Supporting Information

Derivatization of (quinolin-8-yl)phosphinimidic amides via ortho-lithiation revisited†

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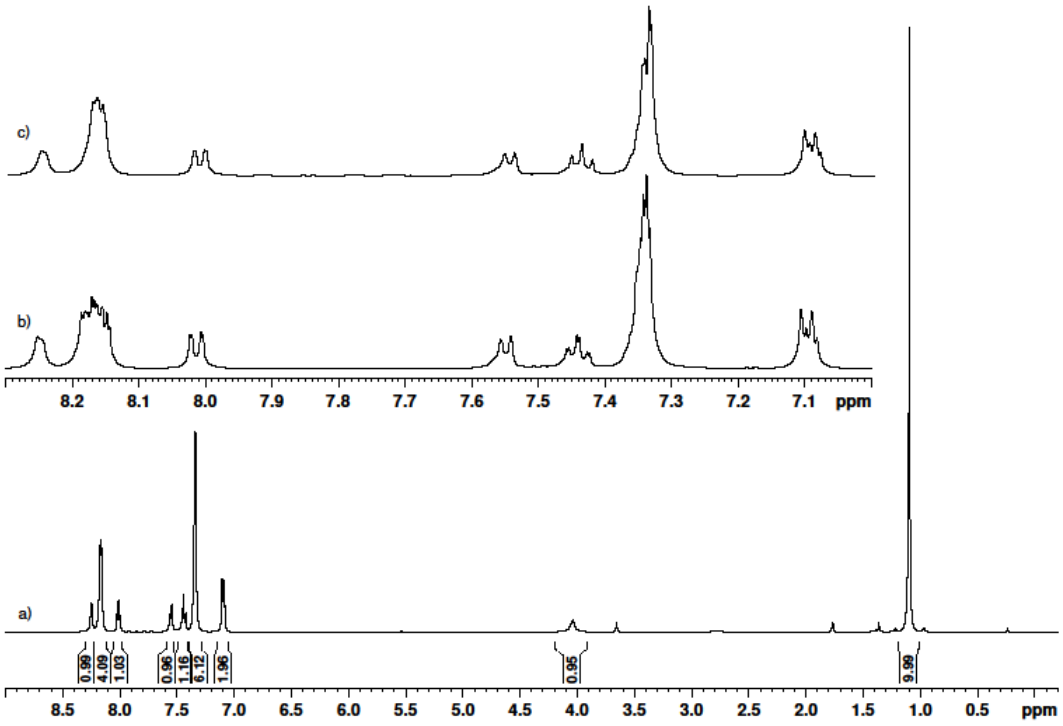

Figure S1. ^{1}H NMR spectra (500.13 MHz) of phosphinimidic amide **5** in THF-d_8: (a) standard; (b) expansion of (a); (c) the same as (b) including ^{31}P decoupling.

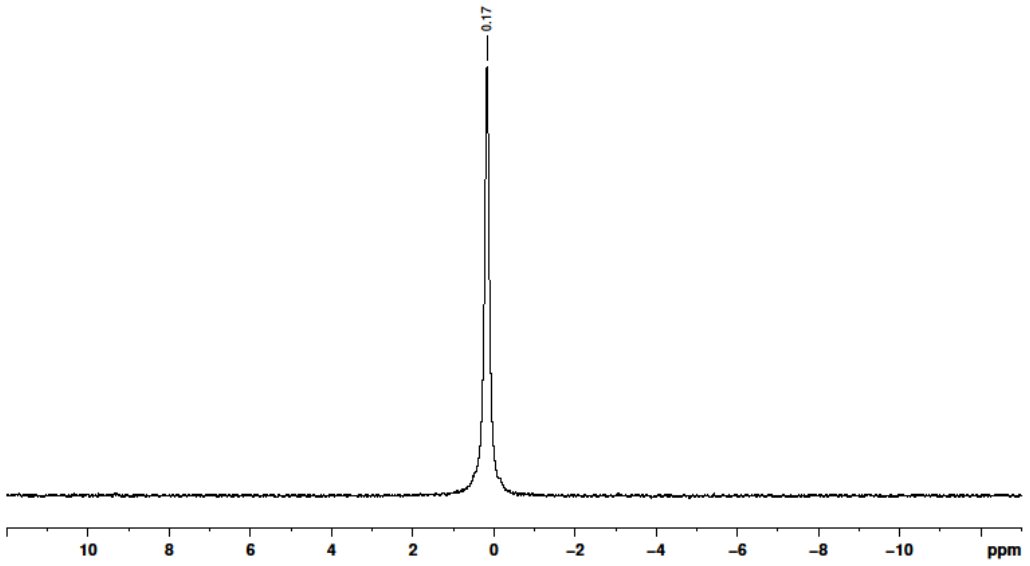

Figure S2. ^{31}P{^{1}H} NMR spectrum (202.45 MHz) of phosphinimidic amide **5** in THF-d_8.

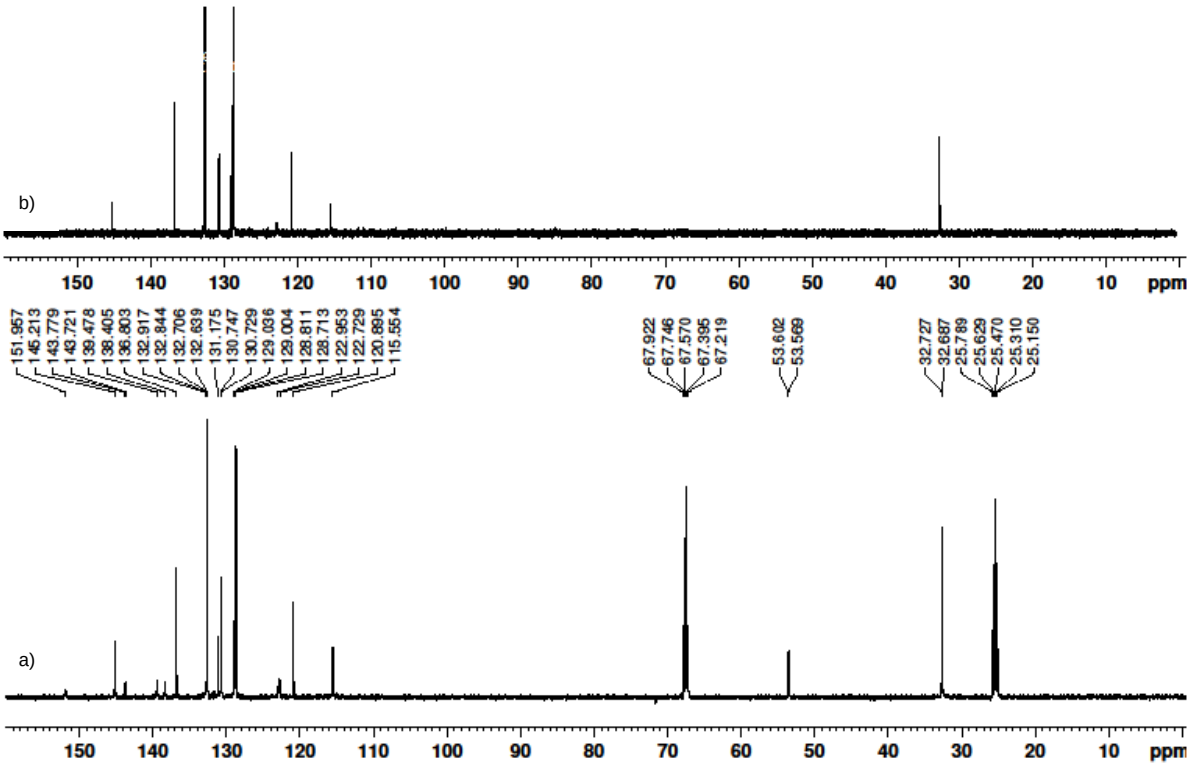

Figure S3. $^{13}C\{^{1}H\}$ NMR spectra (125.76 MHz) of phosphinimidic amide **5** in THF-d_8, standard (a) and dept135 (b).

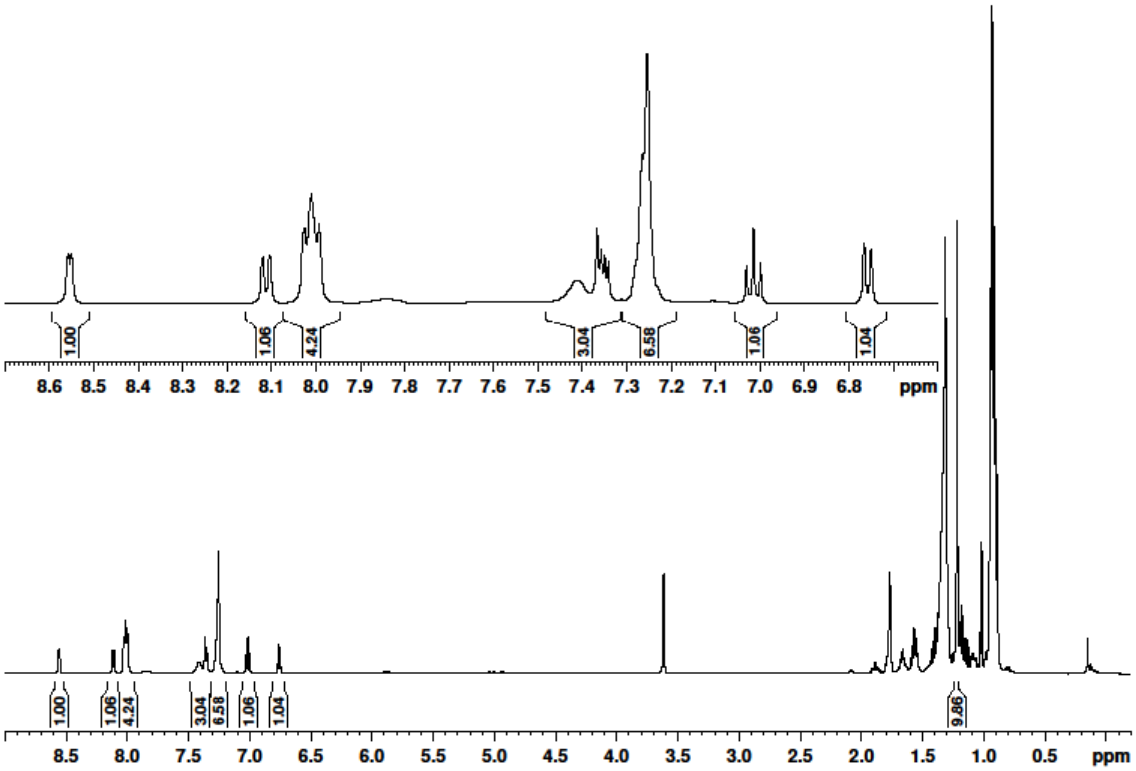

Figure S4. ^{1}H NMR spectrum (500.13 MHz) of a 75 mM solution of lithium complex **9** in THF-d_8 measured at -40 ºC.

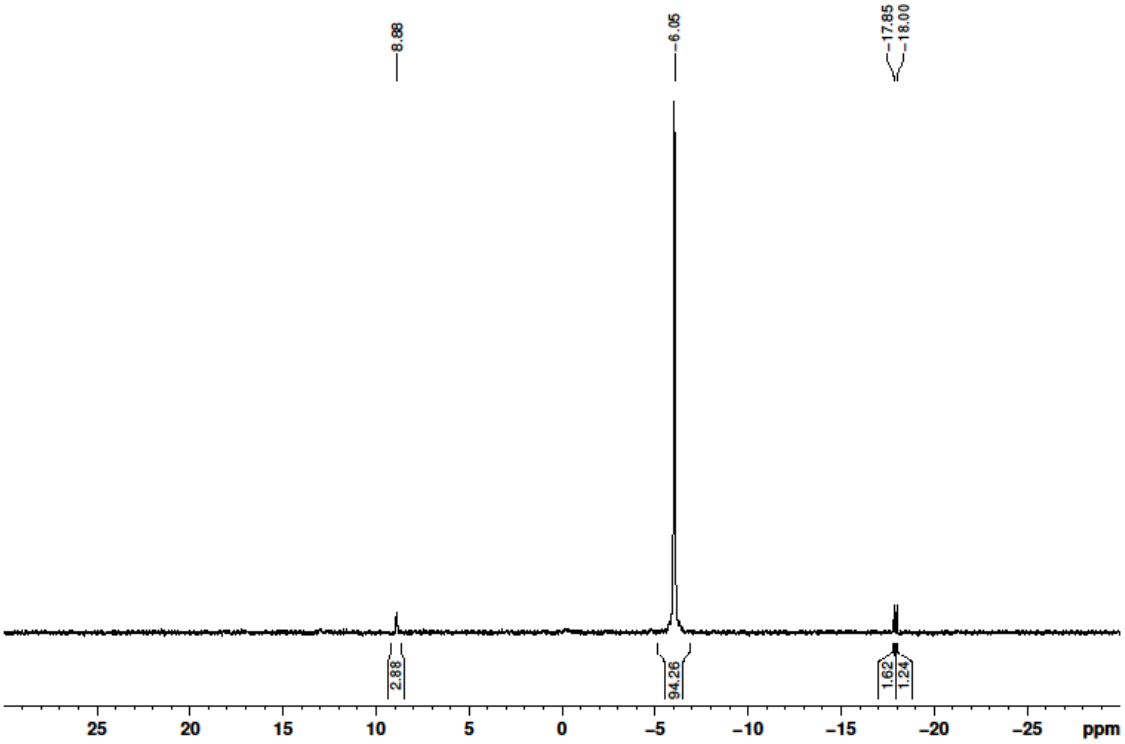

Figure S5. ^{31}P{^{1}H} NMR spectrum (202.45 MHz) of a 75 mM solution of lithium complex **9** in THF-d_8 measured at -40 ºC.

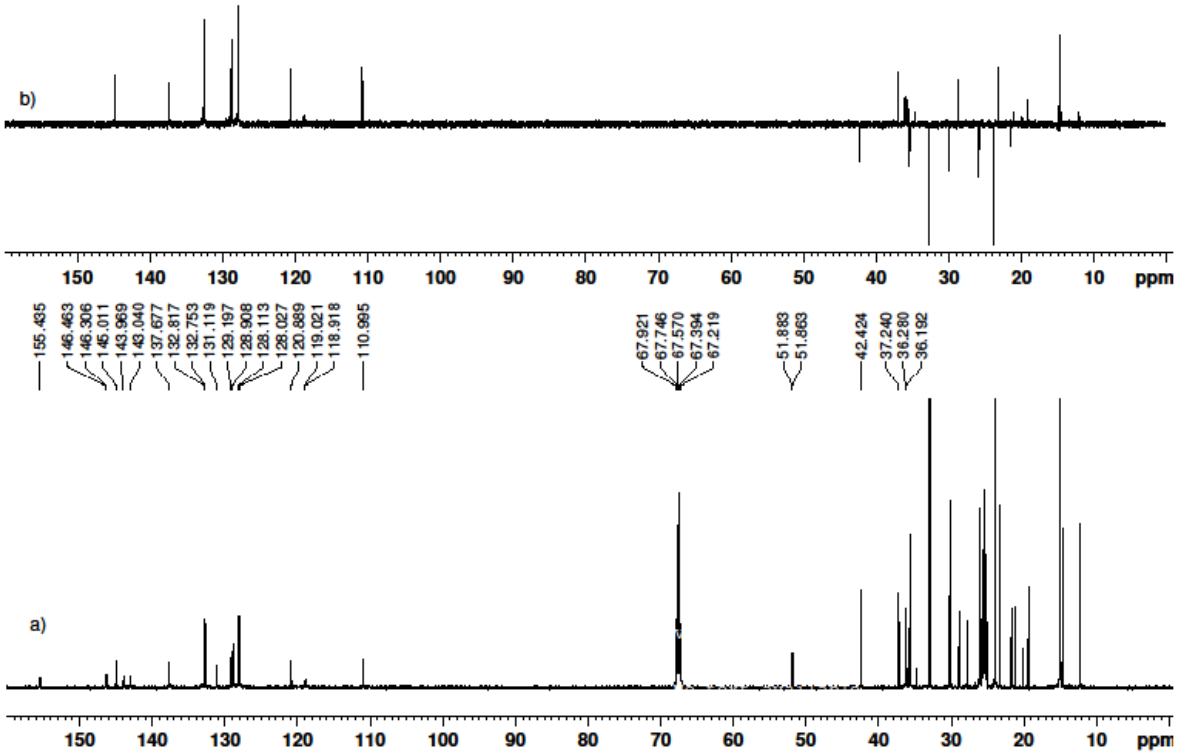

Figure S6. $^{13}C\{^{1}H\}$ (a) and dept135 (b) NMR spectra (125.76 MHz) of a 0.42 mM solution of lithium complex **9** in THF-d_8 measured at -40 ºC.

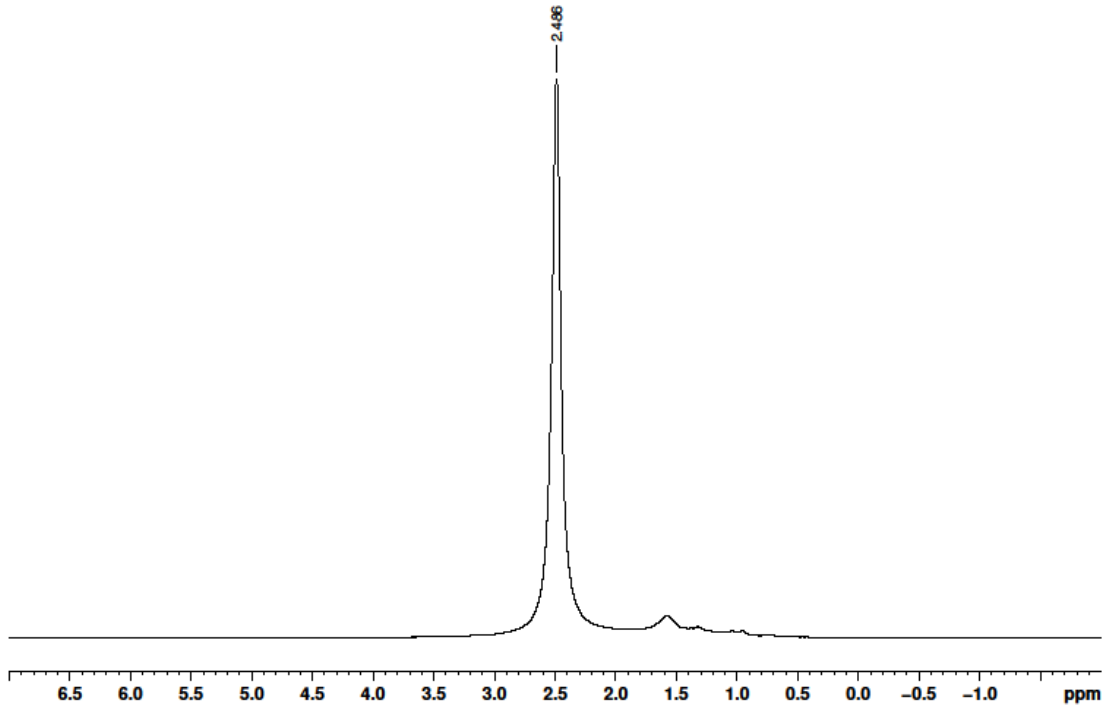

Figure S7. $^{7}Li\{^{1}H\}$ NMR spectrum (194.37 MHz) of a 0.42 M solution of lithium complex **9** in THF-d_8 measured at -40 ºC.

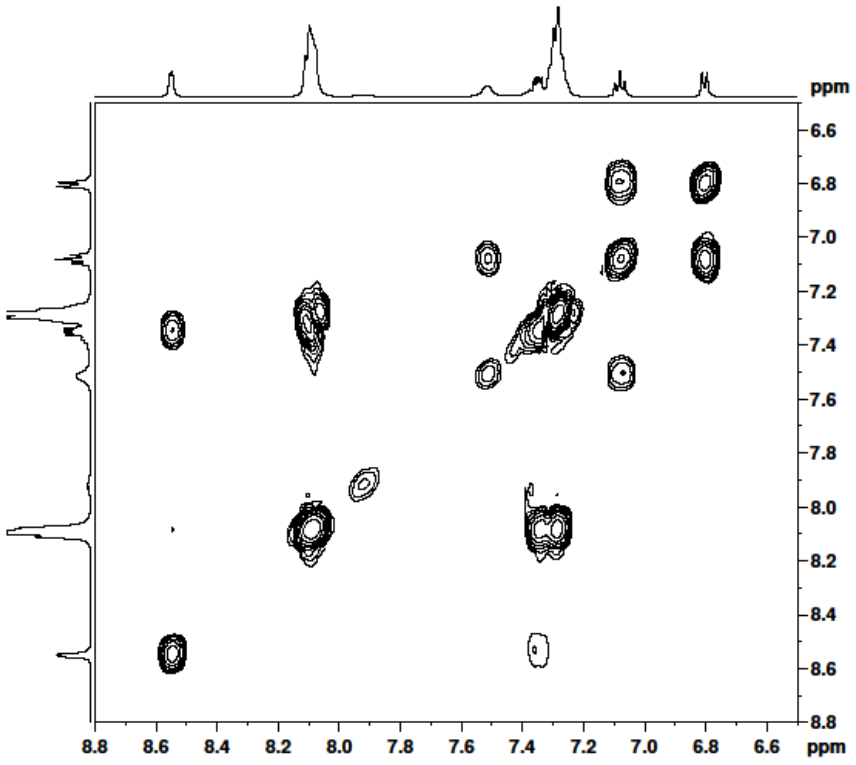

Figure S8. COSY45 NMR spectrum (500.13 MHz) of a 0.42 M solution of lithium complex **9** in THF-d_8 measured at -40 ºC.

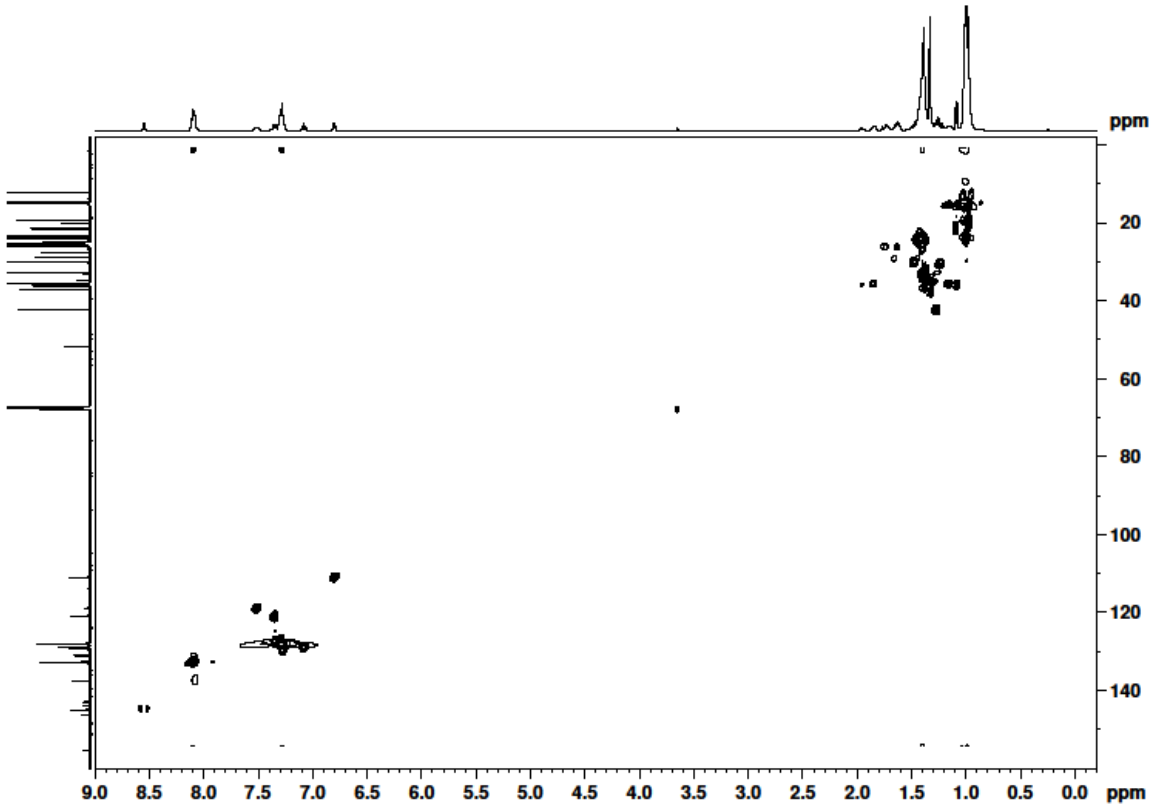

Figure S9. $^{1}H,^{13}C$ gHMQC spectrum (500.13 MHz) of a 0.42 M solution of lithium complex **9** in THF-d_8 measured at -40 ºC.

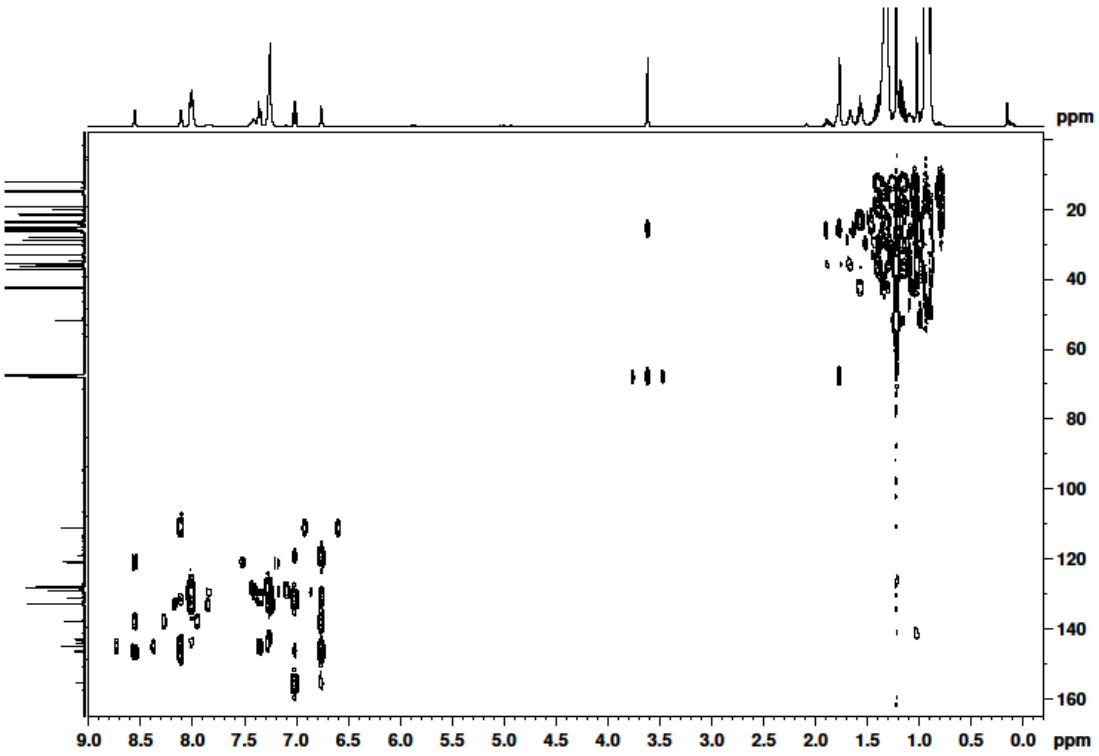

Figure S10. $^{1}H,^{13}C$ gHMBC spectrum (500.13 MHz) of a 75 mM solution of lithium complex **9** in THF-d_8 measured at -40 ºC.

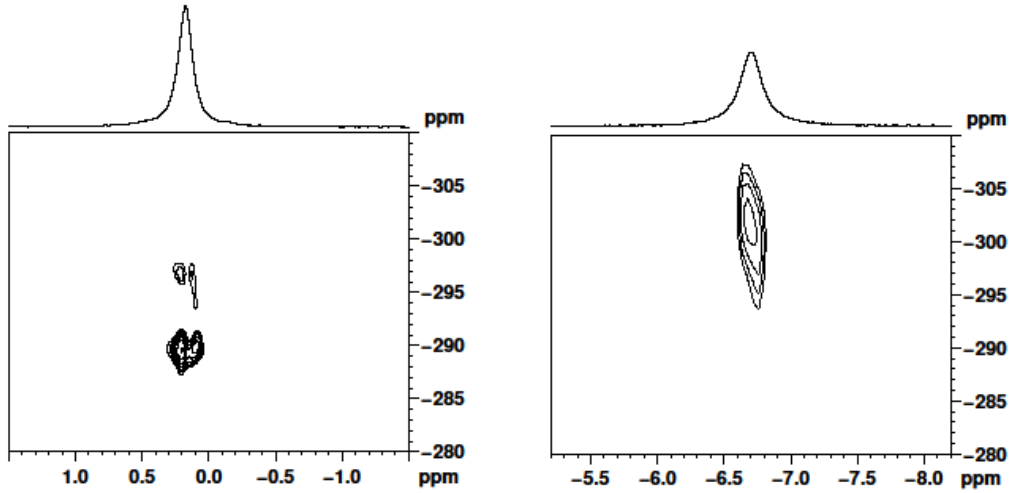

Figure S11. $^{31}P,^{15}N\{^{1}H\}$ HMQC spectra (202.45 MHz) of a 0.42 M solution in THF-d_8 of compound **5** (left) measured at 25 ºC and lithium complex **9** (right) measured at -40 ºC. Slight differences in ^{15}N chemical shifts as compared with the 75 mM sample are assigned to concentration effects.

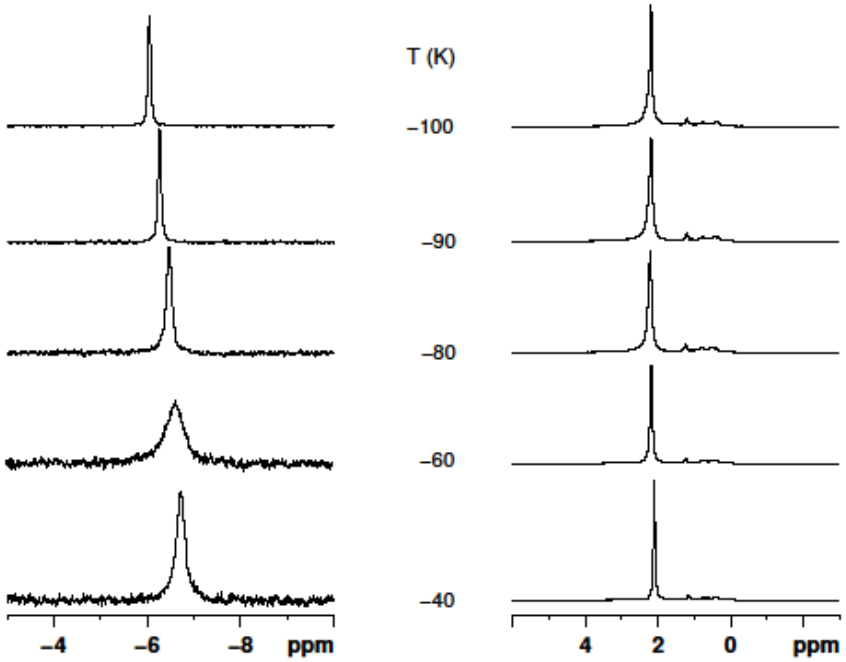

Figure S12. Variable temperature $^{31}P\{^{1}H\}$- (202.45 MHz) (left) and $^{7}Li\{^{1}H\}$ (194.37 MHz) NMR spectra (right) of a 75 mM solution of lithium complex **9** in THF-d_8.

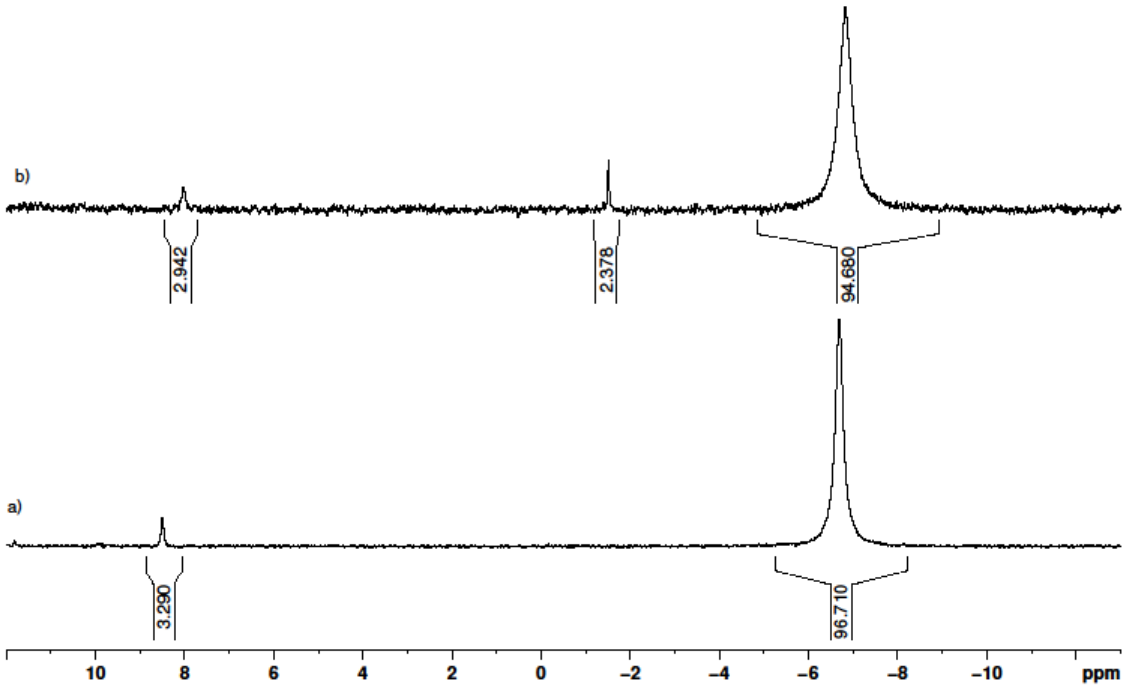

Figure S13. Effect of temperature and time aging of monoanion **9** (0.42 M solution in THF-d_8) determined through ^{31}P NMR spectroscopy: (a) measured at -20 ºC, time elapsed after the preparation of the sample ca. 4 h. (b) Time elapsed after the preparation of the sample of 69 h (49 h at temperatures below -20 ºC, 15 h at 4 ºC and 5 h at rt).

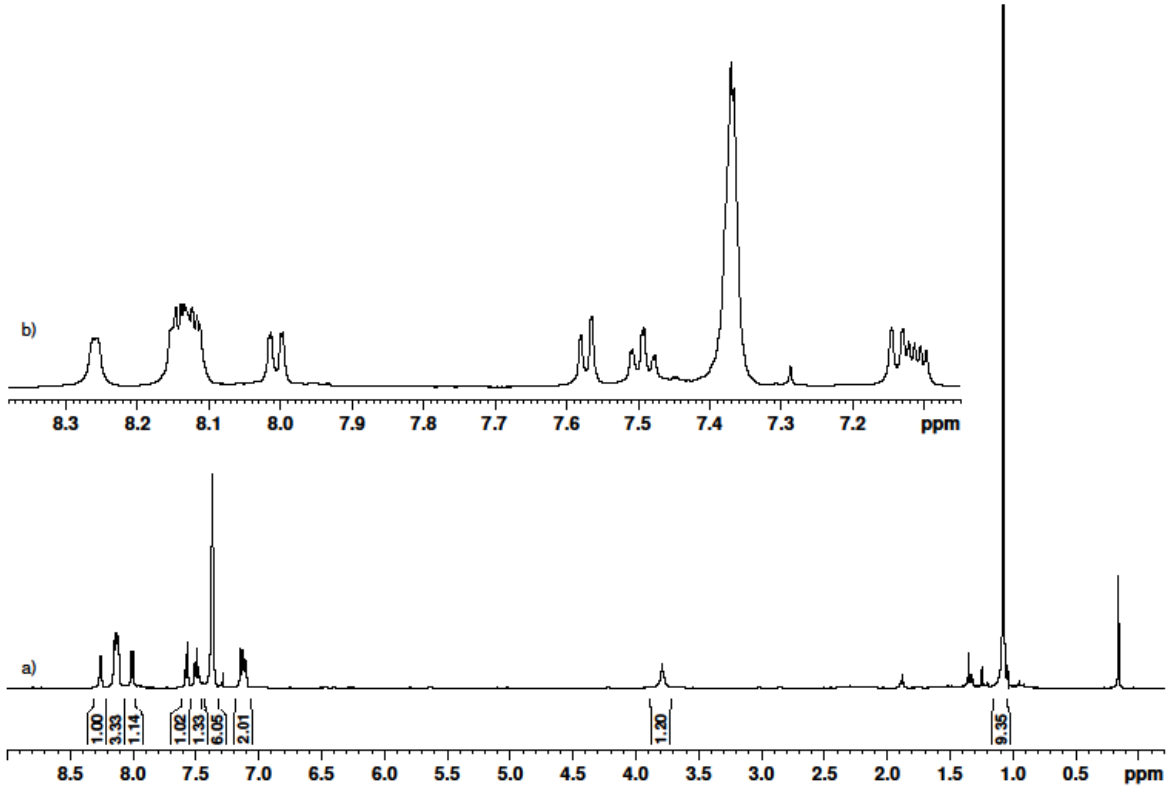

Figure S14. ^{1}H NMR spectrum (500.13 MHz) of phosphinimidic amide **13** in $CDCl_3$.

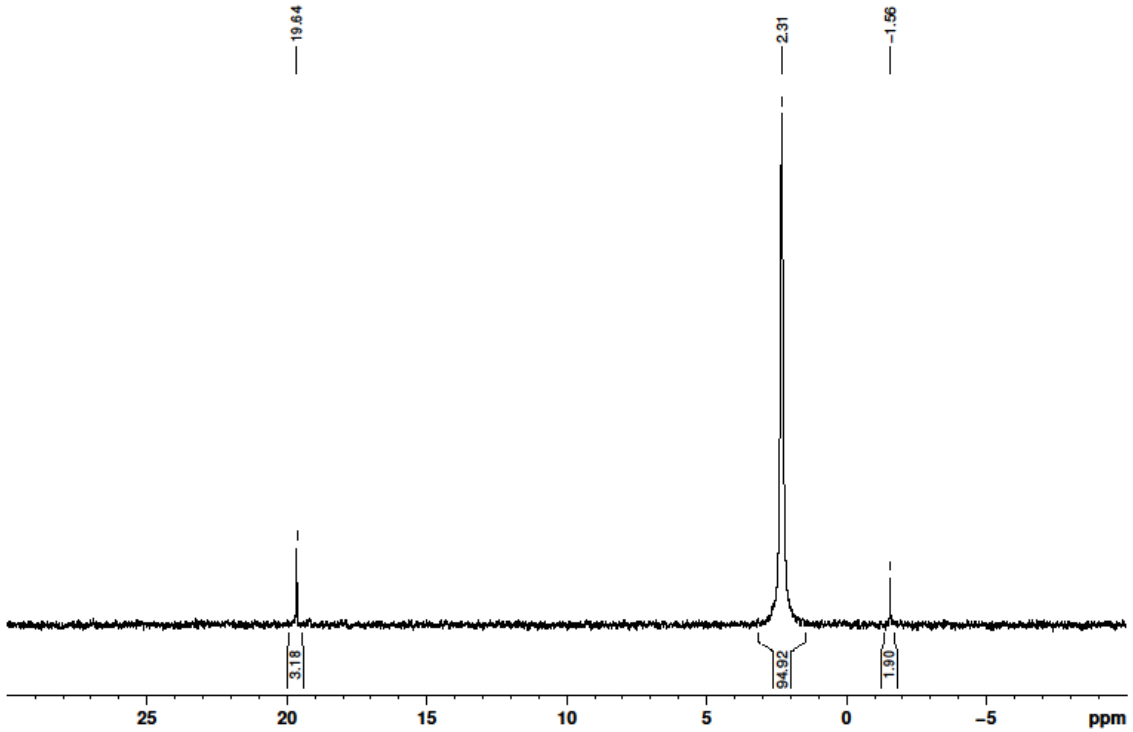

Figure S15. $^{31}P\{^{1}H\}$ NMR spectrum (202.45 MHz) of phosphinimidic amide **13** in $CDCl_3$.

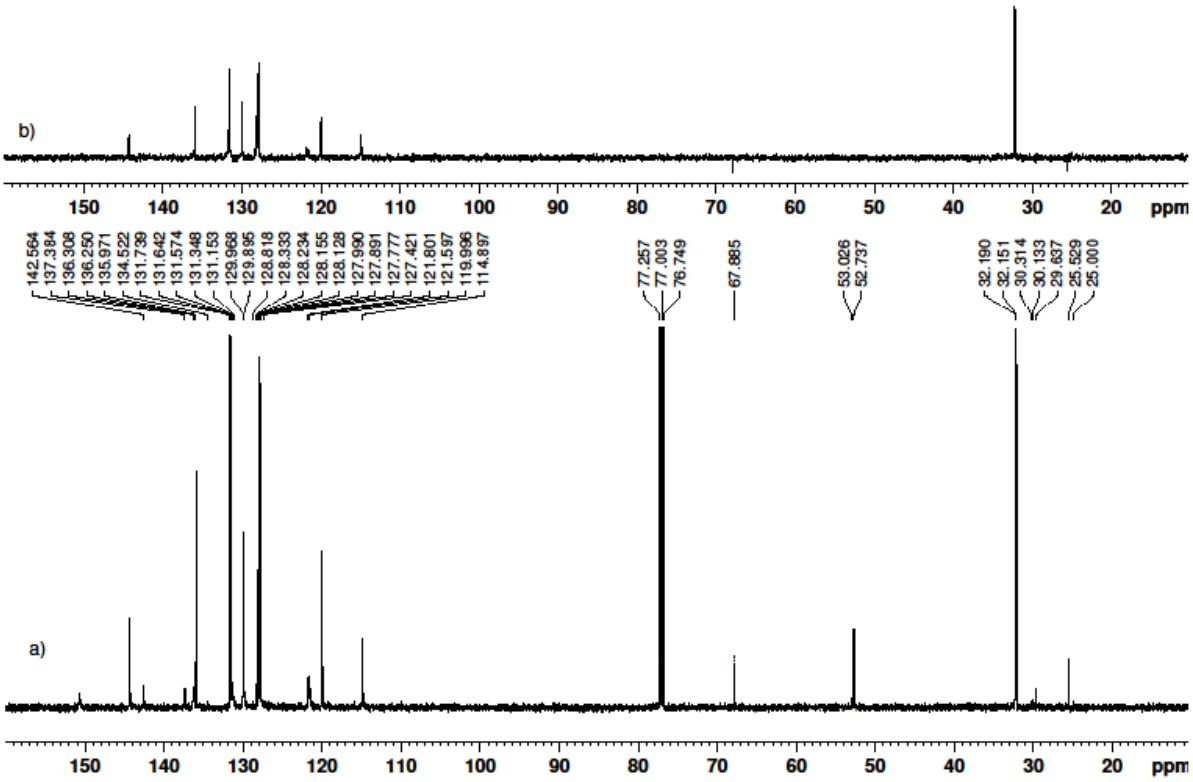

Figure S16. $^{13}C\{^{1}H\}$ (a) and dept135 (b) NMR spectra (125.76 MHz) of phosphinimidic amide **13** in $CDCl_3$.

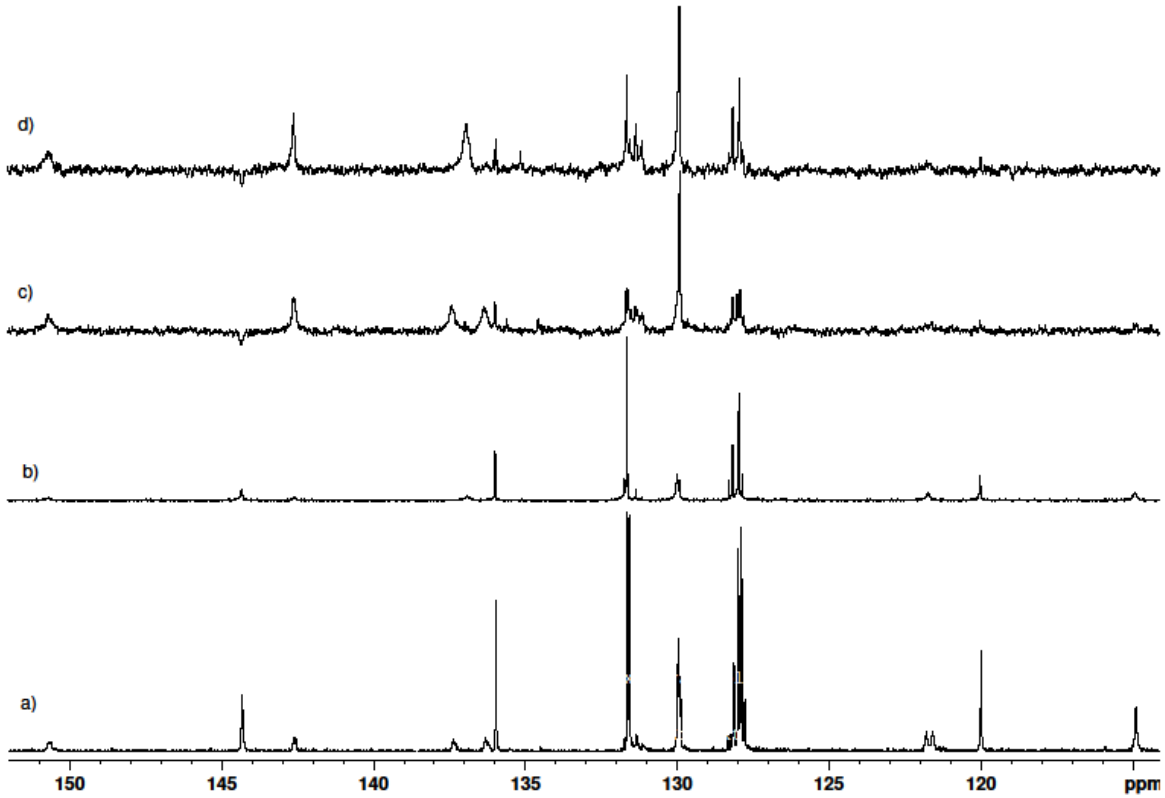

Figure S17. Expansions of ^{13}C NMR spectra (125.76 MHz) of phosphinimidic amide **13** in $CDCl_3$: a) $^{13}C\{^{1}H\}$; b) $^{13}C\{^{31}P,^{1}H\}$; $^{13}C\{^{1}H\}$ jmod; $^{13}C\{^{31}P,^{1}H\}$ jmod.

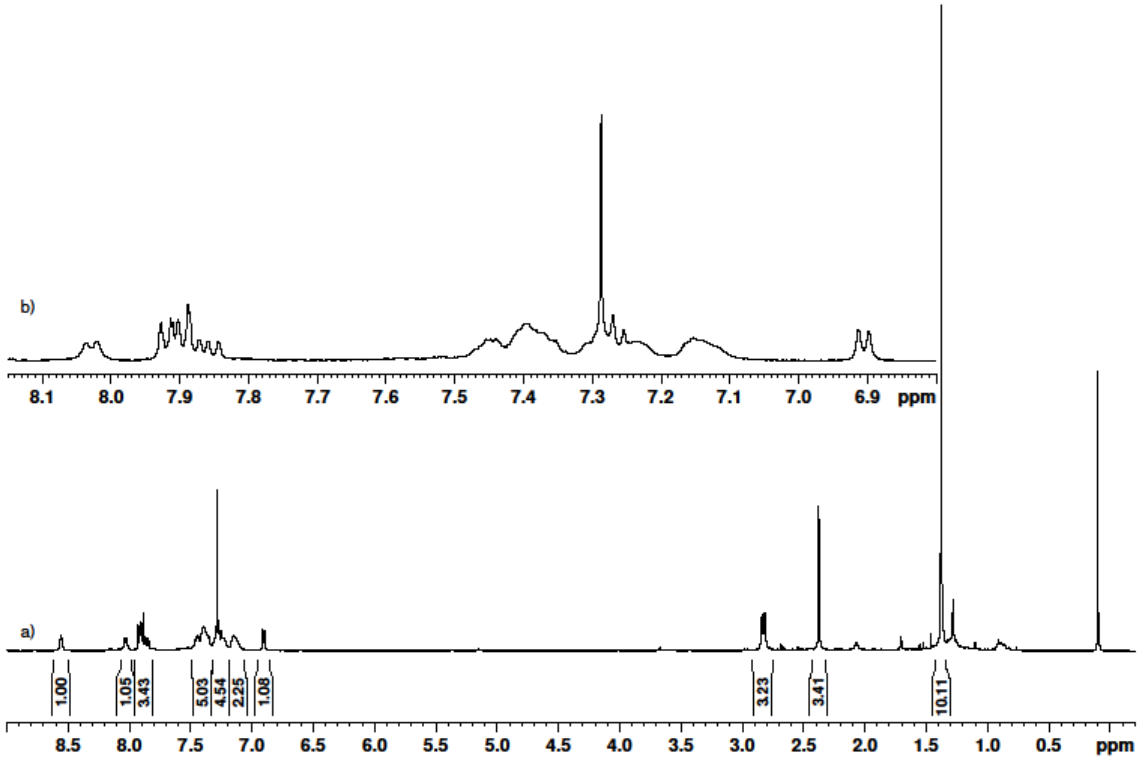

Figure S18. ^{1}H NMR spectrum (500.13 MHz) of phosphinimidic amide **14** in $CDCl_3$.

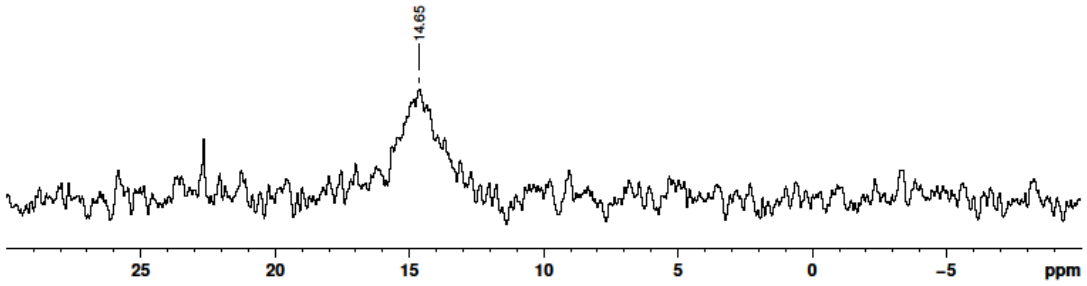

Figure S19. $^{31}P\{^{1}H\}$ NMR spectrum (202.45 MHz) of phosphinimidic amide **14** in $CDCl_3$.

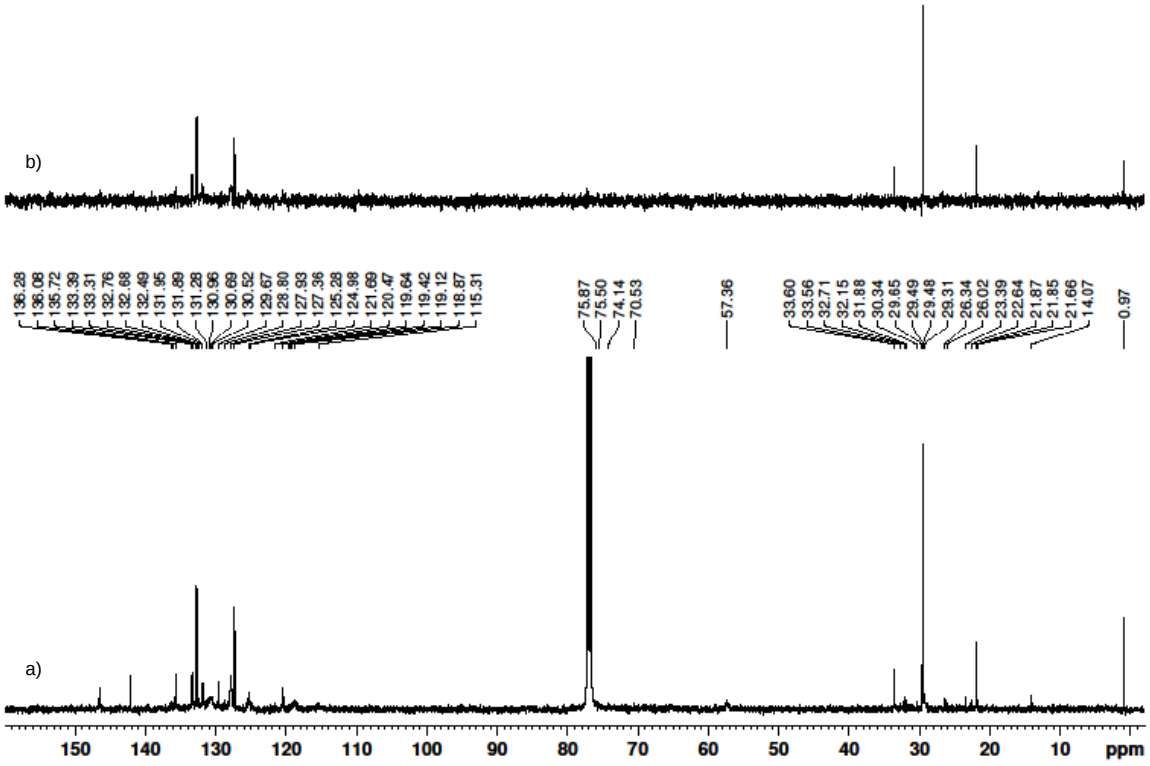

Figure S20. $^{13}C\{^{1}H\}$ (a) and dept135 (b) NMR spectra (125.76 MHz) of phosphinimidic amide **14** in $CDCl_3$.

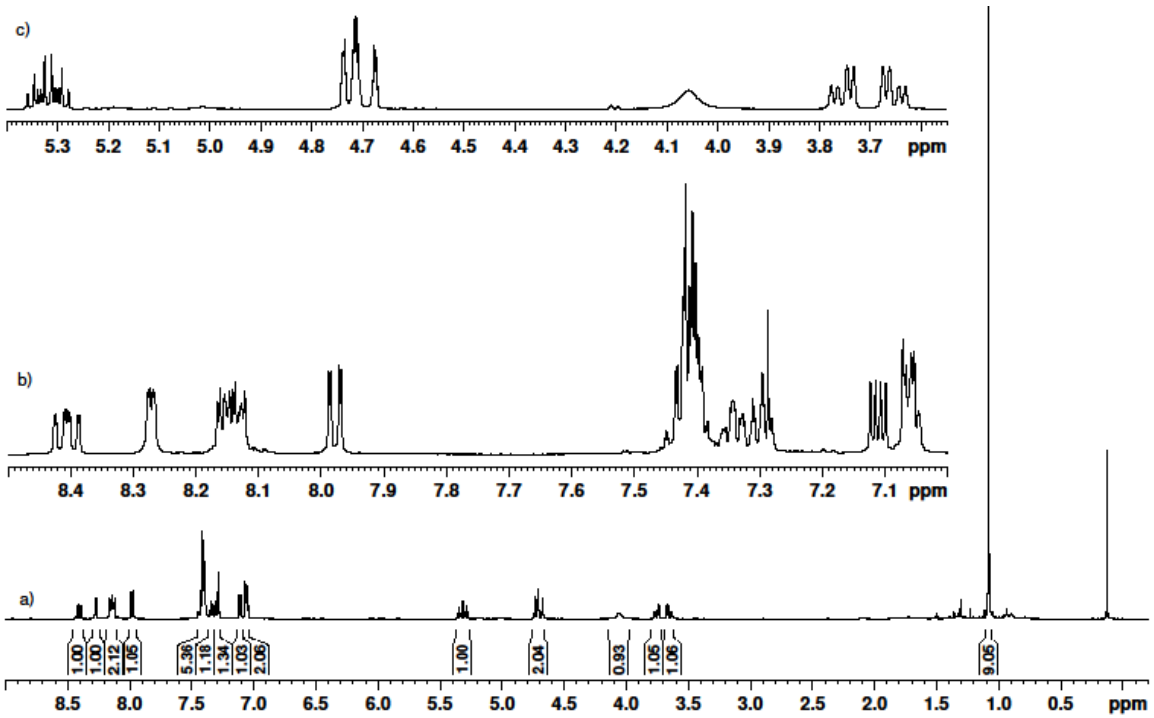

Figure S21. ^{1}H NMR spectrum (500.13 MHz) of phosphinimidic amide **15** in $CDCl_3$.

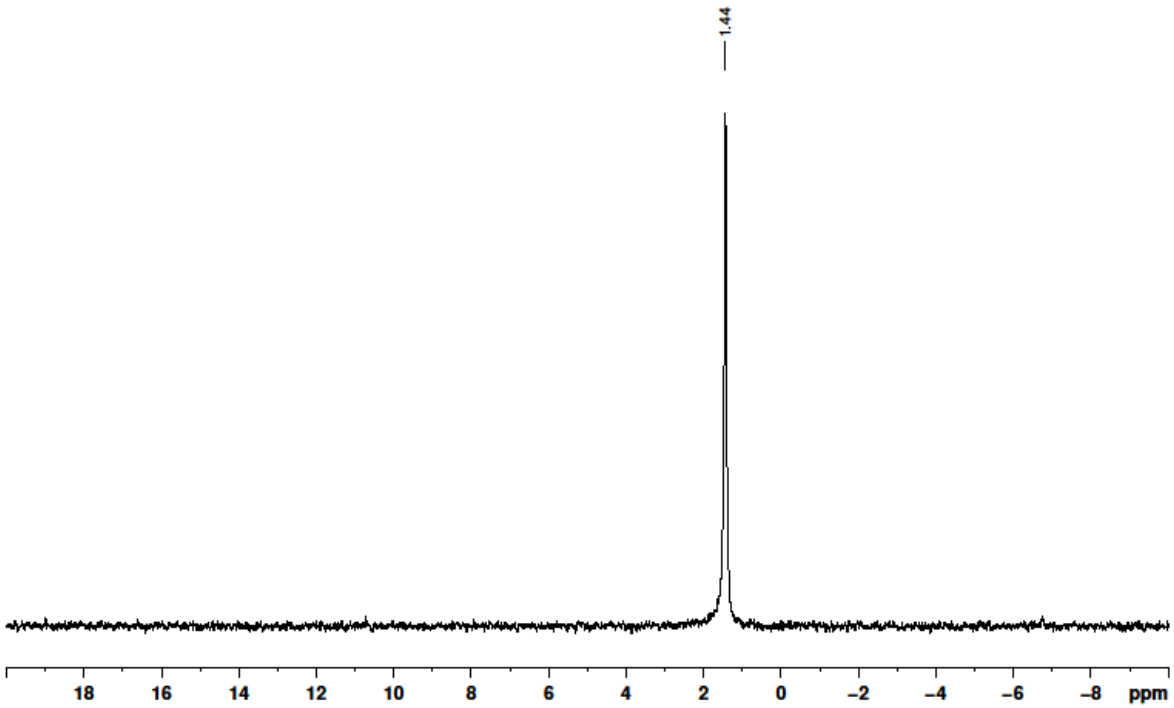

Figure S22. $^{31}P\{^{1}H\}$ NMR spectrum (202.45 MHz) of phosphinimidic amide **15** in $CDCl_3$.

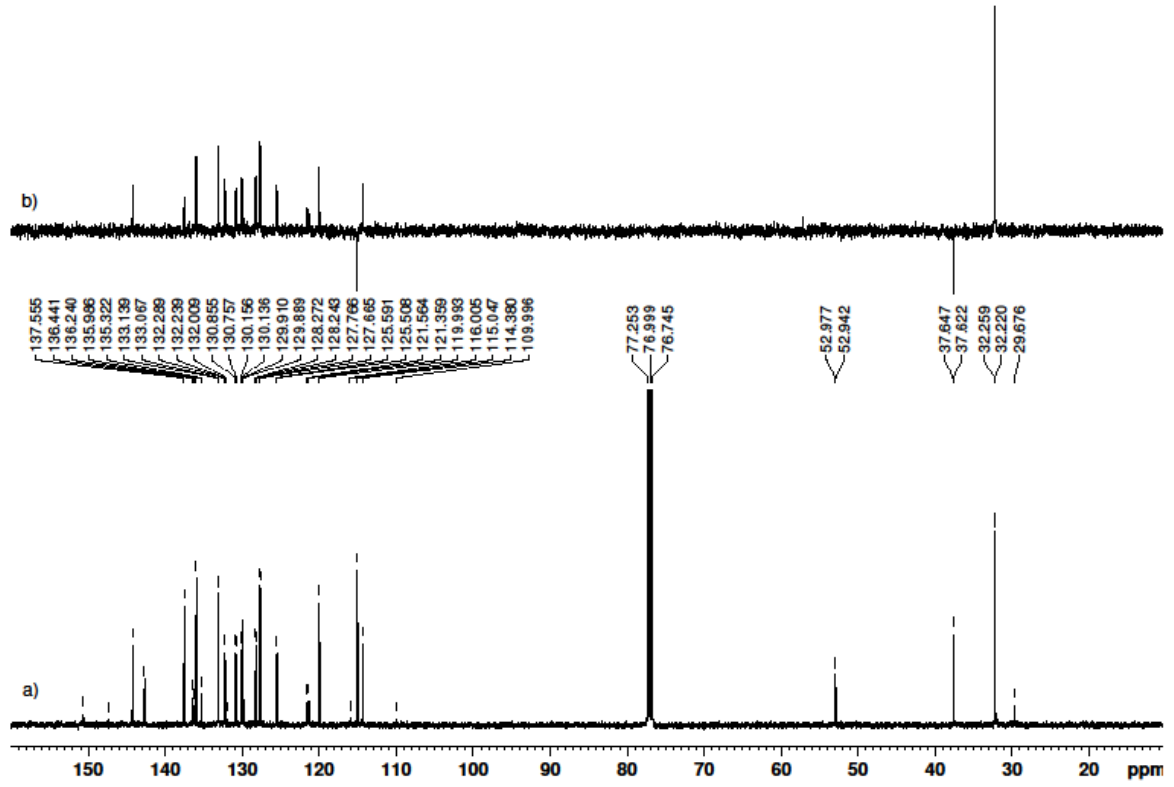

Figure S23. $^{13}C\{^{1}H\}$ (a) and dept135 (b) NMR spectra (125.76 MHz) of phosphinimidic amide **15** in $CDCl_3$.

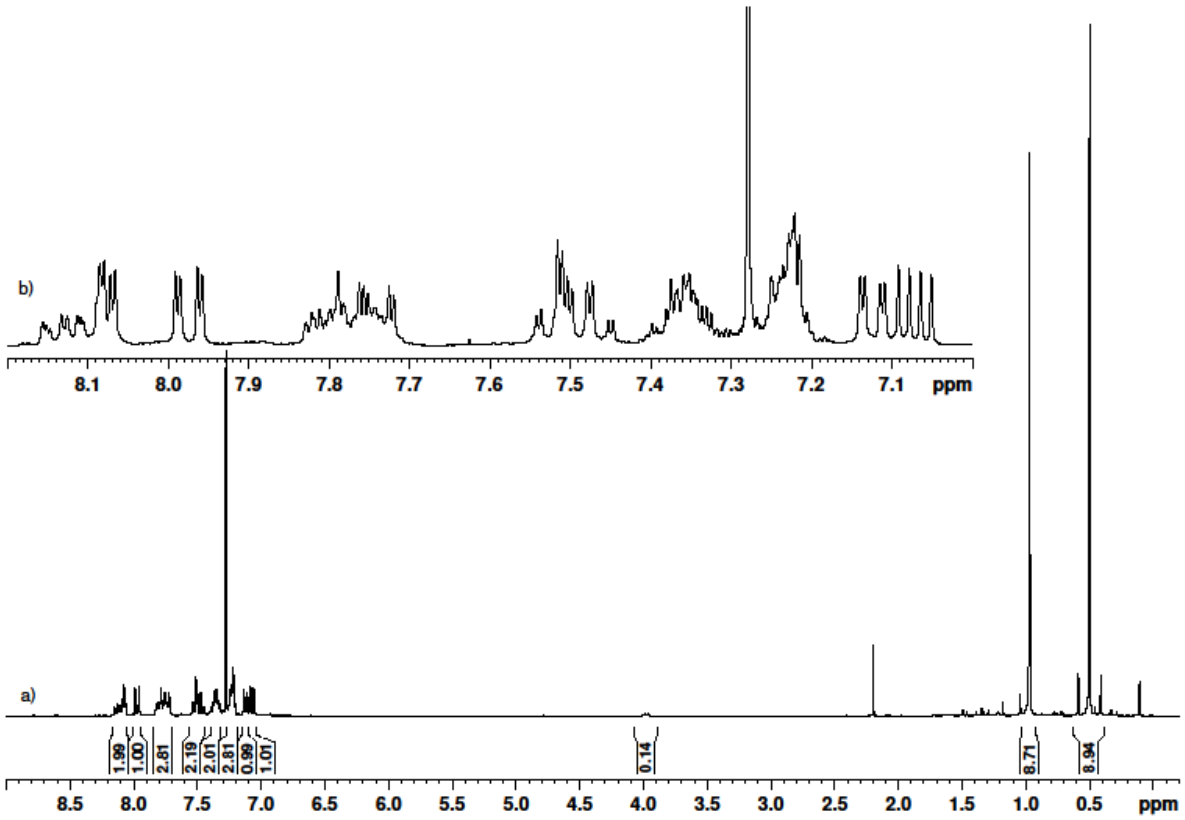

Figure S24. ^{1}H NMR spectrum (300.13 MHz) of phosphinimidic amide **16** in $CDCl_3$.

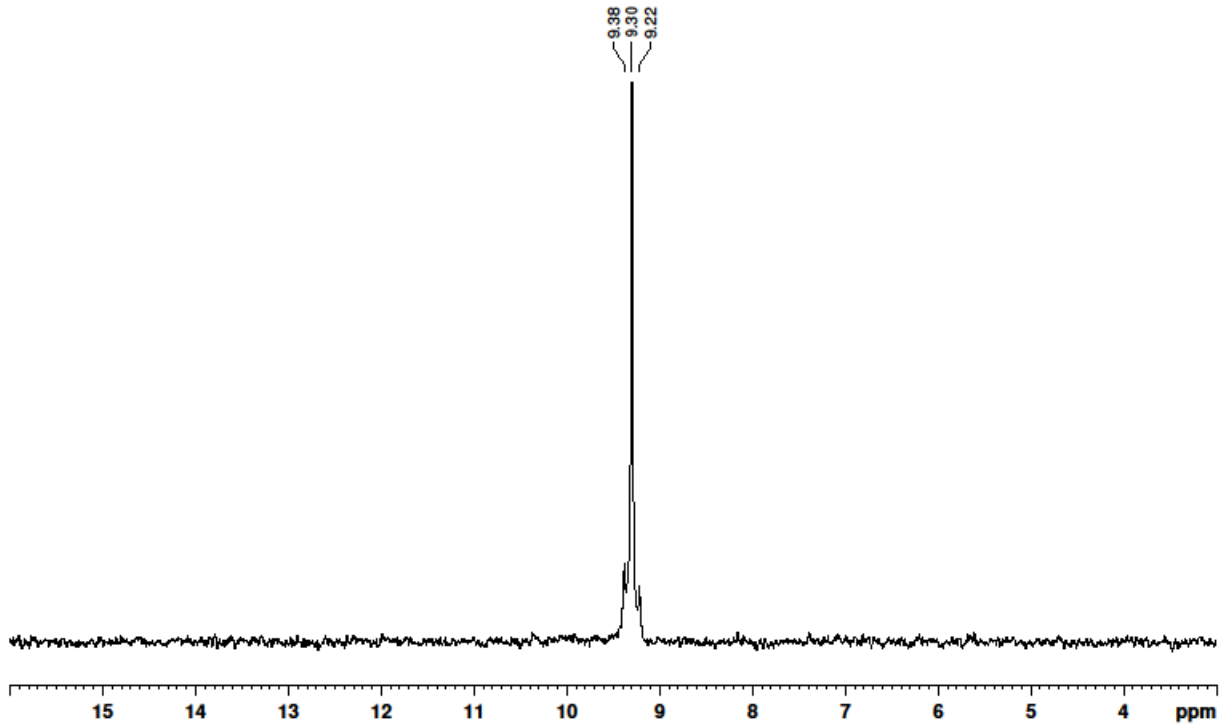

Figure S25. $^{31}P\{^{1}H\}$ NMR spectrum (121.49 MHz) of phosphinimidic amide **16** in $CDCl_3$.

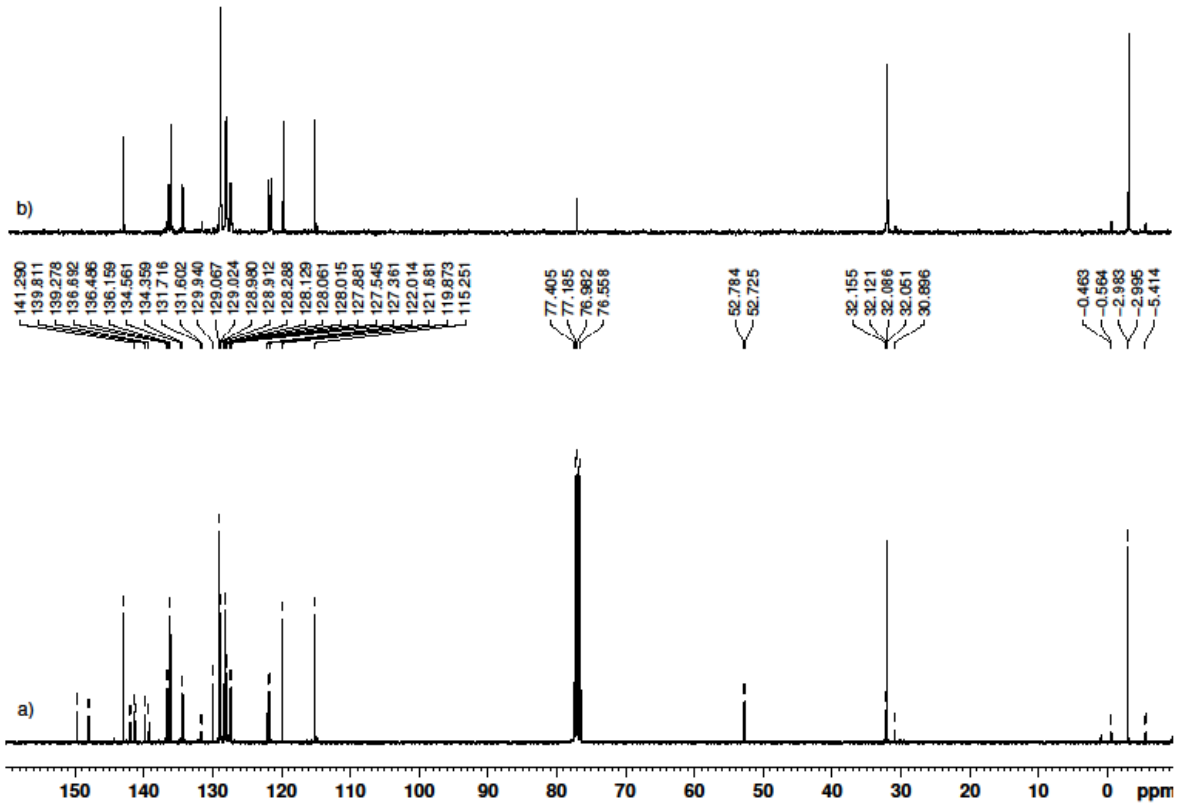

Figure S26. $^{13}C\{^{1}H\}$ (a) and dept135 (b) NMR spectra (75.46 MHz) of phosphinimidic amide **16** in $CDCl_3$.

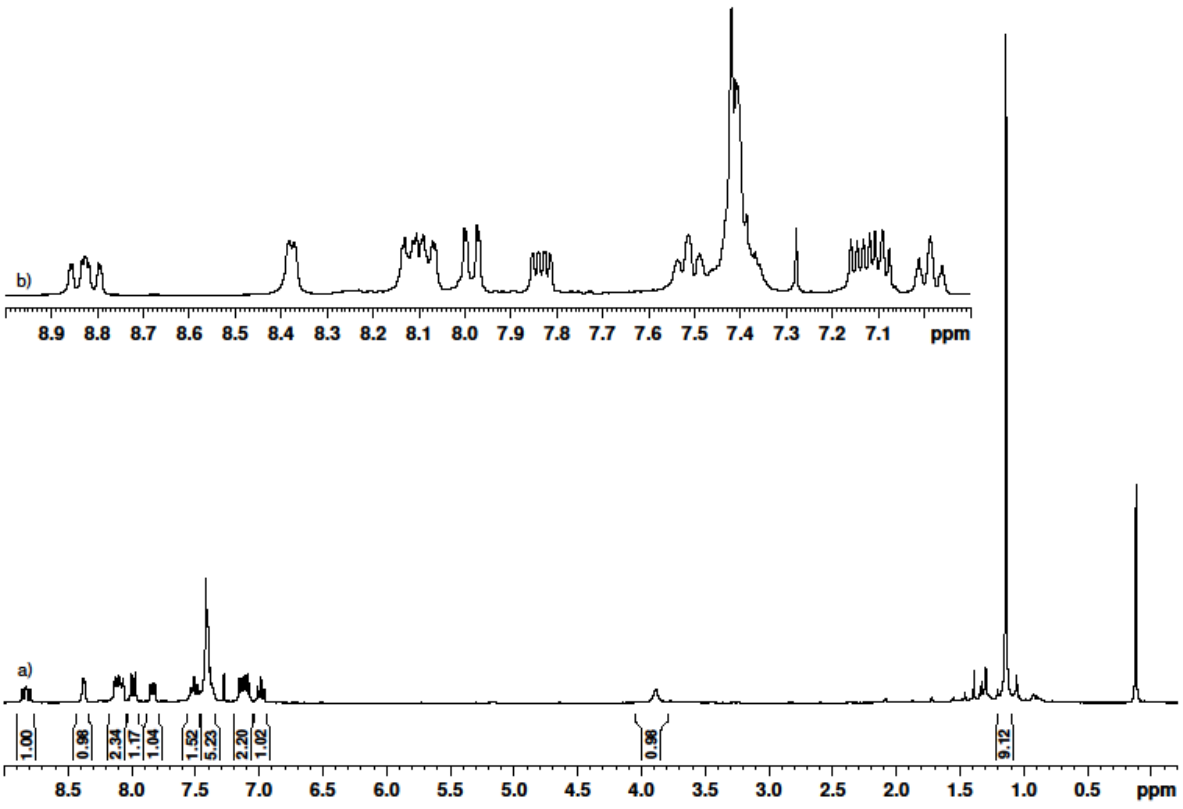

Figure S27. ^{1}H NMR spectrum (300.13 MHz) of phosphinimidic amide **17** in $CDCl_3$.

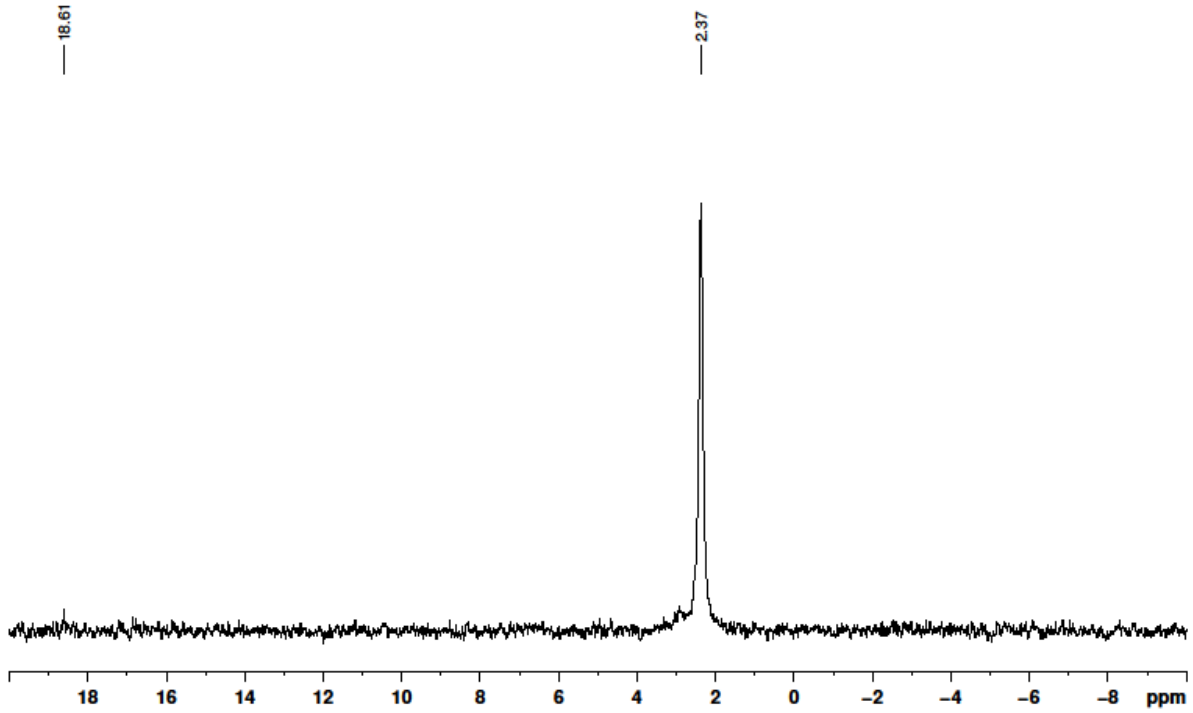

Figure S28. $^{31}P\{^{1}H\}$ NMR spectrum (121.49 MHz) of phosphinimidic amide **17** in $CDCl_3$.

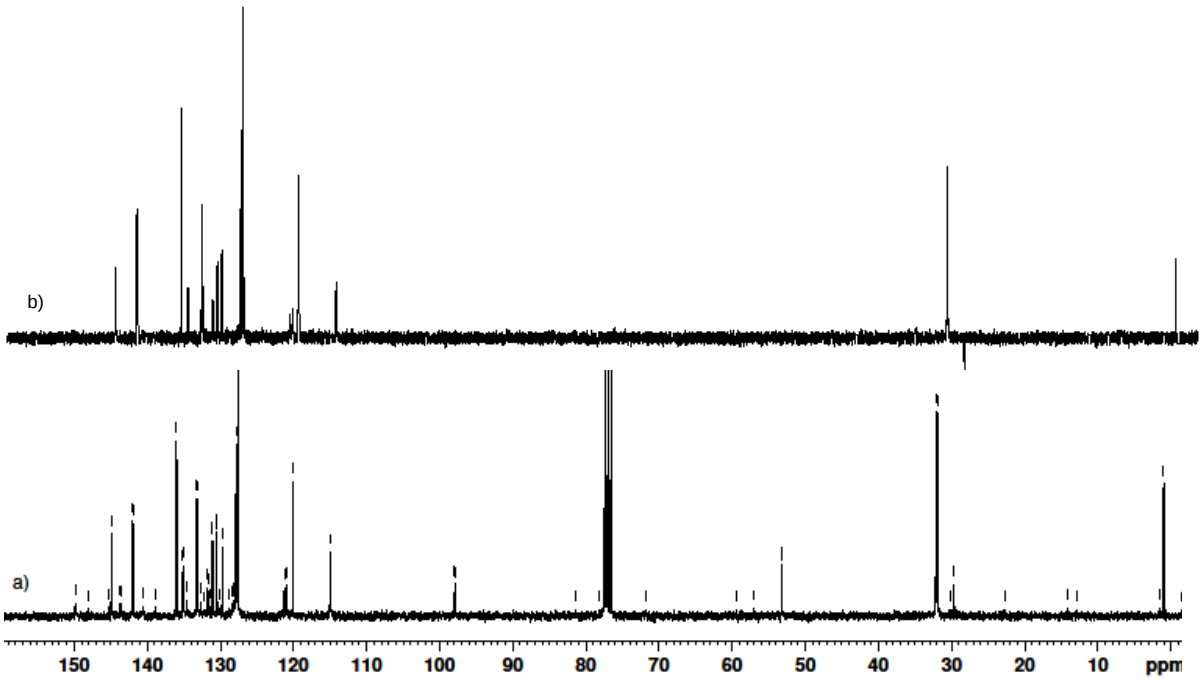

Figure S29. $^{13}C\{^{1}H\}$ (a) and dept135 (b) NMR spectra (75.46 MHz) of phosphinimidic amide **17** in $CDCl_3$.

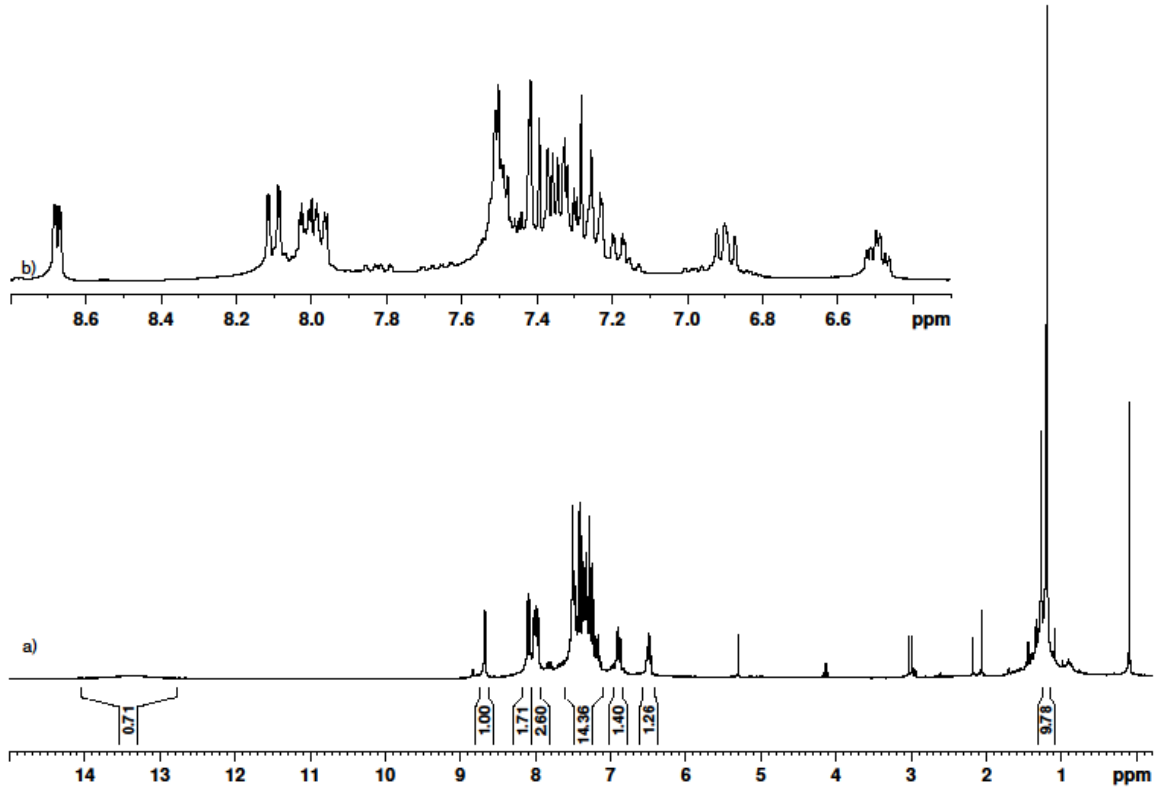

Figure S30. ^{1}H NMR spectrum (300.13 MHz) of phosphinimidic amide **18** in $CDCl_3$.

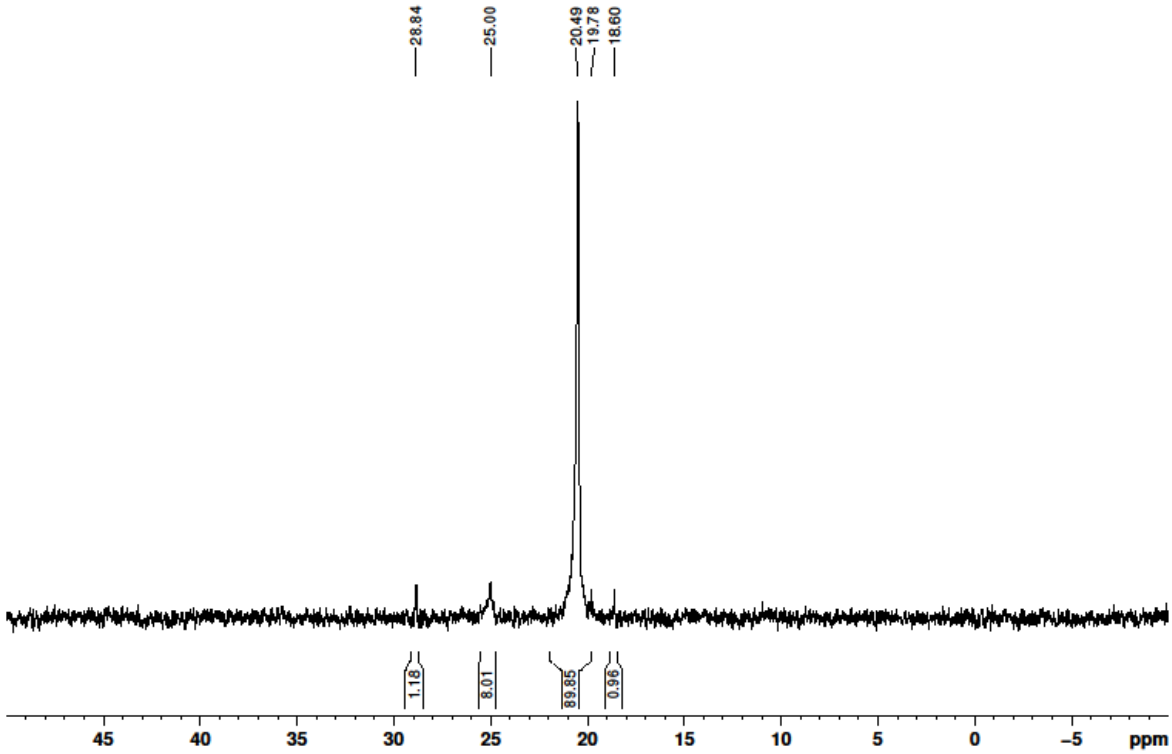

Figure S31. $^{31}P\{^{1}H\}$ NMR spectrum (121.49 MHz) of phosphinimidic amide **18** in $CDCl_3$.

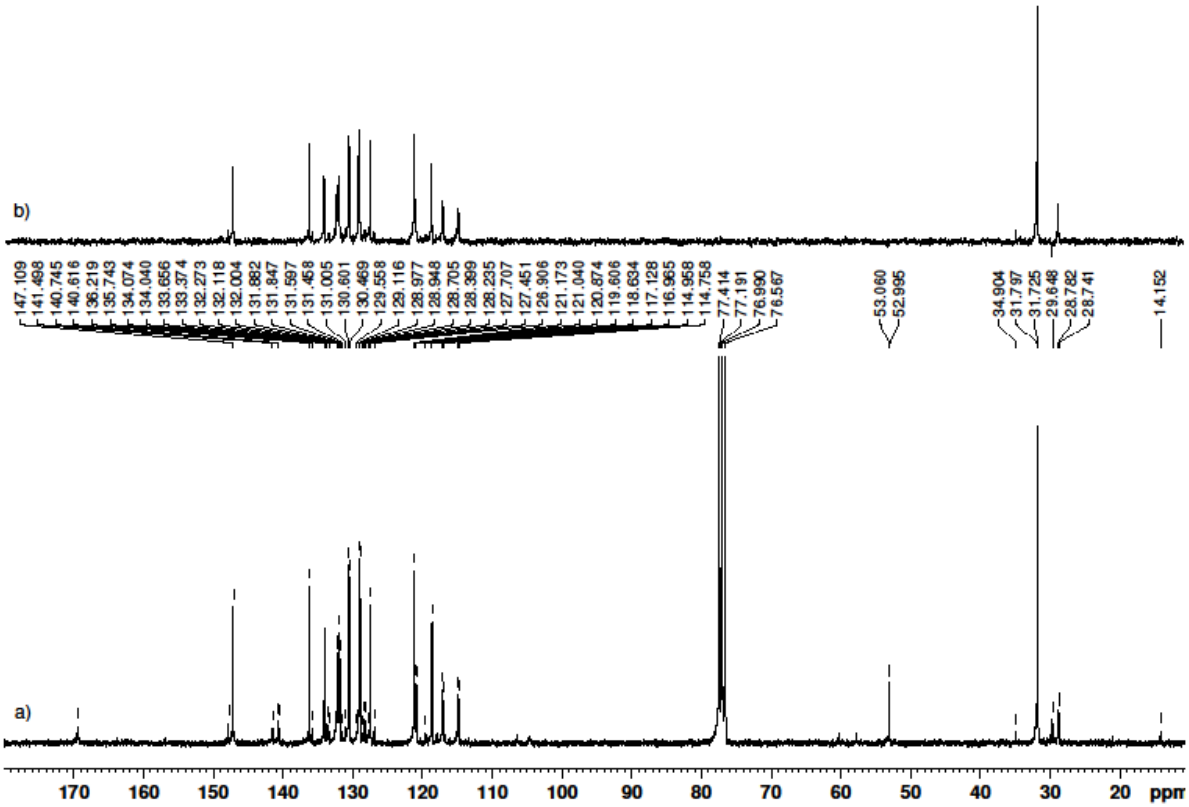

Figure S32. $^{13}C\{^{1}H\}$ (a) and dept135 (b) NMR spectra (75.46 MHz) of phosphinimidic amide **18** in $CDCl_3$.

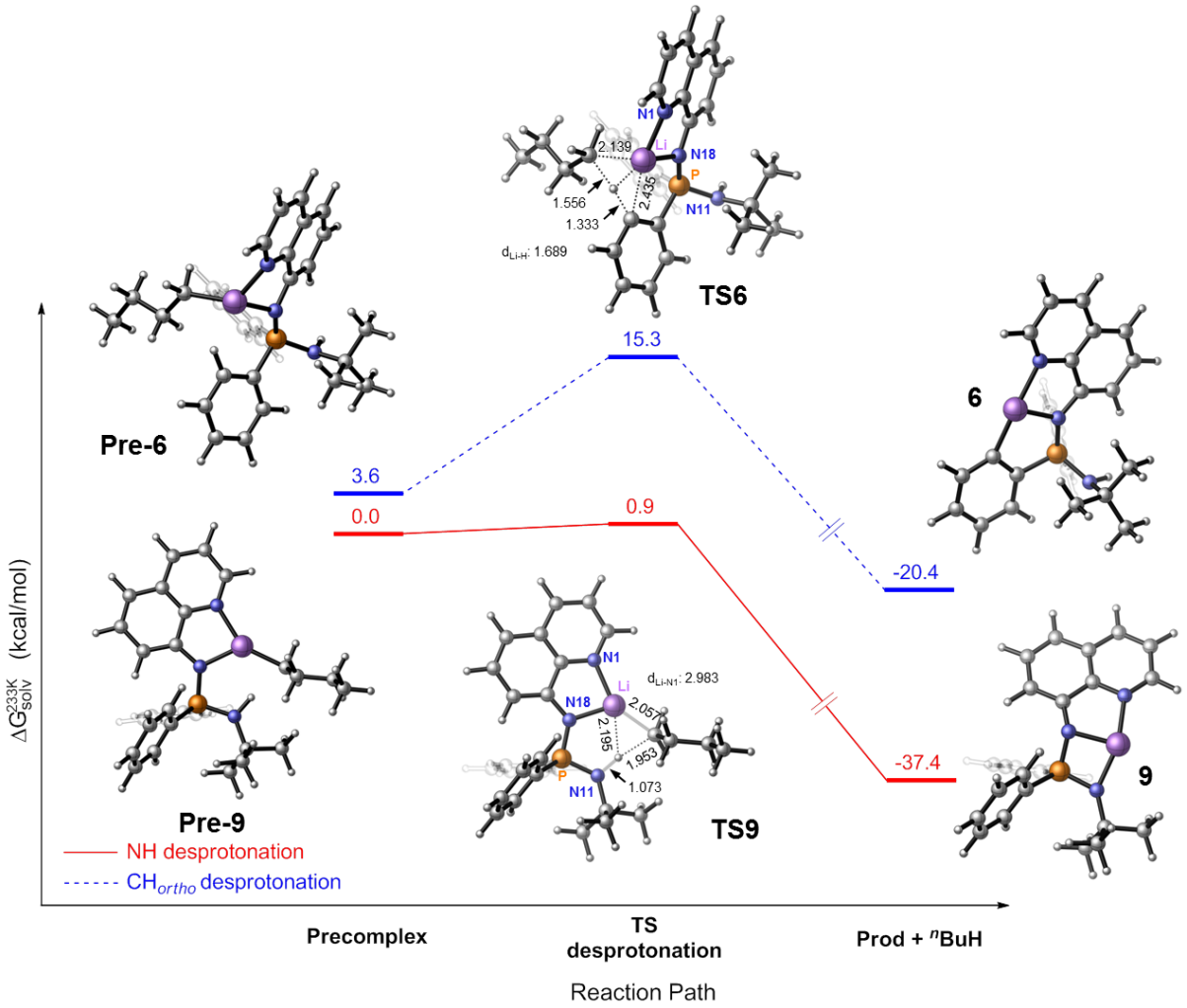

Figure S33. Computed reaction pathway for the NH vs. CH_{ortho} deprotonation of **5**.

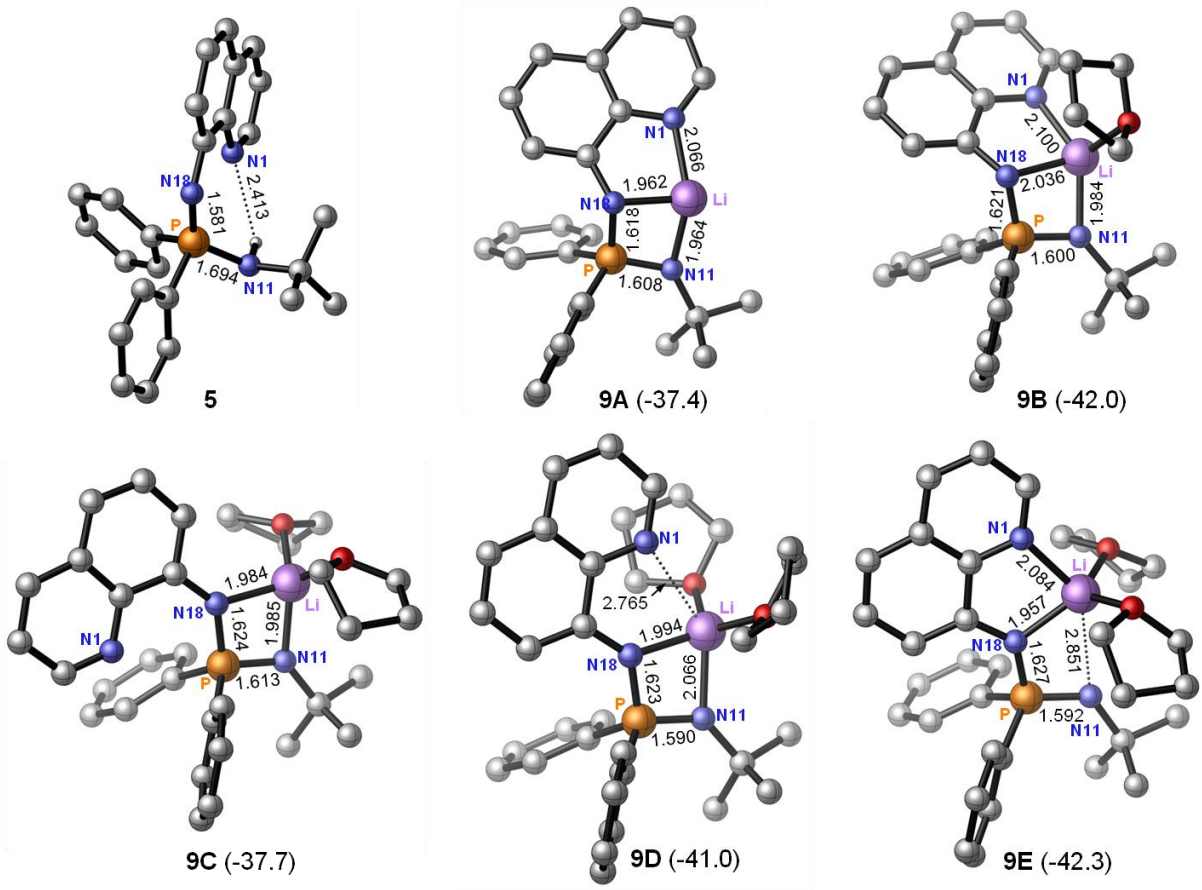

Figure S34. Computed structures of monomers. Hydrogen atoms are omitted for clarity. Free energies and enthalpies (in parentheses) are given in kcal/mol with respect to the equations: a) **Pre-9** → **9A** + **^{n}BuH**, b) **Pre-9** + **THF** → **9A** + **^{n}BuH**, and c) **Pre-9** + 2**THF** → **9B-E** + **^{n}BuH**.

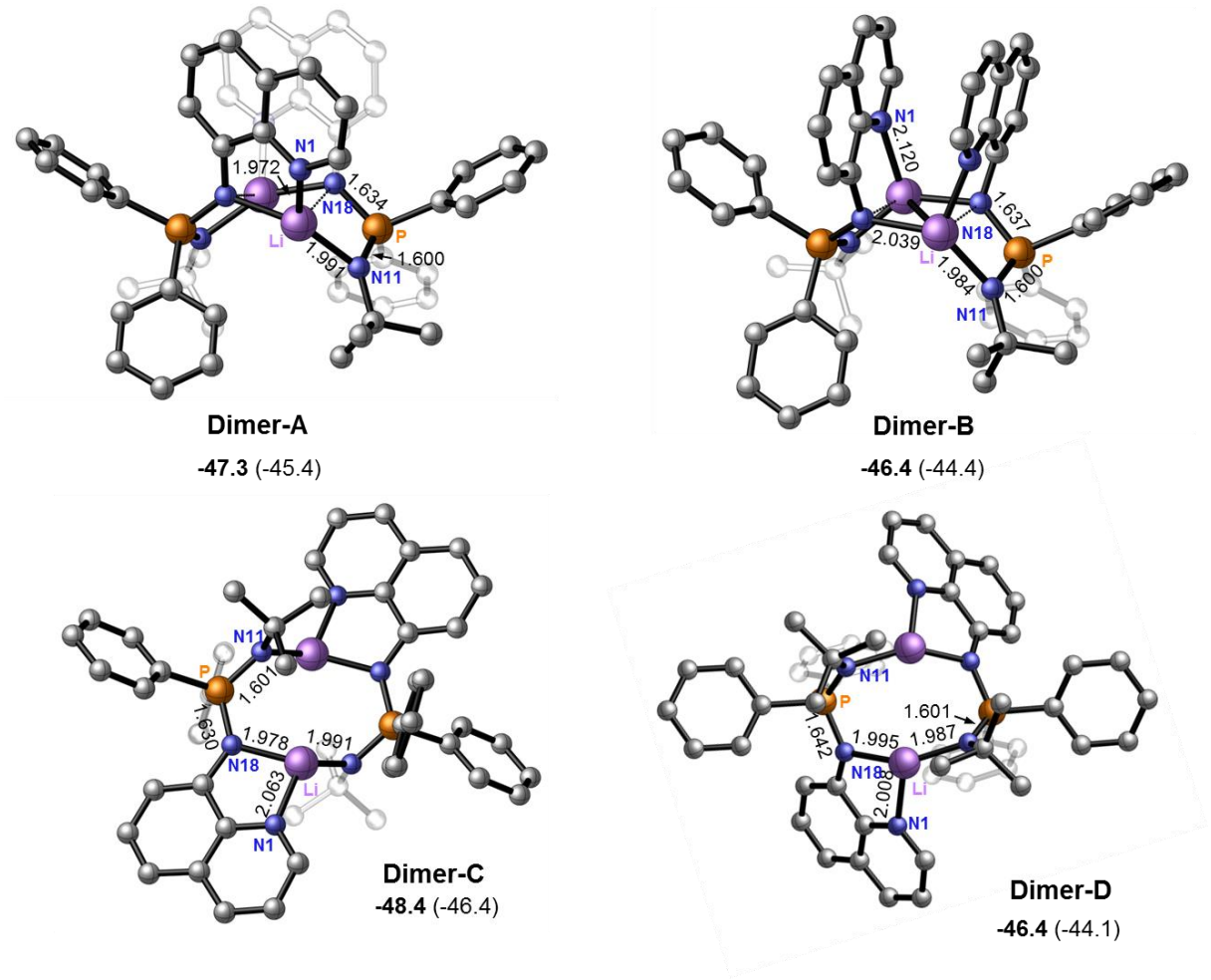

Figure S35. Computed structures of dimers. Hydrogen atoms are omitted for clarity. Free energies and enthalpies (in parentheses) are given in kcal/mol with respect to the equation: **Pre-9** → **½Dimer** + **^{n}BuH**. Selected bond distances are given in Å.

Table S1. The Cartesian coordinates (Å), SCF energies, enthalpies at 233K and and Gibbs free energies at 233K for the optimized structures.

5

M06-2X SCF energy: -1473.43493538 a.u.
M06-2X enthalpy: -1472.95769500 a.u.
M06-2X free energy: -1473.01359900 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	0.75603400	-0.04163400	-0.07254800
C	0.50690700	1.76232700	0.00824000
C	-0.12376400	2.37464100	-1.07717500
C	0.94252700	2.53835700	1.08523200
C	-0.32081700	3.75165300	-1.08339900
H	-0.47032800	1.76274500	-1.90612400
C	0.74165100	3.91654300	1.07619200
H	1.43091200	2.06400300	1.93168800
C	0.11137800	4.52358000	-0.00699700
H	-0.81635400	4.22247800	-1.92675900
H	1.07876700	4.51645400	1.91613800
H	-0.04402600	5.59816300	-0.01200900
C	2.46689000	-0.25613400	-0.63998100
C	2.72386400	-0.81339700	-1.89259600
C	3.52827900	0.17680500	0.16052400
C	4.03735900	-0.94635300	-2.33708100
C	4.83817800	0.04472200	-0.28738700
H	3.32455200	0.59735700	1.14158000
C	5.09321000	-0.51827500	-1.53711400
H	4.23574100	-1.38611400	-3.30971200
H	5.66065400	0.37714600	0.33845500
H	6.11633600	-0.62302100	-1.88551600
N	0.80890900	-0.44080300	1.57240000
N	-0.12542200	-0.81005000	-1.13681400
C	-1.48474000	-0.93416700	-1.27013800
C	-2.45790000	-0.38310400	-0.35401400
C	-1.98250100	-1.64268200	-2.36047300
C	-3.85162400	-0.55622900	-0.59735000
C	-3.35968400	-1.81322500	-2.58365100
H	-1.25989600	-2.06526700	-3.05077400
C	-2.86540300	0.83539400	1.56006900
C	-4.74911300	0.02968800	0.33190300
C	-4.29406500	-1.28190800	-1.72682000
H	-3.68296800	-2.37477200	-3.45560800
C	-4.26735500	0.72907900	1.40565700
H	-2.45031900	1.38597800	2.40382700
H	-5.81844100	-0.08513200	0.17168800
H	-5.35910500	-1.40574800	-1.89845300
H	-4.93032400	1.19244800	2.12825900
N	-2.00260700	0.30109900	0.72861900
C	0.82556100	-1.84636800	2.06001600
C	1.87436200	-2.67174700	1.31512800
H	1.90228300	-3.67793100	1.74523100
H	2.86919000	-2.22673500	1.40545500
H	1.62916500	-2.76605000	0.25220200
C	-0.55461400	-2.49453100	1.89372200
H	-1.32281000	-1.91172100	2.41444000
H	-0.55111700	-3.50732800	2.31110300
H	-0.83029800	-2.55415300	0.83651400
C	1.19253700	-1.77359200	3.54406700
H	1.20923700	-2.77580400	3.98431200
H	0.45922800	-1.17421200	4.09603600
H	2.17757700	-1.31470300	3.67013500
H	0.02475500	0.04507400	2.01102900
H	1.88418000	-1.14683000	-2.49380100

Pre-6

M06-2X SCF energy: -1638.72589863 a.u.
M06-2X enthalpy: -1638.11976300 a.u.
M06-2X free energy: -1638.18754500 a.u.
M06-2X SCF energy in solution: -1639.13149841 a.u.
M06-2X enthalpy in solution: -1638.52536278 a.u.
M06-2X free energy in solution: -1638.59314478 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	-0.50351400	0.98991900	0.12324700
C	-1.16859000	0.22698700	1.62951800
C	-0.90625400	-1.13404100	1.81741100
C	-1.98666600	0.91813500	2.52920300
C	-1.45387700	-1.79423700	2.91423500
H	-0.29568300	-1.67484600	1.09552500
C	-2.52069800	0.25336900	3.62831400
H	-2.21991800	1.96685600	2.36300000
C	-2.25356500	-1.10136300	3.81966100
H	-1.25766300	-2.85253100	3.05329300
H	-3.15412800	0.78878600	4.32854700
H	-2.67921600	-1.61980900	4.67332400
C	-1.83894800	0.97911200	-1.09380000
C	-2.04412200	-0.12727300	-1.92189500
C	-2.75358300	2.03877800	-1.10615400
C	-3.13254100	-0.14373900	-2.79173100
C	-3.83655000	2.01448600	-1.97757700
H	-2.60545100	2.88249300	-0.43830800
C	-4.02203300	0.92561500	-2.82769800
H	-3.28622700	-1.00867100	-3.42940800
H	-4.53667200	2.84394000	-1.99117900
H	-4.86919300	0.90632300	-3.50662300
N	-0.31599600	2.59732800	0.58846300
N	0.75994100	0.20067300	-0.47149000
C	1.93668700	0.02932700	0.24708400
C	2.99529100	-0.71121700	-0.40289400
C	2.20740400	0.50559300	1.52545800
C	4.26395700	-0.85749200	0.21836800
C	3.46660500	0.33893100	2.13998300
H	1.43837900	1.03451000	2.07898400
C	3.66489200	-1.95238800	-2.23263300
C	5.25724300	-1.57645500	-0.49201000
C	4.49164200	-0.31190100	1.50573000
H	3.61488700	0.74448900	3.13646200
C	4.96899800	-2.11779700	-1.71648800
H	3.38899100	-2.40340800	-3.18258300
H	6.24042600	-1.69525000	-0.04369000
H	5.46370900	-0.43373800	1.97342600
H	5.70640200	-2.67836000	-2.27990900
N	2.72377800	-1.27726700	-1.61189300
Li	0.70884800	-1.44438500	-1.66133000
C	0.42362000	3.64602900	-0.16491900
C	0.22011600	3.48516700	-1.67251100
H	0.80155900	4.25722000	-2.18554800
H	-0.82843000	3.60111500	-1.95609600
H	0.57373500	2.50951000	-2.02218000
C	1.92040400	3.57902200	0.15453700
H	2.09256100	3.63116700	1.23609200
H	2.44460800	4.41902400	-0.31314700
H	2.35567700	2.64651300	-0.21430400
C	-0.14787100	4.99023000	0.29275800
H	0.36082000	5.81382900	-0.21761300
H	-0.00981100	5.12682000	1.37177900

H	-1.21786700	5.04869600	0.07173700
H	-0.17661800	2.69582700	1.59162800
C	-0.34573800	-3.13959700	-1.21093800
H	-0.11807600	-3.95591500	-1.92003500
H	0.23807400	-3.41828100	-0.30490200
H	-1.39244300	-1.00152300	-1.87048200
C	-1.82818600	-3.25233900	-0.84068000
H	-2.15550400	-2.39337800	-0.22538000
H	-2.44824000	-3.18719800	-1.75197700
C	-2.24050500	-4.52000200	-0.08201500
H	-1.62174800	-4.59804300	0.82401700
H	-1.99175400	-5.39879400	-0.69164400
C	-3.71894200	-4.54575000	0.30308500
H	-3.99204100	-5.45746300	0.84524100
H	-3.96559400	-3.68841300	0.94091600
H	-4.35459600	-4.48339200	-0.58762800

TS6

M06-2X SCF energy: -1638.70871634 a.u.
M06-2X enthalpy: -1638.10718700 a.u.
M06-2X free energy: -1638.17244700 a.u.
M06-2X SCF energy in solution: -1639.11087147 a.u.
M06-2X enthalpy in solution: -1638.50934213 a.u.
M06-2X free energy in solution: -1638.57460213 a.u.
Frequency: -1242.90 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
P	0.78807200	-0.85304100	0.17409000
C	1.26078600	0.17976100	1.59307900
C	0.57204300	1.38120000	1.78521400
C	2.33512600	-0.14997300	2.42666000
C	0.94819500	2.23869100	2.81543400
H	-0.24404400	1.64793000	1.11755700
C	2.70383400	0.70901800	3.45713100
H	2.89157400	-1.06872200	2.25997000
C	2.01004200	1.90196100	3.65148500
H	0.41525000	3.17374900	2.95807200
H	3.53863300	0.45235600	4.10174000
H	2.30342800	2.57416400	4.45196900
C	1.93644700	-0.54762300	-1.18167100
C	1.60211400	0.43321900	-2.12772900
C	3.15308400	-1.24132100	-1.21267800
C	2.54180900	0.66513300	-3.13928800
C	4.05464000	-0.98885100	-2.24014700
H	3.38112800	-1.98382300	-0.45075500
C	3.74210300	-0.03765200	-3.21226400
H	2.33183200	1.43521800	-3.88158700
H	4.99605900	-1.52830400	-2.28242300
H	4.44714000	0.16183300	-4.01535900
N	1.10018100	-2.39611700	0.78030400
N	-0.67273100	-0.50428100	-0.38774600
C	-1.85390900	-0.49032000	0.31989700
C	-3.01346100	0.00077600	-0.39043900
C	-2.04606600	-0.90324600	1.63310100
C	-4.28711900	0.02065000	0.23609200
C	-3.31643500	-0.87180000	2.24604800
H	-1.19822800	-1.26611400	2.20711900
C	-3.86790000	0.91099800	-2.33318400
C	-5.37730300	0.51342300	-0.52318400
C	-4.42586800	-0.42920100	1.57295100
H	-3.40619200	-1.20984400	3.27423000
C	-5.17629700	0.95622600	-1.80371000
H	-3.67385100	1.27267400	-3.34021700
H	-6.36542100	0.53728400	-0.07056700
H	-5.40375200	-0.40701100	2.04380600
H	-5.98938500	1.34366800	-2.40721100
N	-2.83224800	0.45177400	-1.66572300
Li	-0.81679400	0.66234600	-1.96687000
C	0.64021900	-3.66935700	0.16760100
C	0.75414500	-3.61453800	-1.35650000
H	0.40528700	-4.56723900	-1.76678600
H	1.78567800	-3.45499600	-1.67867000
H	0.13119200	-2.81739200	-1.77550900
C	-0.81327000	-3.95274100	0.56120000
H	-0.92691200	-3.96220000	1.65188000
H	-1.12906700	-4.92959900	0.18003100
H	-1.48005200	-3.18696200	0.15479600
C	1.55550800	-4.76782000	0.71309800
H	1.26391800	-5.74253900	0.30977400
H	1.49110800	-4.82324300	1.80625100
H	2.59567600	-4.56973200	0.43808500
H	1.02811000	-2.43033100	1.79527400
C	-0.14224000	2.66020600	-1.60839000
H	-0.53685400	3.27644000	-2.43256700
H	-0.96375800	2.59999200	-0.86571500
H	0.70107500	1.40318300	-1.96838000
C	1.04261100	3.37315200	-0.95308500
H	1.62231600	2.65851000	-0.34154400
H	1.74794700	3.70485700	-1.73069600
C	0.69532500	4.56761700	-0.06229900
H	-0.03453300	4.23884600	0.69289600
H	0.18128200	5.33073300	-0.66115300
C	1.91382900	5.17236500	0.63242300
H	1.64667900	6.02165300	1.27019400
H	2.41072800	4.42149700	1.25839900
H	2.64696100	5.52269200	-0.10259000

6

M06-2X SCF energy: -1480.39418283 a.u.
M06-2X enthalpy: -1479.92679600 a.u.
M06-2X free energy: -1479.98351100 a.u.
M06-2X SCF energy in solution: -1480.74781926 a.u.
M06-2X enthalpy in solution: -1480.28043243 a.u.
M06-2X free energy in solution: -1480.33714743 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	0.96227700	0.09185900	0.07330400
C	1.21364600	1.74728300	-0.64768100
C	0.28348800	2.20563400	-1.58508200
C	2.32058400	2.54145900	-0.32817400
C	0.45416000	3.44748800	-2.18928600
H	-0.57425500	1.58676800	-1.83343100
C	2.48796200	3.78274900	-0.93492400
H	3.05186100	2.18667100	0.39278400
C	1.55483900	4.23644000	-1.86429400
H	-0.27386300	3.79955900	-2.91327300
H	3.34943700	4.39402900	-0.68453400
H	1.68724800	5.20480400	-2.33704000
C	1.96309300	-1.14399600	-0.77438700
C	1.29928300	-2.16225800	-1.49499000
C	3.35686900	-0.99670800	-0.67652600
C	2.19566700	-3.05314800	-2.12662300
C	4.17464700	-1.91007700	-1.32300900
H	3.79461200	-0.19168400	-0.08766600
C	3.58178200	-2.94479800	-2.05220600
H	1.79233400	-3.88258900	-2.70831100
H	5.25546800	-1.82329700	-1.26092700
H	4.21407700	-3.66893900	-2.56203700
N	1.60378800	0.35834000	1.61479100
N	-0.55941100	-0.39219900	-0.08442800
C	-1.72876000	0.21805400	0.27265500
C	-2.93311600	-0.43115800	-0.19814700

C	-1.88370600	1.37358600	1.02965500
C	-4.20963900	0.09776900	0.12544600
C	-3.15958300	1.89003400	1.33943400
H	-1.00002500	1.89176700	1.39179000
C	-3.86702600	-2.16420300	-1.40392200
C	-5.34283400	-0.59400600	-0.36844000
C	-4.30819500	1.27601200	0.90824000
H	-3.22360700	2.79558800	1.93576300
C	-5.17927400	-1.72197900	-1.12926300
H	-3.70902300	-3.05306300	-2.01044900
H	-6.33469500	-0.21491200	-0.13519500
H	-5.28876100	1.67384800	1.15028200
H	-6.02679000	-2.27253500	-1.52178800
N	-2.78718600	-1.55385900	-0.96338100
Li	-0.74264800	-1.93927300	-1.23420100
C	1.48091000	-0.58697600	2.75226000
C	1.77660200	-2.01629500	2.29782300
H	1.74130700	-2.67670400	3.17007700
H	2.76561200	-2.08933900	1.83779500
H	1.03882500	-2.37154400	1.57114200
C	0.07475800	-0.51290800	3.35849700
H	-0.15695300	0.50987800	3.67913900
H	-0.00171900	-1.16752100	4.23323900
H	-0.67670700	-0.82015300	2.62498900
C	2.52240600	-0.15229300	3.78570300
H	2.48075700	-0.80156400	4.66576200
H	2.33792200	0.87638700	4.11825600
H	3.52709100	-0.20264900	3.35629700
H	1.45190900	1.31693300	1.92495600

^{n}BuH (*n*-butane)

M06-2X SCF energy: -158.35738499 a.u.
M06-2X enthalpy: -158.21879100 a.u.
M06-2X free energy: -158.24411700 a.u.
M06-2X SCF energy in solution: -158.40755233 a.u.
M06-2X enthalpy in solution: -158.26895834 a.u.
M06-2X free energy in solution: -158.29428434 a.u.

Cartesian coordinates

ATOM	X	Y	Z
C	1.94876400	-0.11984200	0.00028400
H	2.08709800	-0.75164100	0.88413300
C	0.56183100	0.51754100	-0.00030300
H	0.45185100	1.16757300	0.87747800
H	0.45233000	1.16699100	-0.87858500
C	-0.56183000	-0.51750400	-0.00030900
H	-0.45182400	-1.16753800	0.87747800
H	-0.45227700	-1.16695700	-0.87857800
C	-1.94880800	0.11983300	0.00027900
H	-2.08717000	0.75291900	-0.88264700
H	-2.74031900	-0.63501800	-0.00082600
H	-2.08746500	0.75071100	0.88473100
H	2.08764500	-0.75209500	-0.88317100
H	2.74039100	0.63488900	0.00028100

Pre-9

M06-2X SCF energy: -1638.73470516 a.u.
M06-2X enthalpy: -1638.12955400 a.u.
M06-2X free energy: -1638.19820000 a.u.
M06-2X SCF energy in solution: -1639.13544842 a.u.
M06-2X enthalpy in solution: -1638.53029726 a.u.
M06-2X free energy in solution: -1638.59894326 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	0.35079100	-0.76587700	-0.11191100
C	-0.18664800	-1.95742600	-1.38049300
C	-0.97544400	-3.07977900	-1.10898000
C	0.10408200	-1.62893300	-2.71044500
C	-1.44714700	-3.87380500	-2.15185300
H	-1.21821800	-3.34698100	-0.08490000
C	-0.37123000	-2.42089200	-3.74937700
H	0.71082800	-0.75022300	-2.91641900
C	-1.14447700	-3.54654300	-3.47013700
H	-2.05364200	-4.74674000	-1.93203100
H	-0.13765500	-2.16109900	-4.77703400
H	-1.51318800	-4.16686000	-4.28127600
C	0.58154100	-1.69401600	1.44074800
C	0.42459900	-0.95576800	2.61978100
C	0.95642700	-3.03918500	1.51475700
C	0.65791700	-1.55149700	3.85438100
C	1.18801700	-3.63315400	2.75289000
H	1.06784100	-3.62803400	0.60869900
C	1.04368800	-2.88900300	3.92115800
H	0.53734000	-0.97297800	4.76471200
H	1.48169000	-4.67686900	2.80382300
H	1.22760900	-3.35316200	4.88518000
N	1.72813200	-0.02278500	-0.59804200
N	-0.70760300	0.43456200	0.05728800
C	-2.04070100	0.32012900	0.37183900
C	-2.84510800	1.50380200	0.15879800
C	-2.68749000	-0.79041000	0.90087200
C	-4.23206900	1.50101100	0.45960100
C	-4.06844400	-0.78037300	1.19266500
H	-2.11664800	-1.68590400	1.12154300
C	-2.92138300	3.70483500	-0.54193800
C	-4.95009200	2.69843500	0.22088600
C	-4.84121900	0.33135300	0.97970000
H	-4.51817500	-1.68087400	1.60084100
C	-4.30466800	3.79968300	-0.27811500
H	-2.37730600	4.56013200	-0.93584000
H	-6.01438500	2.72564600	0.44112600
H	-5.90315000	0.33752500	1.20478500
H	-4.82863600	4.72923000	-0.47003500
N	-2.22070500	2.61042200	-0.33549100
Li	-0.23571400	2.22253400	-0.60487000
C	3.11553000	-0.53260400	-0.58946000
C	3.18794000	-1.95177000	-1.16057900
H	4.22834700	-2.29254400	-1.16068500
H	2.81181000	-1.98300800	-2.18716100
H	2.61172000	-2.66282200	-0.56074000
C	3.70668600	-0.50939200	0.82743100
H	3.60579100	0.49069200	1.25982800
H	4.77077500	-0.76877400	0.79729000
H	3.20201500	-1.22331000	1.48548300
C	3.93206400	0.39628100	-1.49282600
H	4.96046000	0.02835400	-1.56569000
H	3.95562700	1.41421200	-1.09335000
H	3.49834300	0.43282600	-2.49723400
H	0.11856500	0.08562400	2.55613300
C	1.61777500	2.94989600	-1.12140800
H	1.07452400	3.84274100	-1.49944300
H	1.60097500	1.03061600	-0.76001300
C	2.51084000	3.43348600	0.02826800
H	1.88919400	3.88594800	0.81899300
H	3.00222800	2.57724500	0.52459000
C	3.60631900	4.43921700	-0.34488000
H	3.13682200	5.31623200	-0.81018500
H	4.24417200	3.99207200	-1.12078900
C	4.46396400	4.87346200	0.84247100
H	4.95652200	4.00883500	1.30246400
H	5.24268000	5.58612700	0.55179900
H	3.84757500	5.34749600	1.61478000
H	2.25645400	2.67155200	-1.97678800

TS9

M06-2X SCF energy: -1638.73469072 a.u.
M06-2X enthalpy: -1638.13123500 a.u.
M06-2X free energy: -1638.19798800 a.u.
M06-2X SCF energy in solution: -1639.13426088 a.u.
M06-2X enthalpy in solution: -1638.53080516 a.u.
M06-2X free energy in solution: -1638.59755816 a.u.
Frequency: -117.56 cm^{-1}

Cartesian coordinates

ATOM	X	Y	Z
P	0.46073000	-0.72902900	-0.11197400
C	0.02124800	-1.97556800	-1.36910900
C	-0.65288500	-3.16789500	-1.08760000
C	0.26810500	-1.62723700	-2.70283400
C	-1.05445600	-4.00822000	-2.12368500
H	-0.85958700	-3.45357700	-0.06052800
C	-0.13763300	-2.46506300	-3.73525200
H	0.78748100	-0.69567000	-2.91645600
C	-0.79639300	-3.65891700	-3.44571000
H	-1.57150000	-4.93499100	-1.89548600
H	0.06162900	-2.18846900	-4.76580600
H	-1.11022600	-4.31541300	-4.25145500
C	0.76735000	-1.62553800	1.44763100
C	0.53065900	-0.90378800	2.62344400
C	1.27331700	-2.92662300	1.52977300
C	0.81318500	-1.46982800	3.86181900
C	1.55407800	-3.49147500	2.77139700
H	1.44879500	-3.50444100	0.62674400
C	1.32880400	-2.76232900	3.93630700
H	0.62949300	-0.90333000	4.76922100
H	1.94923900	-4.50091500	2.82756100
H	1.55090400	-3.20337400	4.90315900
N	1.74469100	0.14943300	-0.60077200
N	-0.72154800	0.35548600	0.05483100
C	-2.03469100	0.11788100	0.37256200
C	-2.94687100	1.21947300	0.14938200
C	-2.57506500	-1.04313400	0.91379600
C	-4.32677100	1.09210500	0.45610900
C	-3.95009500	-1.15709000	1.20990700
H	-1.92264000	-1.87954000	1.13963600
C	-3.22947300	3.39610200	-0.57676900
C	-5.15290400	2.21542200	0.20802600
C	-4.82346100	-0.12352000	0.98991700
H	-4.31398700	-2.09140500	1.62763700
C	-4.61401300	3.36610300	-0.30614300
H	-2.76968000	4.29350500	-0.98435200
H	-6.21435200	2.14678400	0.43294900
H	-5.88069400	-0.21345200	1.21901200
H	-5.22243600	4.24102500	-0.50556900
N	-2.42920700	2.37354900	-0.36155400
Li	-0.42583900	2.13669000	-0.64906800
C	3.17039000	-0.23639000	-0.59949500
C	3.37595700	-1.64341600	-1.17124800
H	4.44355900	-1.88698300	-1.17472300
H	3.00122200	-1.70964600	-2.19681000
H	2.86905900	-2.40496700	-0.57076300
C	3.76330700	-0.16029800	0.81542800
H	3.56920200	0.82508700	1.24995800
H	4.84720800	-0.31837600	0.78223200
H	3.33036700	-0.91886000	1.47458000
C	3.90701600	0.75798700	-1.50324900
H	4.95956200	0.46850600	-1.58648800
H	3.85905200	1.77233900	-1.09753900
H	3.46391300	0.76807000	-2.50417900
H	0.12344600	0.10199400	2.55458300
C	1.38224700	2.95417800	-1.18638600
H	0.65748600	3.70648000	-1.57274200
H	1.49747200	1.22529800	-0.82585600
C	2.10742900	3.60493800	-0.00239700
H	1.37820800	3.88143800	0.77871400
H	2.76911100	2.87026600	0.48871300
C	2.94736200	4.84513700	-0.32636200
H	2.30119100	5.59799000	-0.79741600
H	3.69565200	4.57225000	-1.08363500
C	3.64121000	5.44446100	0.89541500
H	4.30655800	4.71015600	1.36369100
H	4.24106800	6.32356500	0.63894500
H	2.90672400	5.74871000	1.64975600
H	2.08478700	2.84129500	-2.02605600

9A

M06-2X SCF energy: -1480.42595619 a.u.
M06-2X enthalpy: -1479.95852400 a.u.
M06-2X free energy: -1480.01583700 a.u.
M06-2X SCF energy in solution: -1480.77427182 a.u.
M06-2X enthalpy in solution: -1480.30683963 a.u.
M06-2X free energy in solution: -1480.36415263 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	-0.79407400	0.22167300	-0.12453800
C	-0.50311100	-0.89190800	1.29810400
C	-0.73231900	-2.27033400	1.24289900
C	0.09353600	-0.34482200	2.43817400
C	-0.38735200	-3.08452000	2.31862100
H	-1.18924900	-2.70859700	0.35896500
C	0.44170700	-1.15875800	3.51196200
H	0.27334600	0.72715600	2.47210600
C	0.19794400	-2.52914300	3.45387400
H	-0.57414900	-4.15300900	2.26972700
H	0.90056000	-0.72447600	4.39502300
H	0.46583300	-3.16483900	4.29246200
C	-2.21760800	-0.51134700	-1.01010100
C	-2.22509900	-0.41410600	-2.40479400
C	-3.31888600	-1.07553200	-0.35758900
C	-3.32549100	-0.85469000	-3.13426800
C	-4.41725000	-1.52062500	-1.08846600
H	-3.31527200	-1.18146700	0.72449000
C	-4.42391100	-1.40439100	-2.47678700
H	-3.32437300	-0.77459000	-4.21713100
H	-5.26670800	-1.96002400	-0.57440800
H	-5.28186300	-1.74941300	-3.04593500
N	-0.96004700	1.76878500	0.27984300
N	0.50390100	0.23516600	-1.09050100
C	1.67850700	-0.46080500	-0.97734200
C	2.88932100	0.31060500	-0.80043900
C	1.81684100	-1.83888100	-1.06695200
C	4.15703800	-0.33135700	-0.76060200
C	3.07769100	-2.46760700	-1.00496200
H	0.92144200	-2.43545000	-1.21273400
C	3.85527200	2.39040600	-0.49674900
C	5.29923700	0.48958700	-0.59841300
C	4.23466400	-1.74212900	-0.86642500
H	3.12644900	-3.55002900	-1.08205900
C	5.15698500	1.84684500	-0.46994600
H	3.71344100	3.46265800	-0.37905200
H	6.28225900	0.02560900	-0.57414400
H	5.20640500	-2.22511400	-0.83024100
H	6.01221300	2.50086800	-0.34223300
N	2.76675800	1.66622400	-0.65495300
Li	0.75248300	2.12224600	-0.61514800
C	-2.11080500	2.46410000	0.85120200

C	-2.71881000	1.73356600	2.05722200
H	-3.54914300	2.30908400	2.48177500
H	-1.96817300	1.58102300	2.83892500
H	-3.10943600	0.75251100	1.76630500
C	-3.20226500	2.69086500	-0.20740600
H	-2.77252200	3.19397500	-1.08006700
H	-4.01299600	3.31277700	0.19061000
H	-3.63372300	1.74202100	-0.54106600
C	-1.59650700	3.82920500	1.32420100
H	-2.40002900	4.42690100	1.76856100
H	-1.18165100	4.38848200	0.47731500
H	-0.80536800	3.69415900	2.06986600
H	-1.35392300	0.00139000	-2.90437500

THF (Tetrahydroforan)

M06-2X SCF energy: -232.33665781 a.u.
M06-2X enthalpy: -232.21379900 a.u.
M06-2X free energy: -232.23895500 a.u.
M06-2X SCF energy in solution: -232.41346990 a.u.
M06-2X enthalpy in solution: -232.29061109 a.u.
M06-2X free energy in solution: -232.31576709 a.u.

Cartesian coordinates

ATOM	X	Y	Z
H	1.51204100	-0.46753200	1.17676800
O	-0.00010000	-1.24273400	-0.00022000
C	-1.15814700	-0.42794300	-0.13664500
C	1.15799300	-0.42816300	0.13692400
C	-0.72761300	0.99070700	0.23643900
H	-1.51283900	-0.46742500	-1.17625300
H	-1.94631400	-0.82504900	0.51026500
C	0.72788000	0.99048100	-0.23656600
H	1.94647000	-0.82552600	-0.50943800
H	-0.77136400	1.12876600	1.32200800
H	-1.34345400	1.76009900	-0.23477900
H	1.34389100	1.75985900	0.23445500
H	0.77169400	1.12818800	-1.32217800

9B

M06-2X SCF energy: -1712.79631523 a.u.
M06-2X enthalpy: -1712.20417200 a.u.
M06-2X free energy: -1712.27156400 a.u.
M06-2X SCF energy in solution: -1713.21209329 a.u.
M06-2X enthalpy in solution: -1712.61995006 a.u.
M06-2X free energy in solution: -1712.68734206 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	0.79350200	0.42033200	0.13044500
C	0.37657700	2.20215600	0.17228000
C	0.74526500	3.10145700	-0.83185900
C	-0.47507200	2.63252400	1.19524400
C	0.28908700	4.41738000	-0.79945700
H	1.39138600	2.77399000	-1.64235500
C	-0.93522900	3.94495600	1.22463500
H	-0.76849400	1.92441200	1.96726600
C	-0.54888900	4.84012700	0.22892300
H	0.58612200	5.11179300	-1.57968800
H	-1.59439100	4.27091700	2.02351600
H	-0.90453100	5.86587800	0.25261500
C	2.31788400	0.32481900	-0.88682800
C	2.40699800	-0.68569200	-1.84825000
C	3.41665400	1.16729900	-0.68491800
C	3.58061900	-0.87021600	-2.57510600
C	4.58735700	0.98978200	-1.41700300
H	3.35521900	1.97687000	0.03869400
C	4.67365200	-0.03504500	-2.35755100
H	3.63844000	-1.65876700	-3.32008100
H	5.43218000	1.65233500	-1.25481200
H	5.58806200	-0.17467900	-2.92621800
N	0.89987200	-0.27153300	1.57047300
N	-0.37527000	-0.39623500	-0.63815000
C	-1.58493600	0.13315000	-1.02997800
C	-2.77109600	-0.21995900	-0.28360400
C	-1.75966300	0.96462000	-2.12750700
C	-4.05025000	0.25402400	-0.68716400
C	-3.02956100	1.44178900	-2.51294100
H	-0.87915300	1.24075800	-2.70031500
C	-3.67900100	-1.33825200	1.52576600
C	-5.16678900	-0.13672400	0.09222200
C	-4.16340400	1.09460600	-1.82140100
H	-3.10409500	2.09201300	-3.37993500
C	-4.99016200	-0.93009400	1.19559600
H	-3.50611600	-1.96300900	2.39978600
H	-6.15713800	0.20600300	-0.19778700
H	-5.14312500	1.45517000	-2.12037800
H	-5.82485300	-1.24300300	1.81294200
N	-2.61622100	-1.00446400	0.82557000
Li	-0.61221000	-1.46806300	1.08220600
C	1.88294300	-0.13288000	2.63939700
C	2.22542700	1.32876100	2.96141900
H	2.93163800	1.38710600	3.79745300
H	1.32391200	1.88777400	3.23019600
H	2.68408500	1.82863600	2.10105700
C	3.17692200	-0.89679300	2.31347200
H	2.94872800	-1.95077000	2.12301900
H	3.88553500	-0.84446300	3.14869500
H	3.66642200	-0.48754800	1.42430600
C	1.24931200	-0.76617400	3.88498600
H	1.93006000	-0.73185200	4.74316200
H	0.99872400	-1.81423100	3.68216500
H	0.32658300	-0.23647500	4.14592400
H	1.53492200	-1.31019900	-2.02584500
O	-0.28692200	-3.34817300	0.66524000
C	1.09104600	-3.52276500	0.27120900
C	-1.14847200	-3.80691900	-0.38707800
C	1.06507900	-4.12625500	-1.13629600
H	1.56703800	-2.53717000	0.28663900
H	1.58192400	-4.16714000	1.00682000
C	-0.31222000	-3.69980800	-1.65385000
H	-1.44149400	-4.84535600	-0.18228200
H	-2.03742700	-3.17226500	-0.38770200
H	1.13165800	-5.21834600	-1.09214500
H	1.89284000	-3.75869700	-1.74838900
H	-0.68561700	-4.33332400	-2.46183700
H	-0.29870100	-2.65539300	-1.98109800

9C

M06-2X SCF energy: -1945.15001498 a.u.
M06-2X enthalpy: -1944.43327700 a.u.
M06-2X free energy: -1944.50957200 a.u.
M06-2X SCF energy in solution: -1945.63664832 a.u.
M06-2X enthalpy in solution: -1944.91991034 a.u.
M06-2X free energy in solution: -1944.99620534 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	0.00585800	0.26214000	0.70008500
C	-0.61197600	-0.98039000	1.90948500
C	-1.85196200	-0.94405400	2.55082400
C	0.24578400	-2.05628000	2.16495400
C	-2.22190200	-1.95791800	3.43145900
H	-2.53145500	-0.12225900	2.35470300
C	-0.12714000	-3.07882400	3.03152100

H	1.22316800	-2.06267400	1.68778800
C	-1.36485800	-3.02933100	3.66932200
H	-3.18658100	-1.91353200	3.92820400
H	0.55167800	-3.90616800	3.22004000
H	-1.65845200	-3.82067500	4.35254100
C	-0.93475900	1.80775700	1.01154400
C	-1.24153600	2.60279900	-0.09803100
C	-1.27744800	2.26982400	2.28459800
C	-1.85162000	3.84140900	0.06152200
C	-1.89580600	3.50925800	2.44648100
H	-1.07777300	1.65928900	3.16057100
C	-2.17667400	4.30052700	1.33720900
H	-2.08518300	4.44532700	-0.81042000
H	-2.15802100	3.85371200	3.44239800
H	-2.65530000	5.26686600	1.46399800
N	1.60600200	0.42370500	0.81746800
N	-0.12701300	-0.24029700	-0.83848200
C	-1.12968200	-0.69322300	-1.64292300
C	-2.54228300	-0.61807100	-1.34493500
C	-0.78308300	-1.23760700	-2.88399800
C	-3.50391500	-1.07544900	-2.29326000
C	-1.74343200	-1.69275800	-3.80382000
H	0.27555700	-1.29976900	-3.12874200
C	-4.18060700	0.02780700	0.13303500
C	-4.87081500	-0.94375500	-1.93806700
C	-3.08858300	-1.62175100	-3.53000200
H	-1.40481100	-2.10607300	-4.75015800
C	-5.21664800	-0.38955900	-0.73468800
H	-4.42485000	0.47262800	1.09802100
H	-5.62997700	-1.28424600	-2.63824500
H	-3.83396900	-1.96789400	-4.23965700
H	-6.25401000	-0.26930300	-0.44068200
N	-2.90634900	-0.08713300	-0.15236400
Li	1.84635100	-0.23268600	-1.03992100
C	2.38532100	1.05267800	1.87797900
C	1.89379400	0.74304800	3.30138000
H	2.55367600	1.20738600	4.04303200
H	1.87561600	-0.33595700	3.48216400
H	0.88498600	1.13013900	3.46932100
C	2.43372400	2.57821600	1.68271500
H	2.83878700	2.80700900	0.68972600
H	3.06900000	3.06089200	2.43548000
H	1.43075600	3.01289600	1.74770200
C	3.81560800	0.50633600	1.76696300
H	4.47804000	0.96617600	2.50918900
H	4.22724400	0.70728500	0.77172200
H	3.81671900	-0.57783800	1.92424900
H	-1.01633900	2.22568800	-1.09271500
O	2.45166700	0.94582100	-2.48367500
C	3.59435300	1.75480700	-2.15966800
C	1.39270000	1.79901500	-2.94320700
C	3.13374000	3.21943400	-2.23300700
H	3.91316800	1.48080800	-1.14896800
H	4.40300300	1.52914400	-2.86187500
C	1.60838600	3.09108800	-2.17096700
H	1.49847200	1.95467800	-4.02559600
H	0.45110700	1.28762800	-2.73364600
H	3.43940300	3.67073200	-3.18220100
H	3.54818600	3.82191500	-1.42137300
H	1.08297600	3.94595800	-2.60387200
H	1.27778200	2.95335900	-1.13553000
O	2.47036800	-2.04300700	-1.38025300
C	1.54544300	-3.11234500	-1.09983000
C	3.76438100	-2.40147700	-0.90199600
C	2.26563800	-4.06849000	-0.13219900
H	0.65126500	-2.65447400	-0.66943700
H	1.27576800	-3.60004500	-2.04155400
C	3.49235000	-3.26533700	0.32167300
H	4.30560600	-2.96102600	-1.67748400
H	4.30664500	-1.47683200	-0.68334500
H	2.58114000	-4.97817200	-0.65162000
H	1.62033300	-4.36199300	0.69959500
H	4.34154700	-3.89479100	0.59732200
H	3.24446700	-2.62058600	1.17051400

9D

M06-2X SCF energy: -1945.15454518 a.u.
M06-2X enthalpy: -1944.43791300 a.u.
M06-2X free energy: -1944.51488100 a.u.
M06-2X SCF energy in solution: -1945.64122912 a.u.
M06-2X enthalpy in solution: -1944.92459694 a.u.
M06-2X free energy in solution: -1945.00156494 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	1.44628900	0.00059400	-0.12149900
C	2.14991400	-1.66805000	-0.44544000
C	2.85854300	-2.42587700	0.49165900
C	1.87181700	-2.22946700	-1.69738400
C	3.28073300	-3.71747000	0.18342100
H	3.09898400	-2.00352800	1.46397600
C	2.28777800	-3.52070700	-2.00487200
H	1.33326800	-1.62825900	-2.42714300
C	2.99400100	-4.26708600	-1.06303700
H	3.83495900	-4.29380000	0.91813700
H	2.06855800	-3.94319100	-2.98120300
H	3.32394900	-5.27365900	-1.30217200
C	2.53595100	0.69760600	1.18170400
C	1.93823900	1.42757500	2.21402400
C	3.93129000	0.59598500	1.14150200
C	2.72045800	2.05797500	3.17830600
C	4.71364600	1.22787700	2.10377800
H	4.41026300	0.00875200	0.36180800
C	4.10851500	1.96329500	3.12114100
H	2.24603600	2.61796400	3.97857900
H	5.79536300	1.14359000	2.06200200
H	4.71899900	2.45527500	3.87235700
N	1.23627200	0.85545600	-1.44571400
N	-0.07798000	-0.10793600	0.42393600
C	-0.64567300	-0.79009300	1.44267200
C	-2.09856300	-0.73276400	1.52342500
C	0.01142000	-1.52530000	2.43262100
C	-2.78403800	-1.44710700	2.54920300
C	-0.68904900	-2.21842400	3.43588000
H	1.09548300	-1.56086500	2.42499900
C	-4.07458200	0.09294000	0.68010800
C	-4.19820700	-1.35914500	2.57038600
C	-2.06083700	-2.20045300	3.50525400
H	-0.12040200	-2.78109800	4.17148500
C	-4.85033900	-0.59092500	1.64279500
H	-4.57482200	0.71988200	-0.05907000
H	-4.74712400	-1.90158500	3.33653100
H	-2.59947000	-2.73970200	4.27840000
H	-5.93107400	-0.49641300	1.63720500
N	-2.76226800	0.02690800	0.60537400
Li	-0.81399400	0.74894800	-1.21874900
C	2.18527600	1.55552300	-2.29635300
C	3.44076300	0.73566400	-2.62955700
H	4.10059600	1.29226300	-3.30500100
H	3.17331600	-0.20998100	-3.11080900
H	4.01132000	0.50449900	-1.72305500
C	2.60952100	2.88506800	-1.65093500
H	1.72061600	3.49155000	-1.44645500
H	3.27509900	3.45551900	-2.31022100

H	3.13204800	2.70922400	-0.70426700
C	1.44143300	1.86004400	-3.60323800
H	2.07160000	2.42341400	-4.30112300
H	0.54232400	2.44767300	-3.38671500
H	1.13100200	0.92486100	-4.08223200
H	0.85376500	1.48429200	2.26018700
O	-1.46391500	2.58160600	-0.93500000
C	-0.97430100	2.98129900	0.35727200
C	-2.80761300	3.04624100	-1.10305100
C	-1.79695800	4.21139700	0.70899000
H	-1.15311300	2.16507900	1.06771700
H	0.10148300	3.14515500	0.26224200
C	-3.17250300	3.78953200	0.18496100
H	-2.82968600	3.70681000	-1.97706000
H	-3.46200700	2.19025500	-1.29243500
H	-1.42804400	5.08933200	0.16802200
H	-1.79176100	4.42936500	1.77923900
H	-3.85334700	4.62474900	0.00583000
H	-3.64239200	3.10057800	0.89505400
O	-1.73687400	-0.60150000	-2.35599900
C	-3.07877700	-0.37908200	-2.79935200
C	-1.58925800	-1.95782900	-1.89123500
C	-3.72676500	-1.75826200	-2.88914700
H	-3.59572000	0.23851200	-2.05580000
H	-3.04422600	0.15737100	-3.75161200
C	-3.00633100	-2.50561300	-1.76405500
H	-1.01255800	-2.51643800	-2.63879500
H	-1.03339600	-1.93484200	-0.95163700
H	-3.50802500	-2.22161300	-3.85703100
H	-4.81113900	-1.71621200	-2.76215700
H	-3.04089400	-3.59185400	-1.87346000
H	-3.43106800	-2.23674000	-0.79143400

9E

M06-2X SCF energy: -1945.15822807 a.u.
M06-2X enthalpy: -1944.44122800 a.u.
M06-2X free energy: -1944.51589600 a.u.
M06-2X SCF energy in solution: -1945.64437468 a.u.
M06-2X enthalpy in solution: -1944.92737461 a.u.
M06-2X free energy in solution: -1945.00204261 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	-1.07390400	-0.23963700	0.13767700
C	-1.43154300	-1.09047900	1.73986500
C	-1.87088100	-2.41178200	1.86730200
C	-1.16296200	-0.36463000	2.90599300
C	-2.04047600	-2.98774300	3.12547000
H	-2.09581200	-3.00023100	0.98248400
C	-1.32554900	-0.93638800	4.16292600
H	-0.83579100	0.66637100	2.81144800
C	-1.76705700	-2.25345100	4.27498900
H	-2.38652200	-4.01399200	3.20472800
H	-1.11634000	-0.35353400	5.05555500
H	-1.89967200	-2.70363200	5.25415900
C	-2.01759500	-1.24801200	-1.08783700
C	-1.38529600	-1.57499700	-2.29183000
C	-3.34644200	-1.64767000	-0.89978100
C	-2.06952600	-2.25861300	-3.29421600
C	-4.03209600	-2.33299600	-1.89848000
H	-3.85148800	-1.43227000	0.03832000
C	-3.39585200	-2.63408600	-3.10125400
H	-1.56293400	-2.50547900	-4.22250000
H	-5.06280200	-2.63403000	-1.73700600
H	-3.93084300	-3.16805500	-3.88081000
N	-1.34199800	1.32953800	0.15789800
N	0.51313500	-0.39459100	-0.18607800
C	1.29742800	-1.50766500	-0.18675400
C	2.72515900	-1.26028700	-0.28157100
C	0.90455400	-2.84554000	-0.14294400
C	3.65802800	-2.33106800	-0.30393300
C	1.84390300	-3.89656300	-0.16238500
H	-0.15031100	-3.08988900	-0.10498100
C	4.40362800	0.32011800	-0.43385500
C	5.02973400	-1.98781000	-0.39399300
C	3.19581500	-3.66875400	-0.23832200
H	1.47416200	-4.91754500	-0.11957200
C	5.40906100	-0.67123000	-0.45762600
H	4.66270200	1.37600100	-0.48413400
H	5.77022900	-2.78395900	-0.41228000
H	3.91131700	-4.48505100	-0.25317300
H	6.45247400	-0.38338000	-0.52680100
N	3.12129800	0.04001500	-0.35067400
Li	1.46810000	1.30879700	-0.32058800
C	-2.64103500	2.00168300	0.15549100
C	-3.61881500	1.45820200	1.21066100
H	-4.55598800	2.02680300	1.20633800
H	-3.17742300	1.52497800	2.21080900
H	-3.86498300	0.40739300	1.02799600
C	-3.30136000	1.94346600	-1.23382800
H	-2.61045400	2.34764300	-1.98289000
H	-4.22407700	2.53585700	-1.26027400
H	-3.54677100	0.91732500	-1.52093600
C	-2.40088500	3.48292300	0.48562300
H	-3.34552300	4.03854300	0.48333400
H	-1.73772500	3.94403700	-0.25368600
H	-1.94323200	3.59095900	1.47370700
H	-0.34297500	-1.29956700	-2.43048500
O	1.49847300	2.18777200	-2.04247900
C	0.49896100	3.21323800	-2.20142300
C	1.34725000	1.19472100	-3.07241000
C	-0.13510700	2.96414400	-3.56629500
H	-0.23997200	3.08092600	-1.40317900
H	0.99016600	4.18581900	-2.10908200
C	-0.03801900	1.44012900	-3.65740600
H	2.13514500	1.34481300	-3.82105400
H	1.46966400	0.21114500	-2.60978400
H	0.45129400	3.43719400	-4.36157800
H	-1.16002700	3.33916600	-3.61984200
H	-0.14534500	1.04845300	-4.67186600
H	-0.79902900	0.98339800	-3.01456200
O	1.94897900	2.38570200	1.20750500
C	2.08374400	1.48991800	2.32983500
C	1.17055800	3.53198200	1.57099600
C	1.49559000	2.23366200	3.52826500
H	1.52582700	0.57321800	2.10216200
H	3.14217400	1.24173000	2.44299600
C	0.46433900	3.15034800	2.86450700
H	1.84474300	4.38657500	1.71030800
H	0.47523700	3.74353100	0.75435500
H	2.26545300	2.82747000	4.03200600
H	1.05851900	1.54750400	4.25870800
H	0.19368300	4.01749000	3.47173300
H	-0.44268000	2.59330500	2.61302600

Dimer-A

M06-2X SCF energy: -2960.92407992 a.u.
M06-2X enthalpy: -2959.98714800 a.u.
M06-2X free energy: -2960.07964400 a.u.
M06-2X SCF energy in solution: -2961.60441956 a.u.
M06-2X enthalpy in solution: -2960.66748764 a.u.
M06-2X free energy in solution: -2960.75998364 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Li	-0.39709200	-0.17046400	-1.27889600
N	-1.98374400	-1.37265200	-1.26457100
N	-1.46120900	0.35151900	0.59180800
P	-2.57948600	-0.71922600	0.06882300
C	-2.33985800	-2.64345500	-1.90746500
C	-1.55157300	1.72457000	0.74877400
C	-2.86542400	-1.92570200	1.42506000
C	-4.21431900	0.07848600	-0.12899400
C	-3.84487500	-2.95568300	-1.90517700
C	-1.61004100	-3.81847200	-1.23456300
C	-1.88308200	-2.52923700	-3.36754900
C	-0.58538700	2.34598400	1.63298000
C	-2.40972600	2.59180300	0.07719500
C	-4.12029400	-2.46917600	1.71463900
C	-1.75103700	-2.40496100	2.12124500
C	-4.70574800	0.32343700	-1.41241200
C	-4.90486100	0.58032700	0.97887000
H	-4.03051700	-3.91461300	-2.40199700
H	-4.41573100	-2.18728100	-2.43352400
H	-4.23224700	-3.03393800	-0.88405300
H	-0.53218500	-3.63339300	-1.19078900
H	-1.77873200	-4.75137700	-1.78610300
H	-1.96868400	-3.96182800	-0.20955600
H	-2.05713600	-3.46332000	-3.91424100
H	-0.81611300	-2.28701700	-3.42169000
H	-2.43052800	-1.72329100	-3.86920200
C	-0.54771200	3.75760600	1.80186400
N	0.31263900	1.53771300	2.26186700
C	-2.36993700	3.98836900	0.26513200
H	-3.11446400	2.19693100	-0.64257800
C	-4.25566500	-3.46565100	2.68037700
H	-5.00089000	-2.11605200	1.18499500
C	-1.88037700	-3.40491600	3.07835700
H	-0.76322200	-2.01283200	1.89328300
C	-5.88274200	1.04692500	-1.58955300
H	-4.13868800	-0.03570900	-2.26733800
C	-6.07948000	1.30496800	0.80305000
H	-4.51419700	0.41237400	1.98004300
C	0.44712300	4.28480300	2.66158300
C	-1.46777300	4.58023600	1.11086700
C	1.22957600	2.06285900	3.04232500
H	-3.06872800	4.60071800	-0.29842900
C	-3.13792100	-3.93600700	3.36201200
H	-5.23776200	-3.87560400	2.89561000
H	-0.99944000	-3.77265000	3.59700500
C	-6.56970800	1.53677100	-0.48130500
H	-6.26097000	1.23267400	-2.59031400
H	-6.60914300	1.69569300	1.66636500
C	1.33469200	3.44939500	3.28698900
H	0.49571300	5.36169900	2.80488600
H	-1.42843600	5.65719900	1.24411500
H	1.92911900	1.36328400	3.49662600
H	-3.24356500	-4.71606500	4.10970400
H	-7.48546400	2.10419800	-0.61736700
H	2.11005000	3.82785400	3.94401500
Li	0.39791600	-0.16905200	1.27654400
N	1.98591700	-1.36925700	1.26529500
N	1.46190500	0.35135200	-0.59444400
P	2.58071400	-0.71801400	-0.06955400
C	2.34172900	-2.63929300	1.90984300
C	1.55060100	1.72467700	-0.74979200
C	4.21531800	0.08078700	0.12575400
C	2.86623200	-1.92685600	-1.42369200
C	3.84653000	-2.95254900	1.90658600
C	1.61041700	-3.81477400	1.23939600
C	1.88623100	-2.52258800	3.37012500
C	0.58366000	2.34594600	-1.63330000
C	2.40787200	2.59217700	-0.07739900
C	4.90374400	0.58283500	-0.98334200
C	4.70880800	0.32607900	1.40830000
C	1.75127800	-2.40954700	-2.11661200
C	4.12149200	-2.46865000	-1.71463700
H	4.03199100	-3.91105200	2.40429700
H	4.41837600	-2.18395600	2.43359100
H	4.23293100	-3.03216900	0.88518500
H	0.53273800	-3.62857700	1.19578400
H	1.77836700	-4.74685400	1.79255300
H	1.96846900	-3.96036600	0.21450500
H	2.06045300	-3.45584900	3.91816200
H	0.81935200	-2.27999500	3.42471700
H	2.43431200	-1.71599700	3.87003700
C	0.54451900	3.75770800	-1.80076200
N	-0.31362200	1.53739200	-2.26290300
C	2.36658400	3.98887500	-0.26390700
H	3.11311200	2.19731500	0.64189300
C	6.07838300	1.30793100	-0.80960200
H	4.51140700	0.41463400	-1.98382500
C	5.88584600	1.05002200	1.58335600
H	4.14327000	-0.03305100	2.26423600
C	1.88056600	-3.41103400	-3.07212000
H	0.76314900	-2.01909400	-1.88700400
C	4.25676000	-3.46667800	-2.67880200
H	5.00244000	-2.11311000	-1.18721500
C	-0.45089900	4.28477100	-2.65989500
C	1.46374100	4.58062500	-1.10900700
C	-1.23113800	2.06242700	-3.04276200
H	3.06474800	4.60140000	0.30023600
C	6.57073900	1.54000400	0.47389800
H	6.60639600	1.69881400	-1.67385600
H	6.26568400	1.23604800	2.58345500
C	3.13854100	-3.94028600	-3.35736500
H	0.99927300	-3.78150100	-3.58821000
H	5.23916000	-3.87530800	-2.89516200
C	-1.33766500	3.44909800	-3.28606500
H	-0.50057300	5.36176100	-2.80210900
H	1.42321800	5.65767800	-1.24115700
H	-1.92999700	1.36263900	-3.49778800
H	7.48650800	2.10779500	0.60834700
H	3.24411200	-4.72154000	-4.10381700
H	-2.11345700	3.82741500	-3.94266000

Dimer-B

M06-2X SCF energy:	-2960.91977354 a.u.
M06-2X enthalpy:	-2959.98336800 a.u.
M06-2X free energy:	-2960.07602800 a.u.
M06-2X SCF energy in solution:	-2961.60057944 a.u.
M06-2X enthalpy in solution:	-2960.66417390 a.u.
M06-2X free energy in solution:	-2960.75683390 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Li	0.45049800	0.09840800	1.21903800
N	1.83049800	-1.31062800	1.43035200
N	1.51103700	0.18858000	-0.67035800
P	2.53721600	-0.84963900	0.07130900
C	2.19045200	-2.43965800	2.29309500
C	1.88053900	1.51181400	-0.92130500
C	2.91178400	-2.22982900	-1.06762200
C	4.12309700	0.03734500	0.29955400
C	3.69809700	-2.53065000	2.57772900
C	1.72850900	-3.77925400	1.69186600
C	1.47261700	-2.21256200	3.63001200
C	1.63806300	2.51542000	0.08382500

C	2.39242700	1.93180200	-2.13472300
C	4.14242500	-2.88788700	-1.13043200
C	1.83746900	-2.71565900	-1.81912300
C	4.33090000	0.69083600	1.51721000
C	5.04352300	0.21653000	-0.73827200
H	3.91180300	-3.37394200	3.24443100
H	4.06544900	-1.61562100	3.05203200
H	4.26598500	-2.68720200	1.65374600
H	0.67790600	-3.72487100	1.39063400
H	1.84364300	-4.59163100	2.42018100
H	2.31615200	-4.03793100	0.80530400
H	1.68539400	-3.02267200	4.33701400
H	0.38826900	-2.15637400	3.48617200
H	1.80344500	-1.26625800	4.07302700
C	1.89526000	3.88442300	-0.19425200
N	1.12199000	2.10813700	1.28065400
C	2.65790200	3.29434200	-2.40298200
H	2.57704700	1.17779000	-2.89530800
C	4.29457600	-4.01435700	-1.93790200
H	4.98703800	-2.52278500	-0.55146500
C	1.98618400	-3.84286700	-2.61920600
H	0.87654200	-2.20932900	-1.75291800
C	5.45532600	1.48996400	1.70547000
H	3.59452500	0.56977800	2.30827400
C	6.17047200	1.01153100	-0.54871500
H	4.87753000	-0.26640000	-1.69822000
C	1.60495100	4.82453600	0.82465400
C	2.41097600	4.25981100	-1.46097500
C	0.86985400	3.01270700	2.20110900
H	3.05942400	3.57299700	-3.37316000
C	3.21835100	-4.49347800	-2.67996700
H	5.25498100	-4.51889900	-1.98408800
H	1.13940600	-4.21451300	-3.19026500
C	6.37843900	1.64572600	0.67421900
H	5.61093000	1.99153400	2.65586400
H	6.88392000	1.14043500	-1.35703200
C	1.09850500	4.39576400	2.02316400
H	1.78668600	5.88013200	0.63666000
H	2.60568400	5.30946500	-1.66264700
H	0.44136300	2.64853600	3.13249200
H	3.33843600	-5.37399700	-3.30388400
H	7.25746900	2.26633900	0.82065700
H	0.85671900	5.08782100	2.82214600
Li	-0.45048700	0.09823400	-1.21890700
N	-1.83071900	-1.31052200	-1.43035800
N	-1.51103200	0.18867700	0.67030100
P	-2.53737300	-0.84941400	-0.07132600
C	-2.19077600	-2.43954600	-2.29306300
C	-1.88036000	1.51196000	0.92125500
C	-4.12313800	0.03778200	-0.29954300
C	-2.91209300	-2.22954600	1.06762200
C	-3.69842700	-2.53042700	-2.57769800
C	-1.72895300	-3.77914800	-1.69176000
C	-1.47290400	-2.21258200	-3.62998300
C	-1.63773200	2.51553100	-0.08387600
C	-2.39219000	1.93201800	2.13467200
C	-5.04355200	0.21702400	0.73828300
C	-4.33084100	0.69137800	-1.51716100
C	-1.83782500	-2.71546500	1.81913200
C	-4.14278700	-2.88750700	1.13041300
H	-3.91220900	-3.37376700	-3.24431500
H	-4.06568800	-1.61541300	-3.05209700
H	-4.26633500	-2.68683100	-1.65370100
H	-0.67832700	-3.72485600	-1.39059000
H	-1.84421500	-4.59156700	-2.42000700
H	-2.31657800	-4.03768800	-0.80514500
H	-1.68574400	-3.02270800	-4.33694800
H	-0.38855200	-2.15648700	-3.48612800
H	-1.80363500	-1.26626900	-4.07304900
C	-1.89471500	3.88457200	0.19420800
N	-1.12172400	2.10816600	-1.28070200
C	-2.65746100	3.29459900	2.40293300
H	-2.57692900	1.17803200	2.89525500
C	-6.17040800	1.01216400	0.54875500
H	-4.87762700	-0.26597800	1.69820700
C	-5.45517300	1.49064500	-1.70539100
H	-3.59445800	0.57029600	-2.30821400
C	-1.98663900	-3.84266100	2.61921300
H	-0.87686200	-2.20920300	1.75293200
C	-4.29503700	-4.01396600	1.93788000
H	-4.98736300	-2.52233900	0.55143300
C	-1.60425000	4.82464400	-0.82469200
C	-2.41037800	4.26003300	1.46093300
C	-0.86944500	3.01269900	-2.20115300
H	-3.05894500	3.57331300	3.37310900
C	-6.37828500	1.64644900	-0.67414700
H	-6.88385100	1.14110700	1.35707000
H	-5.61070200	1.99229400	-2.65575600
C	-3.21886000	-4.49317300	2.67995700
H	-1.13989800	-4.21437600	3.19028200
H	-5.25548200	-4.51843300	1.98405100
C	-1.09787000	4.39579300	-2.02320200
H	-1.78581200	5.88026800	-0.63669200
H	-2.60492300	5.30971700	1.66260900
H	-0.44101500	2.64846200	-3.13253800
H	-7.25724100	2.26717300	-0.82056200
H	-3.33902000	-5.37368500	3.30386900
H	-0.85596800	5.08781400	-2.82217900

Dimer-C

M06-2X SCF energy: -2960.92667495 a.u.
M06-2X enthalpy: -2959.98969400 a.u.
M06-2X free energy: -2960.08226800 a.u.
M06-2X SCF energy in solution: -2961.60767953 a.u.
M06-2X enthalpy in solution: -2960.67069858 a.u.
M06-2X free energy in solution: -2960.76327258 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Li	-0.82844900	1.53658300	-0.28271700
N	-0.85409900	-1.71264700	-0.76744100
N	-2.42332100	0.39063500	-0.04417900
P	-2.17016200	-1.21869500	-0.00209900
C	-0.71672000	-1.82379700	-2.23260100
C	-3.51535500	1.14076300	0.29475600
C	-3.70154800	-2.08231900	-0.52080600
C	-1.85267900	-1.74925800	1.72075100
C	-3.41526000	2.56477300	0.03110400
C	-4.70779000	0.70338500	0.87492900
C	-3.96564600	-3.38390700	-0.08879100
C	-4.56320300	-1.47814500	-1.44293600
C	-1.02699400	-2.85077700	1.97508900
C	-2.35448600	-1.01215400	2.79834100
C	-4.50453200	3.43542900	0.30669500
N	-2.23802300	3.03068100	-0.47640900
C	-5.77662100	1.58153100	1.14433800
H	-4.82665900	-0.34792100	1.11629200
C	-5.06829800	-4.07834600	-0.57953800
H	-3.30374900	-3.85874500	0.63124100
C	-5.66344900	-2.17288000	-1.93516500
H	-4.36614700	-0.46129600	-1.77312800
C	-0.68735600	-3.19487300	3.28181100
H	-0.64671100	-3.41818100	1.12890700
C	-2.02354100	-1.36319300	4.10435700

H	-2.98477900	-0.14650300	2.61701700
C	-4.33011000	4.80952100	0.01032200
C	-5.70074200	2.92260000	0.86501600
C	-2.11607900	4.31474700	-0.73382200
H	-6.68103800	1.17235600	1.58585200
C	-5.91515200	-3.47484600	-1.50580200
H	-5.26536000	-5.09069900	-0.24017300
H	-6.32619300	-1.69818500	-2.65222500
C	-1.18370600	-2.44810100	4.34761200
H	-0.03135800	-4.04068300	3.46732600
H	-2.40775900	-0.77630800	4.93309400
C	-3.14517900	5.25496200	-0.51339300
H	-5.14881800	5.49716100	0.20784700
H	-6.52599600	3.59644200	1.07292900
H	-1.15788600	4.64309600	-1.13153800
H	-6.77358500	-4.01707900	-1.89066700
H	-0.91416200	-2.70930400	5.36640800
H	-2.98220600	6.30082000	-0.74885200
C	0.74741100	-2.18990200	-2.50563600
H	0.98627300	-3.15913800	-2.05190400
H	0.93945400	-2.25366600	-3.58281500
C	-1.58535600	-2.95225200	-2.81466000
H	-1.43451700	-3.87076900	-2.23732000
H	-2.65041100	-2.70918700	-2.79809500
H	-1.30255700	-3.14571200	-3.85599100
C	-1.04078900	-0.50599400	-2.95292800
H	-0.40411000	0.30441400	-2.57559300
H	-0.86340300	-0.59615500	-4.03134700
H	-2.08593600	-0.21625400	-2.79878000
Li	0.82840600	-1.53680400	0.28273000
N	2.42313800	-0.39066400	0.04388000
N	2.23806600	-3.03074800	0.47602300
P	2.17010800	1.21870500	0.00208400
C	3.51525100	-1.14069200	-0.29502300
C	3.41528400	-2.56470900	-0.03142000
C	2.11622900	-4.31483700	0.73337900
N	0.85403700	1.71261700	0.76742700
C	1.85272500	1.74953700	-1.72070700
C	3.70154800	2.08206900	0.52098600
C	4.70766100	-0.70317600	-0.87514200
C	4.50465800	-3.43524800	-0.30696500
C	3.14543700	-5.25494300	0.51298700
H	1.15803600	-4.64328600	1.13101700
C	0.71651400	1.82348100	2.23260100
C	2.35435100	1.01243400	-2.79838100
C	1.02741000	2.85136000	-1.97492100
C	4.56316100	1.47761300	1.44297000
C	3.96566700	3.38378000	0.08935400
C	5.77660100	-1.58119800	-1.14450500
H	4.82642800	0.34814900	-1.11648600
C	4.33035700	-4.80937000	-0.01064000
C	5.70084700	-2.92228500	-0.86520600
H	2.98252900	-6.30082600	0.74837800
C	-0.74769600	2.18929100	2.50562500
C	1.04069300	0.50554500	2.95267700
C	1.58487200	2.95196700	2.81498100
C	2.02352400	1.36374000	-4.10435000
H	2.98438300	0.14656800	-2.61716100
C	0.68788600	3.19573200	-3.28160500
H	0.64735300	3.41881300	-1.12867400
C	5.66337400	2.17220900	1.93545800
H	4.36606300	0.46067800	1.77286900
C	5.06828800	4.07808000	0.58036700
H	3.30378100	3.85883200	-0.63054600
H	6.68099400	-1.17191500	-1.58596500
H	5.14914700	-5.49691600	-0.20813500
H	6.52618300	-3.59604400	-1.07306600
H	-1.41786500	1.43507800	2.08151800
H	-0.93980000	2.25269100	3.58281600
H	-0.98667900	3.15864000	2.05220000
H	0.40437400	-0.30491700	2.57484200
H	2.08597200	0.21613200	2.79880300
H	0.86290200	0.59530700	4.03106300
H	1.43415400	3.87048300	2.23760500
H	1.30167600	3.14537900	3.85621300
H	2.64994900	2.70899500	2.79880700
C	1.18401400	2.44893100	-4.34748800
H	2.40759300	0.77685000	-4.93315400
H	0.03213700	4.04175800	-3.46700800
C	5.91509000	3.47430500	1.50649600
H	6.32608800	1.69731600	2.65241700
H	5.26538300	5.09052500	0.24129700
H	0.91456400	2.71033500	-5.36625700
H	6.77350200	4.01642600	1.89156700
H	1.41771100	-1.43564500	-2.08180500

Dimer-D

M06-2X SCF energy: -2960.91879996 a.u.
M06-2X enthalpy: -2959.98153700 a.u.
M06-2X free energy: -2960.07541600 a.u.
M06-2X SCF energy in solution: -2961.60042130 a.u.
M06-2X enthalpy in solution: -2960.66315834 a.u.
M06-2X free energy in solution: -2960.75703734 a.u.

Cartesian coordinates

ATOM	X	Y	Z
Li	0.26054400	-1.68689800	1.22874000
N	1.67870500	1.28192300	1.51330600
N	1.99135600	-1.14781900	0.38825900
P	2.48429500	0.41782100	0.43275500
C	2.02240800	1.44277900	2.93769900
C	2.35851300	-2.07823400	-0.55711000
C	4.30499500	0.47798800	0.64684100
C	2.17859600	1.19807200	-1.20182400
C	1.64183800	-3.33841400	-0.53261100
C	3.32625300	-1.94109900	-1.55176600
C	4.99594400	1.69040100	0.53594500
C	5.01116100	-0.68161900	0.97664300
C	0.84840500	1.43126600	-1.56743400
C	3.18677100	1.53865600	-2.10925700
C	1.92342900	-4.36256800	-1.47483400
N	0.66146000	-3.48004700	0.40124000
C	3.59639900	-2.96742000	-2.48111800
H	3.89729800	-1.02273400	-1.62196500
C	6.37058200	1.74095000	0.74580800
H	4.44890100	2.59823600	0.28981300
C	6.38670200	-0.63066200	1.19206500
H	4.47353200	-1.62169000	1.06960200
C	0.52701800	2.01599800	-2.78820900
H	0.03912300	1.14258500	-0.90416500
C	2.86959300	2.12225500	-3.33429800
H	4.22890800	1.35140800	-1.86816500
C	1.15120700	-5.54767100	-1.39489300
C	2.92295200	-4.16255100	-2.45880500
C	-0.04676400	-4.58645400	0.43432600
H	4.36255300	-2.79381300	-3.23156500
C	7.06657900	0.57861600	1.07488200
H	6.89790900	2.68591400	0.65779000
H	6.92670600	-1.53622900	1.45072100
C	1.54245100	2.36843800	-3.67392500
H	-0.51730000	2.18582400	-3.03997600
H	3.66605900	2.38264700	-4.02504500
C	0.16825000	-5.66738700	-0.44762100
H	1.34729900	-6.35011300	-2.10192500

H	3.13220800	-4.94861800	-3.17778500
H	-0.83358800	-4.63220000	1.18441400
H	8.13887000	0.61770100	1.24138400
H	1.29989700	2.82466700	-4.62895200
H	-0.44429300	-6.55883200	-0.37151900
Li	-0.25101900	1.66651400	1.26002100
N	-1.67065900	-1.30002000	1.48968700
N	-1.98502100	1.15019800	0.41997500
P	-2.48088600	-0.41478200	0.42858800
C	-2.05559400	-1.58186900	2.88452500
C	-2.35367800	2.10296300	-0.50358600
C	-2.17964000	-1.14925800	-1.23005700
C	-4.30268900	-0.47195200	0.63681300
C	-1.62313900	3.35482500	-0.46469200
C	-3.33531100	1.99606900	-1.48797400
C	-0.85210800	-1.40392800	-1.59171200
C	-3.18567800	-1.43168400	-2.15970900
C	-4.99288300	0.67914000	1.02598000
C	-5.01262000	-1.66421600	0.45340000
C	-1.90167500	4.39819800	-1.38624300
N	-0.63069900	3.46851700	0.45960600
C	-3.60424800	3.04218800	-2.39570300
H	-3.91948200	1.08709300	-1.56714600
C	-0.53213400	-1.95205900	-2.82961400
H	-0.04249800	-1.15770900	-0.91221400
C	-2.87036900	-1.97948400	-3.40173800
H	-4.22569300	-1.22799400	-1.92302100
C	-6.36998000	0.63853800	1.23236100
H	-4.44089000	1.60432200	1.17049200
C	-6.38901800	-1.70431900	0.65466100
H	-4.48032200	-2.56530700	0.15601400
C	-1.11114900	5.57047000	-1.29703700
C	-2.91537300	4.22800100	-2.36133900
C	0.09586600	4.56255000	0.50092300
H	-4.38180200	2.89119300	-3.13929200
C	-1.54648300	-2.24685600	-3.73742600
H	0.51027100	-2.13839300	-3.07758300
H	-3.66601100	-2.19490200	-4.10873800
C	-7.06824900	-0.55144000	1.04566800
H	-6.89707000	1.53731100	1.53718800
H	-6.93073300	-2.63411300	0.51054300
C	-0.11374800	5.66023000	-0.36149800
H	-1.30433600	6.38701800	-1.98857700
H	-3.12281800	5.02878100	-3.06446200
H	0.89369000	4.58209000	1.24043300
H	-1.30537800	-2.67460800	-4.70589700
H	-8.14192400	-0.58250400	1.20475600
H	0.51355200	6.54089900	-0.28024700
C	2.99307900	2.61568500	3.14652700
H	3.98071600	2.38736800	2.73891800
H	2.61028600	3.51022000	2.64397200
H	3.11168700	2.83768300	4.21383000
C	2.61898600	0.18673600	3.59144200
H	2.70728600	0.32076300	4.67573300
H	1.99591900	-0.69178500	3.39838200
H	3.61882000	-0.02175400	3.19929400
C	0.71098500	1.79704000	3.65407600
H	0.86507600	1.96124500	4.72569400
H	0.28063200	2.71945000	3.23768800
H	-0.01769600	0.98555500	3.54267100
C	-0.76437700	-1.98375700	3.61268000
H	-0.04512400	-1.15719500	3.60843700
H	-0.95760600	-2.24974200	4.65714100
H	-0.30365400	-2.85816100	3.13046500
C	-2.68210200	-0.38652900	3.61922900
H	-2.06004900	0.50771600	3.51584700
H	-3.67228600	-0.15393500	3.21686700
H	-2.79990100	-0.60795100	4.68627700
C	-3.01930700	-2.77620900	2.97249000
H	-2.61912500	-3.62100000	2.40204000
H	-3.15516300	-3.09005100	4.01432700
H	-4.00201600	-2.52254700	2.56885600