-4.34329131098920
H	-2.51269558024388	2.75392668065330	-3.65746585705705
H	-1.05581815884560	3.67391145716829	-4.17500922820654
O	-1.15010424523213	-1.51258998341353	-4.03300703848434

C	-1.95949887392621	-1.62462008202283	-5.24463964618962
H	-2.48118186392822	-0.67268587784788	-5.36095717372923
H	-1.28419417075159	-1.78656696409687	-6.09194544013309
C	-2.91015972651250	-2.81865441248489	-5.02278950232744
H	-2.79403826844267	-3.55100483744341	-5.82580532112522
H	-3.95180947645017	-2.49233511519827	-4.99652209890730
C	-2.47594989528701	-3.40775603130595	-3.65963182873574
H	-2.49690178177823	-4.50033468531759	-3.64639366429100
H	-3.12175865068009	-3.02941108958034	-2.86209877299933
C	-1.06888056314645	-2.85290955076154	-3.48075472874643
H	-0.32332781579988	-3.42524103134266	-4.04818880566240
H	-0.74312549572659	-2.75935790483199	-2.44382370045562
I	-4.23713220539606	0.31189253670001	-2.73130112342727
C	-1.54866985123631	2.22451694058000	-0.38289328106871
H	-1.84593038144789	2.76658052722679	0.51694586361316
H	-2.39990896063744	1.65724760514221	-0.77607375038680
H	-1.22659107516329	2.95602743400855	-1.13039942412543

7b [W(CO)₅P^tBu(Me)NHMe)]

Energy = -1270.118331986758

ZPE = 0.25293369

G_{corr} = 0.20316884

W	-0.91991722272735	1.21269621268144	1.86710820797053
C	0.36278913723111	1.96493332478655	0.44593833671635
O	1.08729766245268	2.36893181646343	-0.36158300440018
C	-2.42345172076207	2.43682823981283	1.18074934351856
O	-3.25034828628592	3.15950061142865	0.81290171963695
C	-0.43224292762341	2.66248005346259	3.18940257983895
O	-0.15918811052871	3.50707303020242	3.93974503401575
C	0.61977726042219	0.08921786627728	2.64338476510304
O	1.49769590143016	-0.48985322656201	3.12895511174408
C	-2.19110569157267	0.30745990062469	3.20568560542050
O	-2.89866292905103	-0.23379154238958	3.94545549880675
C	-0.58816012144254	-1.97147797987438	-0.23329191289225
C	0.83098635747356	-1.45997366936782	-0.53162770871138
H	0.85065048348641	-0.81960421910050	-1.41953012556929
H	1.24472991888760	-0.89762618974338	0.30944773882411
H	1.48457551663007	-2.31919366434054	-0.72118027304101
C	-0.57778120752725	-2.85120741348062	1.03004734203950
H	-0.32374482082308	-2.27409794830782	1.92448603421940
H	-1.54622257431158	-3.33631626850978	1.19031647744851
H	0.17270607764971	-3.64091261844372	0.91082013701929
C	-1.11135260815608	-2.78383464260184	-1.43029905143639
H	-1.02550140986929	-2.22217431498035	-2.36510334507811
H	-0.50727654834464	-3.69373090719376	-1.52856675561446
H	-2.15592116573154	-3.07337981698235	-1.28712944235888
C	-4.38205359918910	-0.38121400204518	0.49234627080621
H	-5.26144226774957	-1.01113487953662	0.64522009579277
H	-4.30547811216034	0.32672171905107	1.32950811682783
H	-4.51967838738933	0.18526218181467	-0.43138779932590
N	-3.20275709118769	-1.25719078498246	0.35826246830912
H	-3.14695927669394	-1.88638070472257	1.15868133540656
P	-1.68228995713644	-0.49348058178029	0.10599900204554
C	-1.94161915150909	0.28365389425213	-1.52800619367130
H	-0.97141439964359	0.59177976281165	-1.92736486464541
H	-2.42291091912054	-0.41341195931934	-2.21821375034384
H	-2.56002780912667	1.17724872059551	-1.41717699442190

TS(Li(thf)₂-4b+IMe→[Li(thf)₂I]8b)

Energy = -2041.29001515128

ZPE = 0.48376397

G_{corr} = 0.41386426

Imf = -274.28 cm⁻¹

P	0.11030672916272	-0.06103512242715	0.26503252309638
H	1.49161095621970	0.10411505630118	0.56802231714785
W	-0.56116388342559	2.36910254439734	-0.53228996534873
C	1.05440622883461	1.86845984660418	-1.71417342739081
O	1.95849903480005	1.59490973180470	-2.37652607576960
C	-1.66440095680204	2.42398969248038	-2.27306418467442
O	-2.23985553447348	2.53613649813910	-3.26903379025865
C	-0.29477718676230	4.33111732521289	-0.91984317626194
O	-0.09829821122829	5.45665684531812	-1.11611676574086
C	0.68338347578246	2.72975674160350	1.07855505120693
O	1.39516054680145	3.01746765569947	1.94027246789343
C	-2.19630690602057	2.86176932006181	0.62333146884605
O	-3.11489085818275	3.18142348864786	1.24712421805841
C	-0.46203820522442	-0.60638639330015	2.01610196399042
C	-1.36389212636969	0.42693946675740	2.69761619424539
H	-0.87016953351211	1.39712534437488	2.80478939115933
H	-2.29886228308589	0.57698413052662	2.14974804427935
H	-1.62347779747089	0.07223292253278	3.70300603051473
C	-1.21386942131644	-1.93854806216144	1.87083757047387
H	-2.10671236674776	-1.84689962182386	1.24272712423772
H	-0.57536813658420	-2.70889459158236	1.43081196018207
H	-1.53127787153012	-2.27796618374470	2.86503834758115
C	0.80976425255933	-0.81842650256738	2.85723798376550
H	1.36634605631935	0.11611831553799	2.98425389767158
H	0.53035479325364	-1.18695180251238	3.85307866798217
H	1.47610051596409	-1.55415705988008	2.39477659047722
C	1.17495896734616	-2.19852089710517	-0.81540837588066
H	1.25506361127096	-2.68853759091940	-1.79360011265777
H	2.13479718002289	-1.69481339810329	-0.61365386990576
H	1.06412725774400	-2.99592257614337	-0.06200712713048
N	0.04139102134410	-1.25732584845609	-0.82738308691788
Li	-1.39702063447981	-2.00332260198832	-1.93746891132048
O	-1.45520342300852	-0.95686703292160	-3.59021347707824
C	-0.18732868460555	-0.59414604351531	-4.19316400903524
H	-0.20007483288865	0.47932206068086	-4.42367289654993
H	0.58601762005550	-0.80127006688179	-3.45365151041155
C	-0.13158045859796	-1.43972905442238	-5.46322209142505
H	0.25501315138577	-2.43591572571746	-5.22945029066911
H	0.51018172012590	-0.99238823850618	-6.22625537697957
C	-1.61720526923160	-1.51951614557949	-5.90616435244028
H	-1.81008487615356	-0.89167095344092	-6.77946826743471
H	-1.89882291355670	-2.54439242597822	-6.15847916684302
C	-2.40719466444355	-1.00179039670888	-4.68581498730987
H	-3.22811140202187	-1.64445162752644	-4.36601841326186
H	-2.78570058751745	0.01349012842196	-4.85284040915751
O	-1.27839216854129	-3.90916933310008	-2.26857412767331
C	-1.95698977987944	-4.51591107449474	-3.40981095976091
H	-2.88276739746841	-3.95801522001979	-3.59493069190113
H	-1.29235959901450	-4.42637637201958	-4.27230672487916
C	-2.24550968719173	-5.95337395276561	-2.99327343030899
H	-1.37339569588908	-6.58903758529982	-3.18025240865038
H	-3.10429986444630	-6.36939061971725	-3.52586292903234
C	-2.48758423159413	-5.80170157874435	-1.48371945722809
H	-2.36618264075875	-6.73736104623925	-0.93225877441515
H	-3.49224841342058	-5.40789960000581	-1.29847744424686

C	-1.43966764291574	-4.76583689773798	-1.09353429613543
H	-0.46790188060091	-5.22230911249858	-0.87422743941753
H	-1.74405233490684	-4.12957689353090	-0.25866658020145
I	-4.24341255385050	-1.86609106933672	-1.20391719588915
C	-2.62045739485797	0.40090960265975	-0.80682243262860
H	-3.45312153196090	1.07977728796700	-0.92496637374251
H	-2.47874001644476	-0.06057928553009	0.15401335752184
H	-2.11134673000784	0.03227281922617	-1.68004349636517

[Li(thf)₂I]8b

Energy = -2041.3134723197

ZPE = 0.48489085

G_{corr} = 0.41368206

P	0.09684864809816	-0.29168336476944	0.46474323202731
H	1.40378804278904	-0.42071334356969	0.99835305344806
W	-0.19272677779173	2.41529966339190	-0.05161777210966
C	1.35007014144839	2.12119956937380	-1.39233406759508
O	2.21777194496397	2.00373989064529	-2.14171495506446
C	-1.09521678944116	3.60202210067906	-1.50136658396061
O	-1.54159371317639	4.29906039067291	-2.29807542923607
C	0.44507647396722	4.27225276591062	0.46967743434846
O	0.78546842523516	5.33554366202573	0.76042730047734
C	1.14239348630420	2.06399889434344	1.48119486032469
O	1.94055106262396	1.95720072936881	2.30838993174885
C	-1.82284944513359	2.64159253159499	1.19440407222184
O	-2.73875455175835	2.82334064852258	1.86993958298941
C	-0.94318046984144	-0.92066622999481	1.87560507019393
C	-2.43921808584608	-0.82663378492313	1.56036765585581
H	-2.76303742503303	0.20787937466992	1.42429845666522
H	-2.70452482263928	-1.39085664029752	0.66128218880025
H	-3.00138618170595	-1.24560768168349	2.40337812828349
C	-0.54182467536238	-2.39319700882290	2.08856049268097
H	-0.81771311730909	-2.99828854918375	1.22352652991508
H	0.53438736440859	-2.49691947686986	2.26279393513183
H	-1.07264543685701	-2.77376947438861	2.96938300457700
C	-0.59989190096688	-0.10847000793159	3.13406297977237
H	-0.85198351705860	0.94981265774503	3.02434075877866
H	-1.18821531169677	-0.50599220457248	3.96871825086640
H	0.45952962757031	-0.19408552780867	3.39485146145886
C	1.19215085104512	-1.36039859944657	-1.64305211990523
H	1.15481748307317	-0.62670627261574	-2.45950961976380
H	2.12621028044177	-1.20065581474913	-1.08285173611784
H	1.23657067289306	-2.35313496432504	-2.10403760185652
N	-0.00625903877141	-1.29392040850954	-0.79000445542659
Li	-1.47439481533526	-1.94062412395630	-2.05272963109999
O	-1.18377642584452	-1.20924147020251	-3.88103119882817
C	-0.35397113287149	-1.84373561969057	-4.88769624657088
H	0.41705867401906	-1.12881369584203	-5.20179972680012
H	0.11652681079110	-2.70573250408100	-4.41465739883842
C	-1.30144268401471	-2.19805565196815	-6.05281755961655
H	-1.49178252004056	-3.27291529234931	-6.09800814684288
H	-0.86606186084853	-1.89120141015785	-7.00730164832721
C	-2.60201121792464	-1.41324817741858	-5.73637437817371
H	-2.99488769735809	-0.88148262155053	-6.60676903835566
H	-3.37692901388244	-2.08769717743444	-5.36086694358538
C	-2.18045218183663	-0.46079646801840	-4.62052957553352
H	-2.97686648927248	-0.21039925413475	-3.91880030402637
H	-1.71577672994193	0.45416534057641	-5.01394551983905
O	-0.94797413784862	-3.83727606420516	-2.36248041565525

C	-1.86319267022604	-4.69677808237676	-3.09765658846691
H	-2.58954231348808	-4.04053689772309	-3.57956906897216
H	-1.28860100442527	-5.24387358792353	-3.85503686786981
C	-2.48967505021211	-5.64666471325804	-2.05529018045319
H	-2.38345674884626	-6.68755388972553	-2.37226077128725
H	-3.55110535055939	-5.42985941062326	-1.91786759187186
C	-1.69304475834394	-5.36713657046676	-0.75632039434091
H	-1.44665470315285	-6.27908575496587	-0.20625463697710
H	-2.26395586588836	-4.70340860029050	-0.10007617055938
C	-0.45207972675289	-4.64044135786715	-1.26477221263836
H	0.30277604688889	-5.34204909177112	-1.64662561553987
H	0.00811662376936	-3.95303727136089	-0.55333620223671
I	-4.25158128817574	-2.01857904035679	-1.75899400008763
C	-1.67859418142321	1.18250969568092	-1.43304790300396
H	-2.44586214720729	1.76304822826461	-1.94745600633961
H	-2.18237478420816	0.45780569098879	-0.79278298985632
H	-1.03767990001137	0.67905031972662	-2.15483310693502

TS([Li(thf)₂I]8b→[Li(thf)₂I]9b·[W])

Energy = -2041.30090939014

ZPE = 0.48506018

G_{corr} = 0.41642213

Imf = -196.99 cm⁻¹

P	-0.14294924385641	-0.17550536447253	0.33177484626803
H	1.22818153416148	0.02490820312796	0.66736231832313
W	-0.40493769431440	2.38112431248153	-0.55162679238151
C	1.10566597214849	1.52314559602072	-1.65854797957772
O	1.97898438740570	1.09788034508402	-2.28081247769888
C	-1.44692819512523	2.63742644526297	-2.33907849771337
O	-1.98333735791230	2.83407202193488	-3.33624146777151
C	0.44910122073774	4.16134156266748	-0.94548286230644
O	0.94418164901163	5.18292764299577	-1.17336172431777
C	0.75686680650328	2.49682607201155	1.13448719805031
O	1.44752784615990	2.66630721168304	2.04528767728629
C	-1.87721877211864	3.35371985289571	0.54219251989292
O	-2.66479003576003	3.93892208009102	1.14427624528242
C	-0.81979144138160	-0.52163638649110	2.05934987450704
C	-1.70970499362122	0.59538021129359	2.61540684328338
H	-1.17159945224661	1.54316501907460	2.70196059772780
H	-2.59959143529893	0.75150957363531	2.00012798213881
H	-2.04491844014885	0.31003167173508	3.61933320704049
C	-1.59968662702279	-1.84826513961195	2.00262285309834
H	-2.48288847796295	-1.79692010532906	1.35675969245204
H	-0.96634289573671	-2.66130713162655	1.63770352446712
H	-1.93621073652115	-2.09309632477498	3.01700228217446
C	0.42078285786879	-0.71166882589430	2.95331925441166
H	0.99955096372843	0.21106893296711	3.05108924030819
H	0.08924086004119	-1.01588617534422	3.95308744131413
H	1.07903964198438	-1.49514255369952	2.56260940754809
C	1.19459709526567	-2.08663940012794	-0.85023915162589
H	1.33275055436221	-2.38690185127875	-1.89482323505741
H	2.04995779521642	-1.45744076020626	-0.55720893349539
H	1.23627932340105	-2.99654297565484	-0.23519247263891
N	-0.09627932681498	-1.40036631525885	-0.69874180480713
Li	-1.52837633846662	-2.11321249934576	-1.90465449950680
O	-1.57669777971639	-1.00932870996488	-3.53715482399911
C	-0.36468275564870	-0.70717636590644	-4.26976342732093
H	-0.29177165446178	0.38092666431043	-4.39660700022842
H	0.47476009192180	-1.06059774826274	-3.67067858279025

C	-0.53418153743662	-1.41638293255522	-5.61741646608503
H	-0.10549652494100	-2.42079395119879	-5.57421864673583
H	-0.03664742800298	-0.86817697029596	-6.42113861002731
C	-2.07496722306676	-1.48602518857466	-5.81183551421797
H	-2.40595802743269	-0.90634117730517	-6.67687153469402
H	-2.40067526650877	-2.51935566885492	-5.95167546663516
C	-2.64816098879416	-0.90189943738264	-4.51005617079798
H	-3.50181905582564	-1.44204643828083	-4.09850821201431
H	-2.90469717317025	0.15897429155836	-4.62539621660916
O	-1.04489651801001	-3.95046364296171	-2.38633652213882
C	-1.73383599573523	-4.57979056893123	-3.51007848392263
H	-2.70671485575916	-4.08793318381890	-3.62855177143762
H	-1.12409406520874	-4.41808931213983	-4.40236120961600
C	-1.89101077303414	-6.04782023432014	-3.12742016635069
H	-0.99416907695200	-6.61425773133968	-3.40073698747894
H	-2.75624766287820	-6.50569280909415	-3.61351634407397
C	-2.03243995068312	-5.96567322322806	-1.59986329833548
H	-1.80263980178446	-6.90758096251025	-1.09511867208723
H	-3.04524962202719	-5.65027227933617	-1.32989508141164
C	-1.03871755305800	-4.86612570987518	-1.24640829375538
H	-0.01976274078201	-5.25334651277100	-1.12762882579968
H	-1.31978988239848	-4.29057066947827	-0.36026747796911
I	-4.21245342998346	-2.44507379971936	-1.13681693061863
C	-2.05542117681431	0.50279392039474	-0.55775068981891
H	-2.85591010679631	1.19986998037398	-0.31699234757619
H	-2.29135182128071	-0.40725237441990	0.00646003250773
H	-2.01609268741701	0.23387680004329	-1.60939136463669

[Li(thf)₂I]9b·[W]

Energy = -2041.35776402457

ZPE = 0.48507920

G_{corr} = 0.41619172

P	-0.30155715484627	-0.52057311145446	0.48471511093442
H	0.79275268720461	0.36028486674031	0.69172616365919
W	-0.87398732903565	2.94927281160762	-1.10116911737029
C	0.90405862167838	2.15137141613032	-1.76888252183458
O	1.92128866973054	1.75286348277015	-2.14274347092423
C	-1.74046316598895	2.67558579970571	-2.95313890239192
O	-2.20664078830198	2.60132696237559	-4.00589297059953
C	-0.27357465368780	4.72089082224016	-1.71541878213200
O	0.08318381200720	5.76486894563109	-2.08606659181373
C	0.01811945067555	3.33491243878694	0.71666229524535
O	0.53819440121187	3.60230314418657	1.71220368478906
C	-2.63733758503286	3.78701221797985	-0.42554316731175
O	-3.60703182226382	4.29385593090899	-0.06155913977229
C	-0.65866540087014	-1.03424756135989	2.22008864372878
C	-0.80066021770768	0.22357866061234	3.09568491450102
H	0.07771017154234	0.87379879992650	3.01411426375285
H	-1.69324271241785	0.80168026271891	2.83680007922724
H	-0.89390762411600	-0.08139317487768	4.14424687839889
C	-1.93762996453116	-1.88500796781448	2.25146746152013
H	-2.81787097183599	-1.30552466159943	1.95776623436326
H	-1.85877456982682	-2.74111627535615	1.57439531777936
H	-2.09555389835311	-2.25966687467126	3.26941334246061
C	0.55275444208274	-1.86735508688240	2.68577478320706
H	1.48755619481064	-1.30064302600618	2.60636863776414
H	0.41144620721511	-2.14211145602223	3.73721507615715
H	0.64955239600458	-2.78776480913216	2.10307779831146
C	1.21052259605435	-2.32979675525754	-0.73594818080403

H	1.35968928720354	-2.65806170735355	-1.77000026971366
H	2.07442634769680	-1.70990318574262	-0.45343866876691
H	1.22149820859087	-3.22737083509890	-0.10402294749320
N	-0.06163646200887	-1.59442918655663	-0.65321431897724
Li	-1.51587131040973	-2.09128520808319	-1.92731518979710
O	-1.43904768766615	-0.78894468491654	-3.40216881730350
C	-0.12756802540358	-0.55780376106537	-3.97638330712412
H	-0.04806372324691	0.49392172679826	-4.28166185346126
H	0.60275182029394	-0.76939834307567	-3.19477797665126
C	-0.08420506253634	-1.49165961372571	-5.17965077981273
H	0.15480990806746	-2.50652775718812	-4.84823275848378
H	0.65825388848138	-1.18398096511322	-5.92026263008109
C	-1.53159141800872	-1.41540572845978	-5.72144539212423
H	-1.59808356237892	-0.71415319725516	-6.55723578916841
H	-1.88418951262608	-2.38902197380098	-6.06919586737978
C	-2.36263150701568	-0.89979080885098	-4.52500545906452
H	-3.16057203342434	-1.57185738052871	-4.20461572587038
H	-2.78565851379807	0.09004111990675	-4.72316220656903
O	-1.18781658603117	-3.94154430730134	-2.48215373306143
C	-1.97778976547182	-4.54168828647505	-3.55610161443093
H	-2.91862897989376	-3.98441369231108	-3.63358333596662
H	-1.40708700927026	-4.44043849403655	-4.48243230248063
C	-2.21761005801597	-5.98822791702192	-3.13537744783475
H	-1.38272582452035	-6.62364746737181	-3.45003680503498
H	-3.14171480813158	-6.38795077999181	-3.56046425708506
C	-2.25890172071569	-5.87316927665342	-1.60408889125478
H	-2.06971364336926	-6.82244661875563	-1.09627768531232
H	-3.22644909317892	-5.47738379626278	-1.27926360635387
C	-1.16491129098540	-4.84883499546965	-1.33460748302396
H	-0.17132433705503	-5.30954040251228	-1.28525686536033
H	-1.33475005601571	-4.24660711129154	-0.43804011028860
I	-4.20190634123840	-2.17134999384814	-1.15469851343335
C	-1.66325852992326	0.54193884397479	-0.06442734734448
H	-1.89020707171294	1.32918428206793	0.65998004932768
H	-2.57653914786030	-0.04792077209095	-0.22705093029912
H	-1.40585416982126	0.87886547357570	-1.10394100376407

TS([Li(thf)₂I]9b·[W]→[Li(thf)₂I]10b·[W])

Energy = -2041.28707148487

ZPE = 0.48168973

G_{corr} = 0.41139303

Imf = -1333.15 cm⁻¹

P	0.19079435057047	-0.00211414777546	-0.01289468197248
H	1.19119567033444	-0.17666239454854	-1.08796460966751
W	0.89520434383492	3.77865206126503	-0.10862621917248
C	2.16474730521619	3.12821668658673	-1.59466806919251
O	2.93195262977808	2.81832168569284	-2.40081608315138
C	-0.26616659598293	4.79494495238164	-1.47812121171604
O	-0.88744615562494	5.40180896670727	-2.23811564903460
C	2.04342199244689	5.36628143793670	0.07563818347975
O	2.71878337078760	6.30759236392356	0.18911888568710
C	2.08714597459381	2.79558414230181	1.25845061405965
O	2.79270299963999	2.29847478574152	2.02522099648248
C	-0.26768210456352	4.51829318457602	1.42744097282710
O	-0.87246131731541	4.97711683459290	2.29641401457187
C	-0.68482140507649	-0.58902088766924	1.55015670595545
C	-0.71106302143870	0.53715595688668	2.59201571575692
H	0.29726015165149	0.89674888862272	2.82351659576093
H	-1.32400612472197	1.38221545711078	2.26424034726412

H	-1.14810573162990	0.15268424206860	3.52122281995132
C	-2.09576181412176	-0.98996628946663	1.09624269708721
H	-2.70563160454212	-0.11956071908075	0.83960713818739
H	-2.06450249234324	-1.64663781139663	0.21882109355003
H	-2.58915236627191	-1.53397591443905	1.91068080007645
C	0.08802261474739	-1.80278367726412	2.09296343508297
H	1.11800668127377	-1.53541348336721	2.35041064275599
H	-0.41082607340102	-2.16573697911955	2.99929834857492
H	0.11233394286873	-2.62297613448365	1.36959132558736
C	0.47714092703994	-2.27807551773705	-1.42543057943378
H	0.69385482255762	-2.55428013843362	-2.46176920208107
H	1.41352383677647	-2.32650650570033	-0.84461631564795
H	-0.20687345429501	-3.02722506220312	-1.00759258986971
N	-0.14387957975971	-0.94016926947671	-1.40483558412079
Li	-1.38341609839024	-0.31887564906816	-2.86080026166682
O	-0.43399548058473	1.13267482957858	-3.76419904205318
C	0.82842330030158	0.78381460147441	-4.41844756875826
H	1.60849946669781	0.81858054583117	-3.65364750989891
H	0.74906678218235	-0.23808637206310	-4.80011623780005
C	1.03585782115757	1.82530313247520	-5.52338804997552
H	0.68091346529324	1.43753851229263	-6.48335783390262
H	2.08785680132944	2.10014012791457	-5.62956316234296
C	0.15043305864709	2.99867608968836	-5.07108588338743
H	0.66457543108517	3.60682108951435	-4.31999504198851
H	-0.14978617820246	3.64717279549149	-5.89762793303421
C	-1.03076089163718	2.27126382523239	-4.44752678751971
H	-1.73133834436711	1.90848417223728	-5.20984337101895
H	-1.58435150284733	2.83850112314735	-3.69775841362296
O	-1.63065647622094	-1.75827973813251	-4.15203378046749
C	-2.17949086650373	-1.37782219243202	-5.45254967660392
H	-2.77140835263698	-0.46451771852106	-5.31775894665737
H	-1.33660425390647	-1.17811990310307	-6.11918920940460
C	-3.05184776212470	-2.55062290376780	-5.88547180212732
H	-2.44644676173153	-3.31768447840285	-6.38038378702714
H	-3.84798013371742	-2.23848653048683	-6.56602886828465
C	-3.57975484305791	-3.06655095963640	-4.53788881275472
H	-3.93607028675107	-4.09885847739799	-4.58205285148986
H	-4.38898733317092	-2.42355069379847	-4.17715468902161
C	-2.35914720339992	-2.91800378000077	-3.63742506988276
H	-1.69353303624837	-3.78702708982240	-3.69481724738577
H	-2.61012888126061	-2.71502016878170	-2.59246547270674
I	-3.94900241452898	0.55961871537461	-2.29340076083620
C	-0.64304049709178	1.55170618032736	-0.47258647298388
H	-0.57829620149872	2.27142055690502	0.37936037023701
H	-1.72150604118680	1.42505064643751	-0.64314179429551
H	-0.21633677865698	1.89591459725925	-1.42218331897397

[Li(thf)₂I]10b·[W]

Energy = -2041.35776402457

ZPE = 0.48857241

G_{corr} = 0.41923409

P	0.55685623818358	0.05012019600752	0.57562902093480
H	0.95419213749250	0.68529914247582	-1.54976433388136
W	0.91923441175854	3.86668471621864	0.01152172924314
C	2.39253683617051	2.83331695635003	-0.97292883313677
O	3.25111443864243	2.29194283866032	-1.53034424005899
C	-0.04335731182112	4.25459201980941	-1.77412780791248
O	-0.51332203028964	4.55805767756333	-2.78257388920424
C	1.94997099416230	5.52124033367031	-0.28620984372246

O	2.55513196450579	6.49802051860822	-0.47193024490420
C	1.95755656400591	3.57231299482047	1.77020988389963
O	2.57258372795702	3.44562952200434	2.73839409194928
C	-0.53891552430461	4.94354060404147	1.01297089109851
O	-1.33054024358534	5.57496099860776	1.56277555673421
C	-0.65044548981998	-1.23323926005115	1.23220923672158
C	-1.06533787053553	-0.71821688171470	2.62664007031170
H	-0.19099680631423	-0.45739439324587	3.23592432902521
H	-1.71721496654332	0.15772146956672	2.55881516822022
H	-1.61429368305622	-1.51031957387326	3.14929373264961
C	-1.88265419168866	-1.43568254616607	0.34544970458453
H	-2.41725089235705	-0.49757510234989	0.15802619806481
H	-1.61276317612955	-1.87192984033837	-0.62049101891099
H	-2.57859052549367	-2.12370347674944	0.84226293384712
C	0.11088553744866	-2.56209517429339	1.41089206400206
H	0.99624229445205	-2.42783234949696	2.04144924327743
H	-0.54945376405386	-3.29076986366468	1.89702610147879
H	0.43128938823435	-2.98520640769176	0.45464778162116
C	1.07777675291583	-1.33617832007919	-1.73069478546745
H	1.23337197825790	-1.21570849932452	-2.80528762430353
H	2.04534301666014	-1.53181338566143	-1.25071280361483
H	0.42129364550932	-2.19341669717668	-1.57733955025648
N	0.41395565489785	-0.11282519710291	-1.20017488471234
Li	-1.28775888431293	0.27975953502660	-2.38519187762578
O	-0.39678687002410	1.18435513186376	-3.89257880325484
C	0.95028412746298	1.49973225035030	-4.31589463272993
H	1.15005506974424	2.56062659907290	-4.11875062930638
H	1.63775638484251	0.88412285336655	-3.73258769004264
C	0.96038784111806	1.19318607052803	-5.81331894033563
H	1.19848259482532	0.13875265360398	-5.97779884609606
H	1.69850968472329	1.79845726739903	-6.34466873153055
C	-0.49498720583750	1.50065183050240	-6.25697899266883
H	-0.54791124973699	2.39973158870824	-6.87525625817785
H	-0.91014727347673	0.67002775280241	-6.83250737572390
C	-1.26329815275029	1.70848646203768	-4.93855042438065
H	-2.20581631533439	1.16431927875717	-4.87029501994819
H	-1.44772871307472	2.76792728512438	-4.73362418039427
O	-1.98489559076330	-1.36669923923311	-3.15302826685140
C	-1.49210170816683	-1.97252490657058	-4.37772233229977
H	-0.67051128681284	-1.34851440539818	-4.73117601219199
H	-1.11368274772126	-2.97390271612187	-4.14115096296639
C	-2.69852881145196	-2.03331820033819	-5.33966976521404
H	-2.81483124939382	-3.04376223632195	-5.73926547242913
H	-2.57546522103600	-1.34961976475524	-6.18286080803151
C	-3.90893884342350	-1.63046702793670	-4.45900413845839
H	-4.78536716799803	-2.25805776219916	-4.63845818780297
H	-4.18635709009368	-0.58718138039076	-4.63644326944109
C	-3.37308646201033	-1.77617263247411	-3.03926560455133
H	-3.40712825572545	-2.81709580654842	-2.69048508030649
H	-3.84046110773078	-1.11465945633072	-2.30833232991218
I	-3.38487030817251	1.91529953795414	-1.68583160302614
C	-0.47093011271436	1.58822354328034	0.69125783122023
H	-0.28185708231697	2.11092381024518	1.63070014849675
H	-1.54976150619780	1.44360680226360	0.57329144749395
H	-0.24701431170042	2.17841386230749	-0.24503981908710

TS([Li(thf)₂I]10b·[W]→[Li(thf)₂I]7b)

Energy = -2041.35699874136

ZPE = 0.4872217573

G_{corr} = 0.4190279648

Imf = -122.37 cm⁻¹

P	0.77199531397702	0.10531366532806	2.32134652109296
H	1.11331484111859	0.49519743663567	0.13460774804407
W	1.97925878795360	3.11048577827548	1.86855104870668
C	3.24761302942391	1.76275196229916	0.97013595069755
O	4.01765130574371	1.06173760708307	0.46671590712682
C	1.28063484469633	3.74035515046527	0.04005390987295
O	0.92413876595132	4.14452675353329	-0.98330013154409
C	3.42654319207034	4.41895908800406	1.71983219192101
O	4.28516343422443	5.20298157047045	1.62822453421123
C	2.68930455721898	2.49498911309368	3.71636190165101
O	3.11334197618474	2.17791934219070	4.73986483160393
C	0.83171649001377	4.56546939021702	2.78255146491185
O	0.24914827220081	5.42892203239035	3.27894446958548
C	-0.20266780395834	-1.27508215991940	3.15229142191267
C	-0.75798231868177	-0.66902214660353	4.45667587752456
H	0.02613935186934	-0.16309861149700	5.03353340100340
H	-1.56400917881974	0.04382097077277	4.26134611975085
H	-1.16192042090348	-1.47716529871401	5.07751672353518
C	-1.34480460138998	-1.80347866332781	2.27800003355497
H	-2.02299188242330	-1.00470841341698	1.95837020356782
H	-0.96641358179579	-2.31011498152248	1.38556788286818
H	-1.93174238826935	-2.53038018111707	2.85406652889049
C	0.77902970332627	-2.40622930013791	3.51520670937725
H	1.59635172105745	-2.03232627673736	4.14084198256059
H	0.24119229963074	-3.17880101548232	4.07811415453200
H	1.21230554955741	-2.87698734391507	2.62852649919411
C	1.59483885039483	-1.48351418443500	0.25096198612796
H	1.79161213343609	-1.46736083106434	-0.82272006529864
H	2.55199206416968	-1.45994665785134	0.78655522469608
H	1.07289842194762	-2.41130406584662	0.48704593332694
N	0.71750604053655	-0.32942859296197	0.59680537780214
Li	-0.98123052093825	-0.31442698995041	-0.67392949117203
O	-0.16023921092785	0.77470924403974	-2.10939233670244
C	1.22559829743024	0.89993417846351	-2.55215732874048
H	1.80727606213310	1.36593838867507	-1.75035361930648
H	1.61478598526513	-0.10684986703296	-2.73981755272591
C	1.19140427881693	1.74445766940721	-3.82458731901488
H	1.99064242692998	1.46709607685943	-4.51567176754144
H	1.29249517958790	2.80601795629217	-3.57995723543901
C	-0.21435391849825	1.45726826132113	-4.37331702630509
H	-0.56880768389822	2.22961578060956	-5.06013222662888
H	-0.23818580448432	0.49025697261775	-4.88759231237521
C	-1.03999911022692	1.40170091065193	-3.09716823472808
H	-1.94151421923354	0.79006789646743	-3.15972004211054
H	-1.30748560274728	2.40056572238299	-2.73559716129122
O	-1.23179950667782	-2.12074308166768	-1.35950046594460
C	-0.68224696590877	-2.53454511832385	-2.63744553055028
H	0.05219474548784	-1.78467094626085	-2.93201228784538
H	-0.18317073701925	-3.50177470055050	-2.50130220663188
C	-1.88628987007035	-2.64775490091651	-3.59159792154833
H	-1.81105568510382	-3.55225604535576	-4.20011135255833
H	-1.93824478917086	-1.78988316779169	-4.26632668304965
C	-3.11733388780660	-2.68407516918328	-2.64511245433324
H	-3.79704595023184	-3.50884207146475	-2.87284141821846
H	-3.67473021529528	-1.74529027809924	-2.70456843832202
C	-2.50078636504359	-2.81967177417332	-1.25374609417357
H	-2.30017128359634	-3.86678204805552	-0.99087537689490

H	-3.07061096428226	-2.33141138273584	-0.46218744888233
I	-3.46880292877212	0.77716286727544	-0.17464156944581
C	-0.46481833530909	1.47241647907277	2.24582747879907
H	-0.62847418922483	1.89291952958977	3.23846099267358
H	-1.42350616262307	1.17883766945791	1.79422873992268
H	-0.10465183902238	2.28553080216955	1.57054934827711

K-4b [W(CO)₅P^tBu(H)NMeK]

Energy = -1830.532815133371

ZPE = 0.21124458

G_{corr} = 0.15895209

P	-1.33172634949443	-0.21242232068444	0.12577092712561
H	-0.46690593036400	-0.06636174006069	-1.01228267680592
W	-0.50033232082024	1.25346151200537	2.08587909592454
C	-1.36022664714947	2.76326501741842	0.99288527523343
O	-1.86673474750360	3.62461580791761	0.40208738995820
C	-2.28895717207177	0.82747090526056	2.97545504496936
O	-3.32169249091267	0.56587745901109	3.44656182404631
C	0.05240272395722	2.60560534875239	3.47761214520197
O	0.35814841822630	3.40444845540778	4.26986903503870
C	1.24372299184643	1.41453745271509	1.00201175715983
O	2.20973066161657	1.46052443050377	0.36486259371660
C	0.37057542634805	-0.19595088609189	3.25918757673559
O	0.87297413846249	-0.96028711801437	3.97233399595585
C	-1.02632480338600	-2.06662089429112	0.33046523475901
C	0.48766745157018	-2.29091667816013	0.43632832787354
H	0.99699289217643	-1.96767409306161	-0.47911624566186
H	0.92055456394377	-1.74158445927812	1.27762180261881
H	0.69873654225299	-3.35805453064455	0.58399008145468
C	-1.75048241698559	-2.55375023698275	1.59139744590772
H	-1.35135222503520	-2.07445094873482	2.49058135278243
H	-2.82151561347853	-2.32814388690129	1.53285939084291
H	-1.63311073644074	-3.63951439840337	1.70137131369165
C	-1.57066195757437	-2.81121406524843	-0.89971381535398
H	-1.13348681654834	-2.42454312185922	-1.82744313465081
H	-1.32046642853993	-3.87819531981502	-0.82491223845664
H	-2.65844786070200	-2.72202626939654	-0.96555489083235
C	-3.22626664485331	-0.07849329924605	-1.72995056978596
H	-3.93900900152746	0.68678138902236	-2.07833061737450
H	-2.37571312292915	-0.06463516618284	-2.43587187127381
H	-3.72601785219101	-1.05263341086912	-1.85609178344990
N	-2.82697391109461	0.20909017996300	-0.34835625799544
K	-4.73370076079799	1.66189488594892	0.73709249064445

Li-4b [W(CO)₅P^tBu(H)NMeLi]

Energy = -1236.570681351172 (CPCM_{THF}/TPSS-D3/def2-TZVP(ecp))

ZPE = 0.21372213

G_{corr} = 0.16362457

P	-1.40906532054806	-0.18494598231817	0.17948650102334
H	-0.70112300051913	0.07582367019789	-1.03546330214679
W	-0.48831176141966	1.30019220188251	2.07899186207226
C	-1.11786168591634	2.82132982728504	0.84073619073208
O	-1.48635472870915	3.67891968217958	0.15741709897776
C	-2.37743139372422	1.13392872159852	2.77658279183025
O	-3.51013717168678	0.99206933766312	3.04628879957246
C	0.12792252892308	2.66586318439769	3.43793985203162
O	0.46266939427995	3.46733523271140	4.21279526495027
C	1.31828029566149	1.22917642277160	1.07772660654770
O	2.30683579905535	1.15941490665076	0.48136368494487

C	0.13729845430585	-0.17644403625815	3.36746997174418
O	0.49956530758143	-0.96540669787347	4.13611114604057
C	-0.97888604397824	-2.01804129798830	0.27746348105398
C	0.54264577835363	-2.15072666556748	0.42251405945159
H	1.06252886275007	-1.68625830866999	-0.42389319446899
H	0.90262502020584	-1.68265759718826	1.34331384216349
H	0.82197636022276	-3.21174350897762	0.44910037497054
C	-1.70655734217925	-2.62122342524288	1.48552702442381
H	-1.39738146902861	-2.14125143547120	2.41926889811390
H	-2.79114592304213	-2.50108653118137	1.38146202865616
H	-1.48652335849399	-3.69336476474442	1.56329923686385
C	-1.43632525447281	-2.72136273502477	-1.01164814301793
H	-0.99010110898223	-2.25878480418942	-1.89925919618425
H	-1.12612552061160	-3.77447023070522	-0.98501150814176
H	-2.52424833376705	-2.69238556428704	-1.11512443842572
C	-3.47995397173826	-0.10609637194639	-1.49497183370126
H	-4.27815891354231	0.61463079925098	-1.72126048847441
H	-2.69151137228331	0.03022727779818	-2.25396661710697
H	-3.90082722300107	-1.11226576729557	-1.64840474493673
N	-2.98397528636960	0.12364173180484	-0.12850741402636
Li	-4.33894161732566	0.39606272873764	1.18125216446647

Li(12c4)-4b [W(CO)₅P^tBu(H)NMeLi(12c4)]

Energy = -1852.292046717501 (CPCM_{THF}/TPSS-D3/def2-TZVP(ecp))

ZPE = 0.45703893

G_{corr} = 0.39420169

P	-0.94771263397968	-0.18058829251124	0.14309520623575
H	-0.28994058034368	0.11189839460396	-1.09221414028854
W	0.40471944432115	1.03157203277760	2.00409808612210
C	-0.86597032164187	2.60209167252766	1.61804210234222
O	-1.52228652922296	3.53108260445335	1.39696455805635
C	-0.69102394934993	0.20026103156472	3.53187211769565
O	-1.19127971586772	-0.31485678099286	4.44251891844514
C	1.39024335175668	2.20848438458875	3.30287373545171
O	1.95291659277946	2.90921266124046	4.04736661227732
C	1.59790417786290	1.62132259090027	0.44118829032513
O	2.27949405207466	1.91480690873456	-0.44941060285596
C	1.77105916266107	-0.44414054672597	2.41631280003383
O	2.57626905711820	-1.22834722863053	2.70680858384126
C	-0.65455977653246	-2.05275161925268	0.04802857045664
C	0.80151896017626	-2.28900497714626	-0.37271075469848
H	0.97696688612016	-1.92878429182834	-1.39242040973097
H	1.50273204986563	-1.77765251999217	0.29329004251397
H	1.03291568429161	-3.36192256620128	-0.34326713579128
C	-0.93237964271646	-2.67658479936213	1.42125678398798
H	-0.21387907264606	-2.32238672499539	2.16671223444831
H	-1.93485861541065	-2.41666444891322	1.77663776494846
H	-0.85838675433897	-3.77023962186140	1.36374184029099
C	-1.59918906725097	-2.65205758274187	-1.00335818461078
H	-1.39946994485465	-2.23846038050595	-1.99764859667825
H	-1.46110146478619	-3.74060665131202	-1.05075268280022
H	-2.64498888006579	-2.44907335958168	-0.75334412331450
C	-2.87748633999143	0.35434723945030	-1.53602848639525
H	-3.67367632040764	1.09562062855305	-1.66295420835638
H	-2.03011090414740	0.65672954791111	-2.17632520346656
H	-3.25055557688550	-0.59853755285925	-1.94858165786116
N	-2.49865208314288	0.28266268585868	-0.11245271445119
H	-6.86443970998491	-1.50496887048226	-0.65478117028405
C	-6.07051207803372	-0.78324942079128	-0.42123798812302

C	-6.58129764038103	0.63362964287622	-0.62320838218851
H	-5.19979490294345	-0.99143152653999	-1.05558952551352
O	-5.69677499330613	-0.86201036365968	0.96281684791982
O	-5.54194286943773	1.55024526778438	-0.22842718225061
H	-7.46598326885197	0.79842100877337	0.00290040192161
H	-6.85109202716803	0.79329470984050	-1.67469599744905
C	-5.00275474883336	-2.04731806955788	1.38048089330791
C	-5.98454370673625	2.73681165330330	0.46017832823014
H	-5.64210993385062	-2.93536211432868	1.29355455858787
H	-4.10614746712122	-2.18344569016337	0.76055811684437
C	-4.63292868127218	-1.80058976120059	2.83384567272269
C	-4.98827387635137	3.02381352549957	1.57123024127842
H	-6.97608756117868	2.55673446492189	0.89125073121605
H	-6.04132375198397	3.58237430475563	-0.23625744888921
H	-5.54281318875730	-1.71776065600835	3.43884343826508
H	-4.02030824446942	-2.62394186676068	3.22064106920663
O	-3.89879838832390	-0.56270263149473	2.90100340569100
H	-3.99712517236248	3.26913007964230	1.17148761614461
H	-5.34286375373942	3.85360337538525	2.19583780855288
O	-4.93175159607253	1.80055032568155	2.32081423575128
C	-4.26513534656202	0.31409682018772	3.98577666851335
C	-4.10109408632306	1.73896740995821	3.48942016055264
H	-5.31389556270758	0.13949149144993	4.25302263279694
H	-3.63127833293330	0.12866591886166	4.85926721751050
H	-4.43757118981043	2.45209565930448	4.25247289336258
H	-3.05738905758022	1.95630779935726	3.22909256040396
Li	-4.09560010836861	0.45961507565401	1.05996284974434

K (18c6)-4b [W(CO)₅P^tBu(H)NMeK(18c6)]

Energy = -2752.569821183483 (CPCM_{THF}/TPSS-D3/def2-TZVP(ecp))

ZPE = 0.57387940

G_{corr} = 0.50181279

P	-0.96377892243590	-0.43274827264555	-0.21198252584879
H	-0.26529199457699	-0.61983130688275	-1.45472266408883
W	0.62016751492244	0.60334932838235	1.53893743443307
C	0.10815192293762	2.33762636478882	0.54693975076305
O	-0.15246164223890	3.32817731754177	0.00735774544368
C	-1.05990195833238	0.67823992649561	2.69787742376971
O	-2.03034300075548	0.64744708540102	3.33580238280710
C	1.78054776699544	1.68340554714049	2.78394678841983
O	2.43976589523585	2.32947151138370	3.49955422172672
C	2.11069835755277	0.21878124155921	0.18010391724637
O	2.91394155350315	-0.04742897678248	-0.61420941585046
C	1.16374047260884	-1.07659240782402	2.58111750239954
O	1.49880919624696	-1.99050561089053	3.21635582060820
C	-1.36250792881167	-2.26770510699864	0.03398499596795
C	-0.06013977315907	-3.06847104590454	-0.07734968578399
H	0.38185780293549	-2.96155202835494	-1.07491346350990
H	0.67889723987114	-2.73713651489975	0.65847552456591
H	-0.25586179118856	-4.13521670108099	0.09559309810857
C	-2.01470939251659	-2.45781572585621	1.40901022825736
H	-1.32767942070536	-2.18391665718526	2.21592967515723
H	-2.91526076878570	-1.83947932361786	1.49972860221820
H	-2.30522906512714	-3.50758250999196	1.54865264114065
C	-2.34382613813578	-2.70581982013044	-1.06394527441770
H	-1.93281986850860	-2.52578822178855	-2.06390160007761
H	-2.55562144952184	-3.77981129688815	-0.96927297672641
H	-3.28941049642219	-2.16278789138959	-0.97650328983586
C	-2.75994658495639	0.49786276821841	-1.88687329050747

H	-3.21390954805136	1.46864247511671	-2.12317630045413
H	-1.97404430944741	0.30281438358004	-2.64207848458406
H	-3.54063252494233	-0.26522052515548	-2.05750925657200
N	-2.23544036046920	0.52277305670732	-0.52101299301254
H	-3.46683289547414	5.80095774898255	-0.76831856688676
C	-3.72579471348378	4.74084470420292	-0.63316420096403
O	-4.08923792540888	4.49383334060459	0.73160357393769
H	-2.85758375280223	4.12689301152171	-0.91212682380150
C	-4.92143148228988	4.40307087304883	-1.49174222925538
C	-3.10567346666879	4.94838759515394	1.66994929838882
H	-5.80410914356532	4.95683852663883	-1.13923101051441
H	-4.72255341854167	4.68375098455678	-2.53676611724774
O	-5.15972281337221	2.99515712922765	-1.39826185244157
C	-3.69384945964017	4.80535713529157	3.05256013275666
H	-2.86647179650606	6.00542845496859	1.48355447956533
H	-2.18312759357385	4.35957622355038	1.57210510491913
C	-6.37806327061948	2.60481341855471	-2.03877985714073
O	-3.87831791971501	3.41275405437510	3.33414196413194
H	-4.66206451268324	5.32522041171431	3.09836923652843
H	-3.01780319065833	5.25372482657642	3.79565554190293
H	-7.23647853193307	3.02827115486865	-1.49596346356218
H	-6.39977105887655	2.97744260140687	-3.07370844307888
C	-6.44685124288643	1.09692226423924	-2.06393273476947
C	-4.67969839375735	3.21834824940559	4.50581717227526
H	-7.34370158364088	0.78020238151984	-2.61665568332635
H	-5.56071991153590	0.68719782791732	-2.56603270641747
O	-6.50991047030959	0.60902591185755	-0.71596981053093
C	-4.72296205359820	1.74808031197240	4.84191036448813
H	-5.69308413994829	3.60807317489676	4.32641763017521
H	-4.24281944305366	3.76151806347754	5.35719726449792
C	-6.42454868687580	-0.82190843128685	-0.66814622025870
O	-5.37911478494837	1.04253757429457	3.77825211612063
H	-5.28278456550514	1.60988744856525	5.77924383518667
H	-3.70717650785296	1.35889623022653	4.97682571727898
H	-5.40656076877465	-1.14155352696419	-0.93395119173386
H	-7.12767282315077	-1.26694170651194	-1.38695039974836
C	-6.79501076916942	-1.28616272959973	0.71869570027803
C	-5.32887238512384	-0.37710918410743	3.97828768851590
H	-7.80029195971253	-0.92305808129603	0.97823793505838
H	-6.80234578784527	-2.38624110338960	0.74480346242063
O	-5.84740607568499	-0.77785496472490	1.66494602065516
C	-6.27456381016087	-1.03990883070345	3.00737048541739
H	-5.64907062239942	-0.62563858095798	5.00079840068796
H	-4.29987761207807	-0.73572333444919	3.83827807093514
H	-7.29343182241941	-0.64956663604493	3.14733250958358
H	-6.28589796794742	-2.12410265078040	3.19512687820943
K	-4.31489964952908	1.58447706515184	1.03400419599963

Li(12c4)-5b [W(CO)₅P^tBu(Li(12c4))NHMe]

Energy = -1852.293347561089 (CPCM_{THF}/TPSS-D3/def2-TZVP(ecp))

ZPE = 0.45932080

G_{corr} = 0.39772005

W	-0.33078516310348	0.80202301940875	2.70703214075596
C	0.99873148460549	1.75351554412369	1.46893305719489
O	1.82098015682542	2.27176095591995	0.83113753254056
C	-1.86819992628800	2.07354975524735	2.21482051343027
O	-2.73658671378873	2.79818843563529	1.95165578413600
C	0.19608622320846	2.00404461928996	4.22096375942870
O	0.47939088034621	2.71129737143205	5.10951897688203

C	1.21985424699472	-0.44543444888301	3.20874061860531
O	2.11738627806563	-1.10450014123985	3.54348092864424
C	-1.51988509540188	-0.30823715486340	3.96077255904536
O	-2.15513935548304	-0.94944657087468	4.69237530428944
C	-0.61776458476370	-2.30440309925106	0.58405697528415
C	0.85563420114806	-2.18009345963256	0.18083068647079
H	0.96874744286437	-1.68465037857405	-0.78996301472673
H	1.42000243716382	-1.59991574884183	0.91692457208121
H	1.31500020603026	-3.17442469826587	0.10376810508642
C	-0.74396698004838	-3.04516283107397	1.91934014889431
H	-0.15465924832175	-2.55969765992025	2.70161901604568
H	-1.79025318980425	-3.06911138897239	2.24155202457139
H	-0.39001466232814	-4.08085467790102	1.81460384416422
C	-1.39930862887175	-3.08863792914927	-0.48437059345416
H	-1.34902633550318	-2.59841882559120	-1.46159936783536
H	-0.99171718491271	-4.10445511044130	-0.58444947568924
H	-2.45367054665256	-3.16901333842571	-0.19961274129664
C	-4.10657676634515	-0.65366966595577	0.30763369128639
H	-5.02131539248897	-1.12663958141752	0.68545715888757
H	-4.30635028748192	0.42660901215046	0.20475947413937
H	-3.89583394960663	-1.06158351002002	-0.68530270047053
N	-2.98692782113004	-0.96167539468146	1.19426666587950
H	-3.18664016054968	-0.66811487469907	2.14458652006965
P	-1.36170407115357	-0.55294643058975	0.66749224263897
H	-1.60525729587428	-2.03331461999526	-4.16579210958202
C	-1.54883602774283	-0.95168270688751	-3.99752704589681
C	-0.21371896326632	-0.58196215593926	-3.37237084198447
H	-1.66629783937697	-0.43257684609752	-4.95472253700226
O	-2.60429443305916	-0.53490985093391	-3.09975190939526
O	-0.30687301896850	0.82046034579006	-3.07216491050162
H	0.60446373864741	-0.78409162207360	-4.07503476690079
H	-0.03854442098221	-1.14354028607301	-2.44633792037535
C	-3.73068039932351	0.10123060901725	-3.74667521993471
C	0.76127102962856	1.40007552153183	-2.29653654617669
H	-3.39020897739282	0.56049349675894	-4.68146313920559
H	-4.50819696982394	-0.63895457086523	-3.97004381767253
C	-4.27228907273398	1.17696426471595	-2.81907216809303
C	0.27312721596001	2.79082999076704	-1.93704624718808
H	1.68618373886895	1.45654954814448	-2.88339515942340
H	0.93613337570558	0.79356271597982	-1.39830815150310
H	-5.02512070345591	1.77743284439986	-3.34509287174449
H	-4.72293279066580	0.75217834708966	-1.91543286421308
O	-3.13072917466274	1.97674946100953	-2.47424841913423
O	-0.95395637222986	2.64213554995522	-1.18878758294593
H	0.07094689310345	3.35812380386131	-2.85299716610698
H	1.02125104028676	3.32017970755765	-1.33876776869863
C	-3.30313090131739	3.02186752458150	-1.50179660481833
C	-1.93484804500044	3.68065558716866	-1.39892089487018
H	-3.62281506795590	2.59245039470193	-0.54393327244189
H	-4.05074242609178	3.75197235590240	-1.83521749807401
H	-1.70735404068615	4.20561616684150	-2.33316167012596
H	-1.91156588806223	4.39383589806474	-0.56735560022691
Li	-1.74237169675296	0.78046673108345	-1.67176970274341

K-5b [W(CO)₅P^tBu(K)NHMe]

Energy = -1828.981371840752 (CPCM_{THF}/TPSS-D3/def2-TZVP(ecp))

ZPE = 0.22167708

G_{corr} = 0.17118149

W	-0.69056375430749	1.20607671430705	2.08647506198705
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C	0.21891082073670	2.22867843427773	0.57770699613918
O	0.69045664166057	2.74567757753331	-0.35743889724370
C	-2.43794277138541	2.22858209605661	1.74034269761996
O	-3.41975729335704	2.81665972955828	1.54321350903164
C	-0.21879193440454	2.50897888913796	3.53981796616217
O	0.03887419454878	3.26975432282702	4.39002586747305
C	1.06953940764250	0.22304549839883	2.48372798649098
O	2.07527791854928	-0.29123928632766	2.75555422332648
C	-1.67333780898897	-0.11681276973775	3.31481960866727
O	-2.23912993741741	-0.89206554700708	3.96805456763812
C	-0.64378781186646	-1.94217335894502	-0.04525064333310
C	0.77686208611100	-1.61448621709994	-0.52208753499732
H	0.75620388519327	-1.10576408621450	-1.49450601870307
H	1.29880145330838	-0.96607613509230	0.18833724354892
H	1.36296392623628	-2.53575366236426	-0.63627535733920
C	-0.61431911036853	-2.71945060452609	1.27420532896073
H	-0.06135858676775	-2.17124745748619	2.04238903749736
H	-1.63274597872879	-2.88941662308976	1.64024241034706
H	-0.13249657336727	-3.69785387963174	1.13443944108796
C	-1.36443891673616	-2.78109460522217	-1.11498657519560
H	-1.37264823616283	-2.26293041706109	-2.08156004739192
H	-0.85526778225769	-3.74621186810335	-1.24546847074315
H	-2.40039385595486	-2.97333743451158	-0.81749208570886
C	-4.27248450087479	-0.44802933915075	-0.38754195238653
H	-5.20312692606815	-0.92552293647991	-0.05869985322654
H	-4.44238577599086	0.64046649782603	-0.43283322341463
H	-4.04621672075004	-0.79888075011224	-1.39940369619106
N	-3.17964886085144	-0.84052936588210	0.51020089338423
H	-3.43214412316878	-0.66803382525941	1.47855259262335
P	-1.57233707066346	-0.29427974224162	0.08774641336705
K	-1.31906600354807	1.55927015162375	-2.54120748947784

K(18c6)-5b [W(CO)₅P^tBu(K(18c6))NHMe]

Energy = -2752.580917412071 (CPCM_{THF}/TPSS-D3/def2-TZVP(ecp))

ZPE = 0.57708842

G_{corr} = 0.50476082

W	-2.57808710767234	0.90523878494237	2.56979561596108
C	-1.89183584254214	2.68654182153737	1.82816046309493
O	-1.43861703702790	3.66783970740917	1.39862394209684
C	-4.29281110190659	0.97970878639319	1.44669081839002
O	-5.31196639653633	1.06371348678445	0.88887249446340
C	-3.67226735748196	1.67574914776722	4.05596922789095
O	-4.31982955930119	2.10932493398314	4.93134485983981
C	-1.01323703884131	0.92871766569005	3.89554099522718
O	-0.18773765807333	0.97876428920185	4.71475451831537
C	-2.86308454032424	-1.07475770498578	2.96767240352877
O	-2.94734920329142	-2.22869682769289	3.10671999547428
C	0.47811072718253	-0.53615367199392	0.84820343757020
C	1.17361034876809	0.78869508523109	1.18851897501397
H	1.05754753593900	1.50962389649156	0.37044405466908
H	0.75988483447943	1.24049779412642	2.09388492813679
H	2.24733314475013	0.62177397412901	1.34576954757453
C	0.61671163938754	-1.52498529724551	2.01311846898549
H	0.12264888634480	-1.14969757727194	2.91305991925937
H	0.18147517176306	-2.49917223717624	1.76264020966233
H	1.67853030020747	-1.69065164771783	2.24444778137141
C	1.13725618223119	-1.13843441508122	-0.40630428532215
H	1.14298834838561	-0.42424413679091	-1.23562878308379
H	2.17925462618749	-1.41182565929966	-0.18681767550092

H	0.60041481159381	-2.03571085574161	-0.72857243269895
C	-3.24643358482924	-1.85680669476741	-0.41404681371854
H	-3.46363350218672	-2.89274588927093	-0.69877533146467
H	-4.00374819211892	-1.53591221338878	0.31984179556977
H	-3.34440120690681	-1.22405508598704	-1.30065446914487
N	-1.87278351661234	-1.76531084006712	0.09322974907665
H	-1.77912367583975	-2.37811126173867	0.90445086361906
P	-1.32276640771694	-0.12889581181974	0.41542696244520
H	-5.93741144590916	1.90562940210691	-2.82887041324003
C	-4.93951677666461	1.45585746076771	-2.72139037122801
C	-4.71792568886058	0.45834481465118	-3.83192010329622
H	-4.88486957197319	0.95695429465144	-1.74507094046362
O	-3.93304288785584	2.47607758695641	-2.80367639141780
O	-3.47198425692931	-0.21148916022984	-3.60295322144664
H	-4.69546581846014	0.96085314652543	-4.81002098754640
H	-5.54164752521319	-0.27029098169850	-3.82892880476240
C	-4.05656274928058	3.42610672996491	-1.73365245526082
C	-3.23252979535638	-1.25035078901804	-4.55887343152934
H	-3.89998248106633	2.92163130431924	-0.77086206273888
H	-5.06278049138943	3.86938217840414	-1.73926717738722
C	-3.03108082639244	4.51633119966204	-1.92611541091948
C	-1.89132420233105	-1.87884320961296	-4.26614820001882
H	-3.24417877909068	-0.83101700713418	-5.57560035068500
H	-4.01820236901875	-2.01655877524683	-4.48467581737351
H	-3.14928959848274	4.99121973828969	-2.91152238477427
H	-3.17146666408435	5.28038231106457	-1.14744035797332
O	-1.72610758580124	3.94096563834592	-1.81535875605389
O	-0.86876001417323	-0.89699997989855	-4.48942857488900
H	-1.74038267573117	-2.73642919639682	-4.93768073484788
H	-1.84536743086312	-2.23348774132642	-3.22640244049084
C	-0.69238006350961	4.92575657210799	-1.89579215196935
C	0.44498840952097	-1.45059143512633	-4.33093039086403
H	-0.71693177541047	5.41453793257469	-2.88125140333362
H	-0.84018998258481	5.69040087786578	-1.11925726351591
C	0.63879844773310	4.24979263317742	-1.67246707835359
C	1.46197842487943	-0.36687981094466	-4.59525860034201
H	0.59461017569802	-2.26969887834137	-5.04939863955720
H	0.56168354632706	-1.84978860256507	-3.31390173069610
H	1.43599345619282	5.00707999430331	-1.68301455971318
H	0.65076623528536	3.73939228412349	-0.69928809054339
O	0.85413710723367	3.29679664916711	-2.72434784864313
O	1.34521178779688	0.63669867519404	-3.57945716693915
H	1.29425344086818	0.08415609402393	-5.58438387763427
H	2.47073918695223	-0.80481004515855	-4.57485279354495
C	2.14524007768935	2.68075242901200	-2.62935655617460
C	2.29559879352060	1.69322085756224	-3.76078025162296
H	2.93238378568983	3.44483838072568	-2.70592573485758
H	2.24725254139891	2.17128900580608	-1.66030245037362
H	2.12343472627159	2.18671209741231	-4.72864093888259
H	3.31688338786163	1.28503485752184	-3.75065919885815
K	-1.28482570249795	1.31961892076095	-2.65865612153978

Li(thf)₃l

Energy = -1004.15784099119

ZPE = 0.35050582

G_{corr} = 0.30047251

Li	0.15006035680157	0.17314553959747	-0.26893851781143
I	-0.68886265153951	-1.38954481501624	1.80037384819178
O	2.08289882771686	0.06894219624505	-0.37749324489848

O	-0.30314762938663	2.05314057750172	0.03591828658091
O	-0.58872499977425	-0.41309850119143	-1.95723901827077
C	-0.24098859869555	2.90307584104572	-1.13947431557710
H	0.10508269510139	3.89689157820514	-0.82884545607340
H	0.48925878823374	2.46242675874234	-1.82052596376218
C	0.13626591551115	-0.47914404544210	-3.22412163245028
H	0.38936962228800	0.54139894957679	-3.52477322683999
H	1.05772644693408	-1.04537894191590	-3.05377453972935
C	-1.84615966000629	-1.14351164717877	-2.07425212599231
H	-2.00903663949086	-1.65255126123003	-1.12175768330517
H	-2.65409939878488	-0.42194015648944	-2.25080447428297
C	-1.65024575719657	-2.06615893255465	-3.26833949167182
H	-1.09590507309385	-2.96194708106881	-2.96846825651740
H	-2.59909630688848	-2.37177181901178	-3.71617285401731
C	-1.55939750484081	2.40018877835524	0.67680213897844
H	-1.78321747426357	1.60426203230038	1.38895446670803
H	-1.42684976545586	3.35284528194162	1.20608326560663
C	-2.55789389482769	2.52845965516328	-0.47793952030180
H	-3.03715664608365	1.56493615132031	-0.66972590570943
H	-3.33877813559759	3.25925111038035	-0.25395590507557
C	-1.67777853995761	2.95107821945283	-1.68790977228041
H	-1.92445463858265	3.95348793333296	-2.04618149140480
H	-1.80041006761086	2.25142468925714	-2.51764026668782
C	2.62865980700848	-1.28360064061291	-0.49226249895101
H	1.78421248733298	-1.97227441173214	-0.58311318915577
H	3.24329886186788	-1.32702419941922	-1.39936066401449
C	3.45546247582514	-1.49350983121993	0.76920761889204
H	2.80505965518085	-1.81161181766064	1.59040310145076
H	4.24375387408758	-2.23722879607810	0.62771076179537
C	3.99797082993663	-0.08035711837822	1.03260807585594
H	4.31597823289507	0.07010296274765	2.06727440742520
H	4.84385444958210	0.13420780258237	0.37074044559199
C	2.80126216660703	0.79479612515764	0.67346367302695
H	3.06940115554006	1.77506778134084	0.27198211085024
H	2.11996566530795	0.91934181083280	1.52284326474568
C	-0.79981736847322	-1.18963166144858	-4.20137244228716
H	-1.43506608675003	-0.46357712937739	-4.71948478649391
H	-0.24762154645819	-1.76479309805340	-4.94853203213774

Computed ³¹P chemical shifts:

Table S1. GIAO TPSS-D3/def2-QZVP computed ³¹P chemical shifts (in ppm) using TPSS-D3/def2-TZVP + CPCM optimized geometries, using the experimental ³¹P NMR shift of **3b** [W(CO)₅P^tBu(H)NHMe)] at 67.3 ppm as reference.

Compound	Shift (ppm)
3b	67.3
3f	86.9
4b⁻	43.6
4b-Li	67.9
4b-Li(12c4)	72.6
4b-K	43.6
4b-K(18c4)	62.4

Compound	Shift (ppm)
5b⁻	95.2
5b-Li(12c4)	68.1
5b-K	86.3
5b-K(18c6)	77.1
6b⁻	78.3
7b	101.2