SUPPORTING INFORMATION

Understanding the directed ortho lithiation of (*R*)-$Ph_2P(=NCO_2Me)NHCH(Me)Ph$. NMR spectroscopic and computational study of the structure of the *N*-lithiated species

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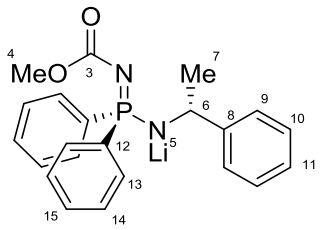
Table S1. NMR parameters of monolithiated intermediate **I** measured on a 0.3 M sample in THF-d_8 at -20 ºC (δ in ppm, *J* in Hz). Coupling constants are given in parentheses.



Position	δ ^{31}P	δ ^{15}N	δ ^{13}C	δ ^{1}H	δ ^{7}Li
1	19.0				
2		-256.5 ($^{1}J_{PN}$ 16)			
3			164.09		
4			53.44	3.68	
5		-320.1 ($^{1}J_{PN}$ 36)			0.98
6			55.35	4.22 ($^{3}J_{HH}$ 20/$^{3}J_{PH}$ 6.4)	
7			28.64 ($^{3}J_{PC}$ 8.7)	1.32 ($^{3}J_{HH}$ 20)	
8			151.53 ($^{3}J_{PC}$ 12.1)	-	
9			126.50	7.44 ($^{3}J_{HH}$ 7.3)	
10			127.32	7.17 ($^{3}J_{HH}$ 7.3)	
11			124.81	7.06 ($^{3}J_{HH}$ 7.3)	
12			135.60 ($^{1}J_{PC}$ 109.9)	-	
12'			137.23 ($^{1}J_{PC}$ 117.8)	-	
13			132.07 ($^{2}J_{PC}$ 8.1)	7.66	
13'			132.29 ($^{2}J_{PC}$ 8.9)	7.79	
14			127.03 ($^{3}J_{PC}$ 11.5)	7.20	
14'			127.48 ($^{3}J_{PC}$ 11.1)	7.38	
15			129.47	7.28 ($^{3}J_{HH}$ 7.1)	
15'			129.67	7.38	

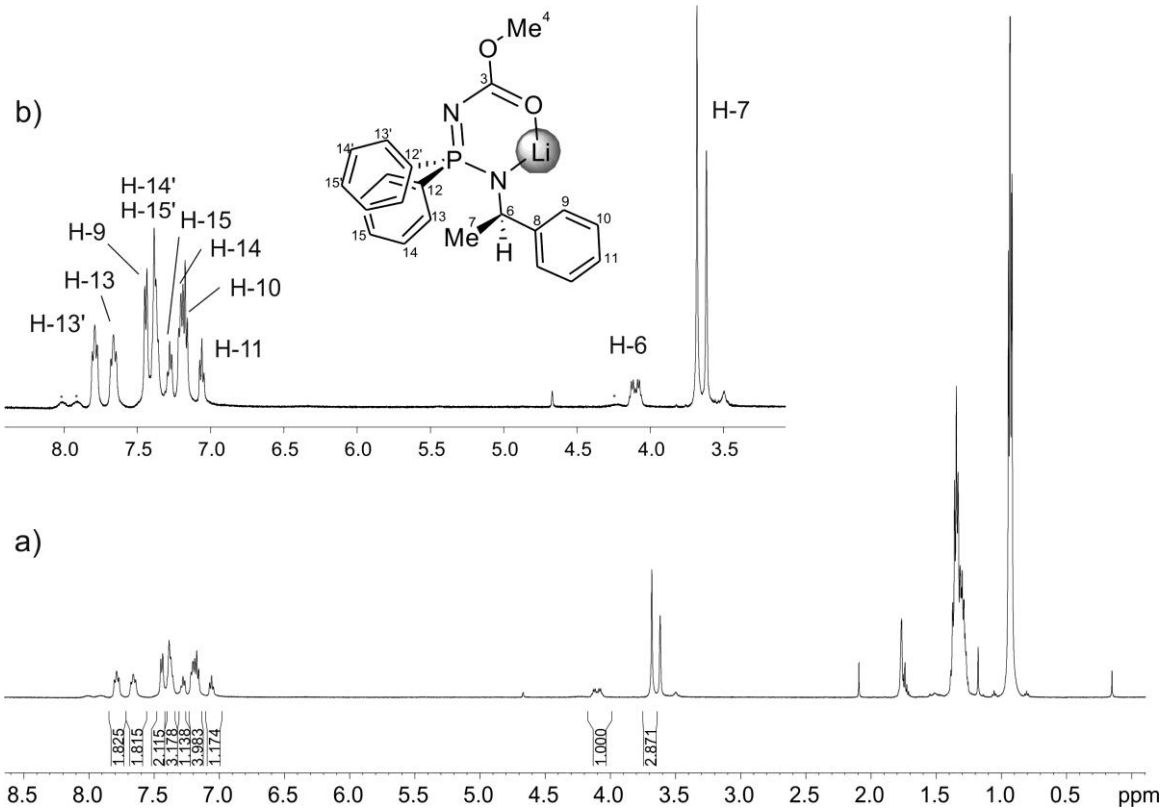


Figure S1. (a) Full spectrum (b) expansion of the ^{1}H NMR spectrum of species **I** (0.3 M, THF-d_8) measured at -20 ºC.

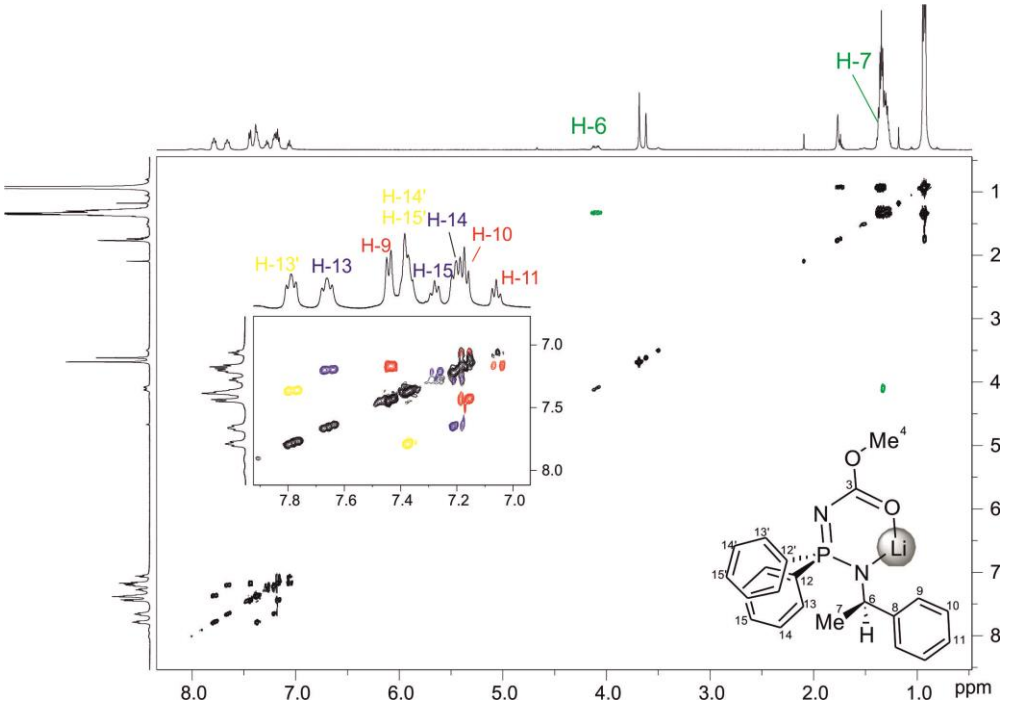


Figure S2. 2D COSY45 spectrum of species **I** (0.05 M, THF-d_8) measured at -20 ºC. An expansion highlighting the three different spin-systems observed for aromatic protons is included.

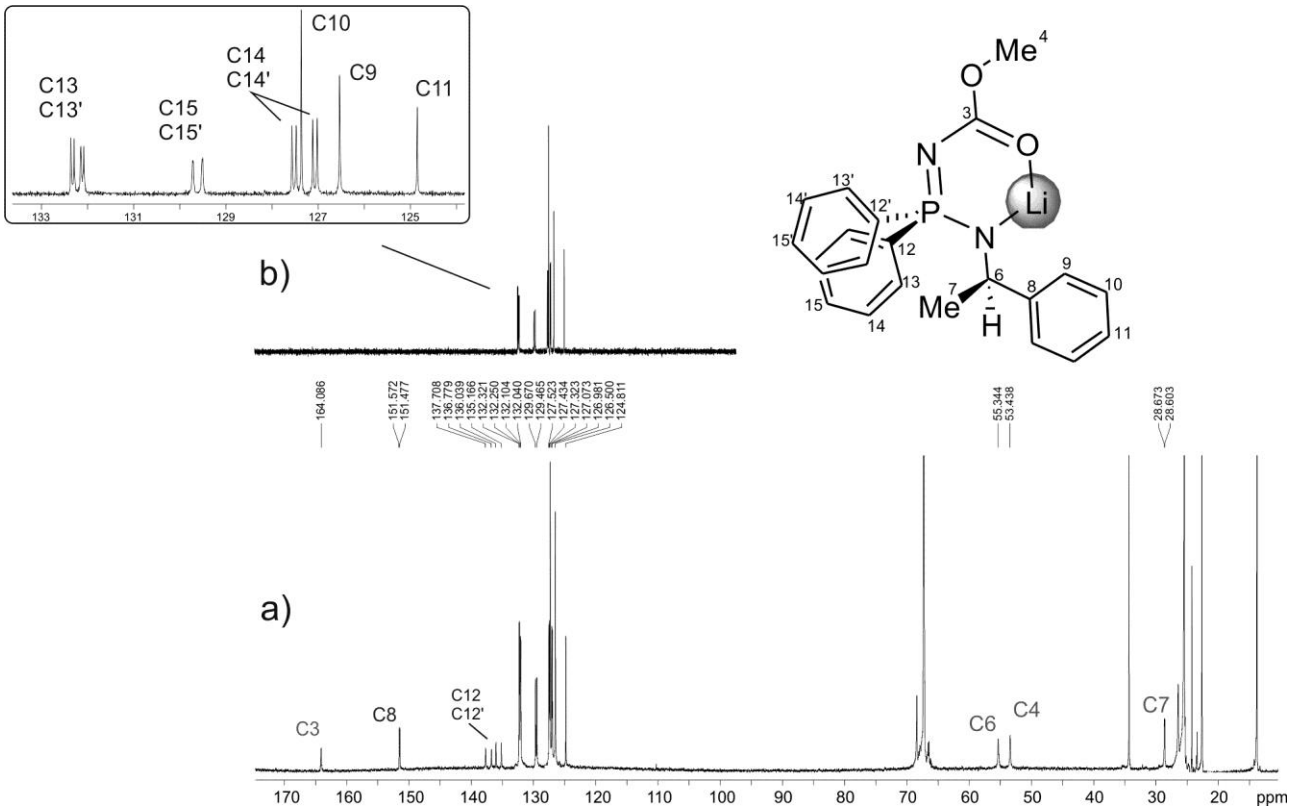


Figure S3. (a) ^{13}C NMR and (b) DEPT135 NMR spectra of species **I** (0.3 M, THF-d_8) measured at -20 ºC.

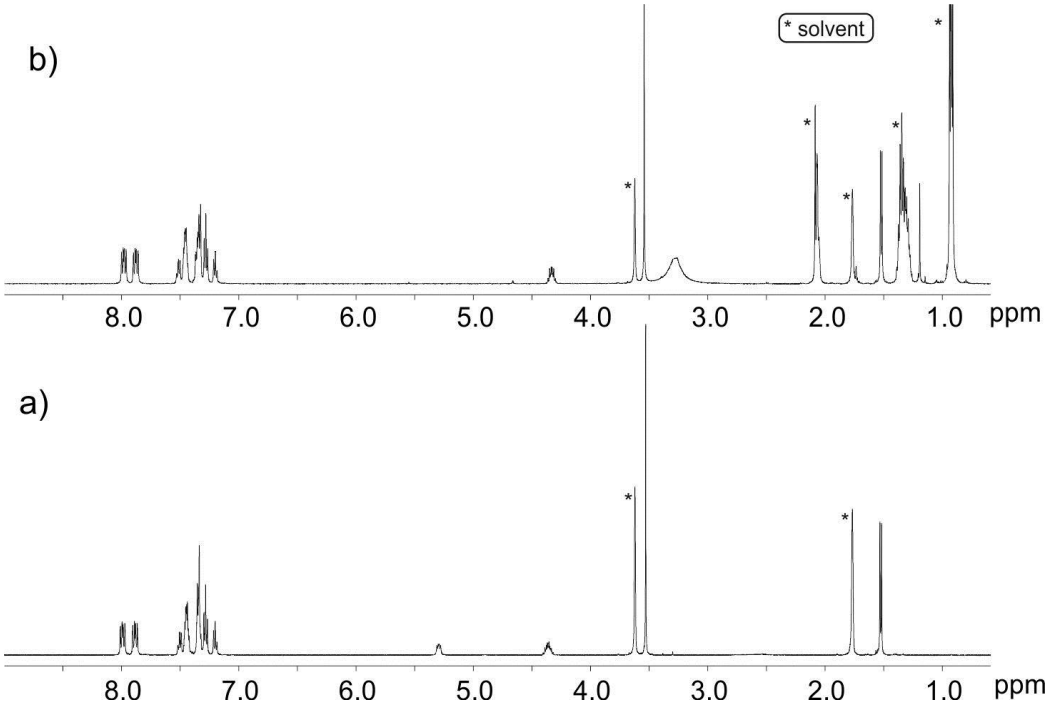


Figure S4. (a) ^{1}H NMR for the aminophosphazene **13** in THF-d_8. (b) ^{1}H NMR measured after quenching with CD_3OD the monolithiated species **I** in THF-d_8.

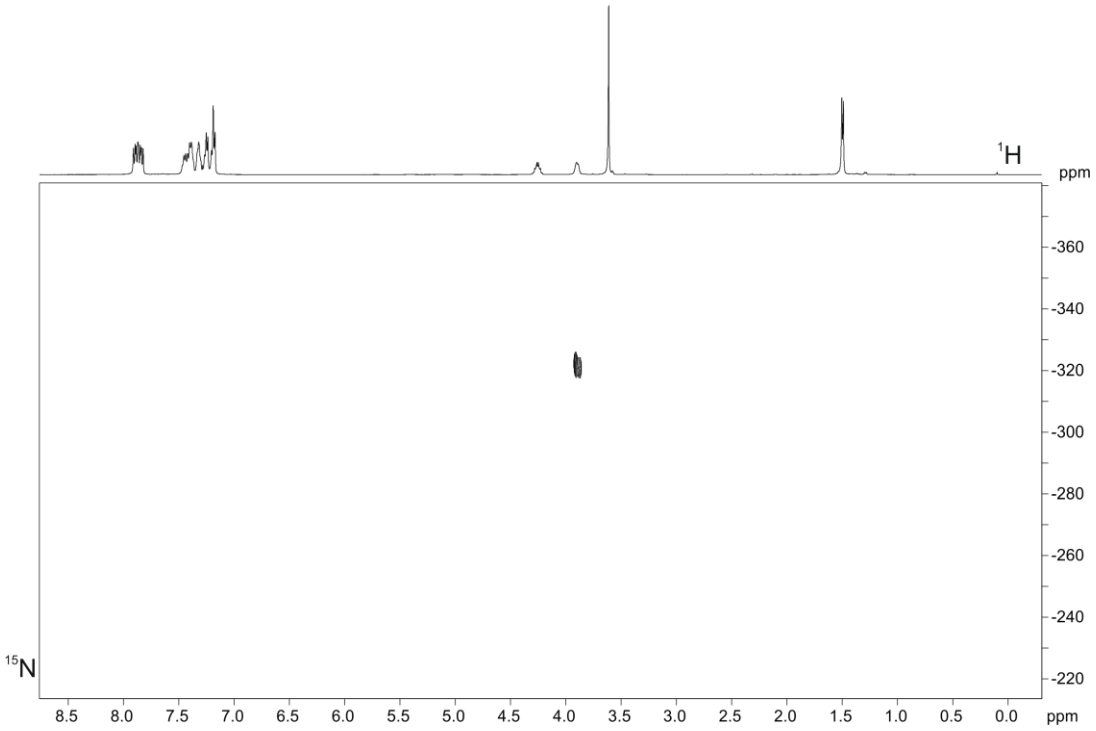


Figure S5. ^{1}H,^{15}N HMQC NMR spectrum of **13** (0.3 M, THF-d_8) measured at 25 ºC.

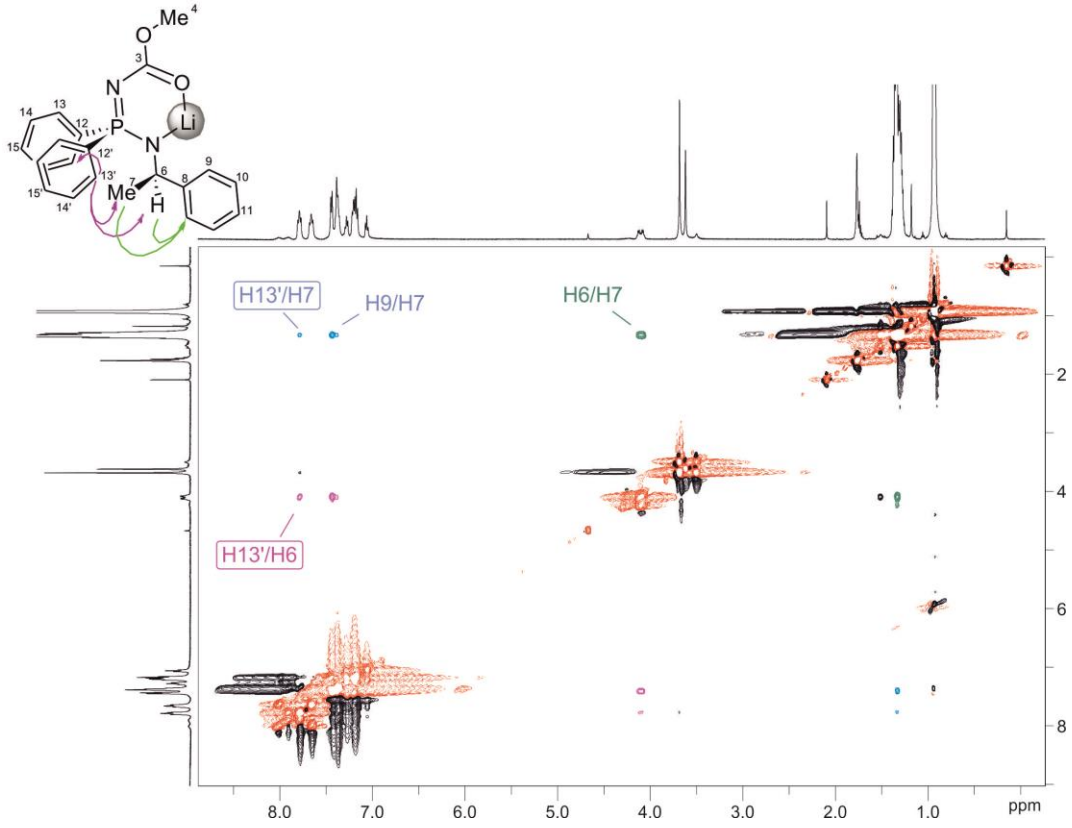


Figure S6. 2D ROESY spectrum of species **I** (0.05 M, THF-d_8) measured at -20 ºC. Key NOE correlations for conformational assignment are highlighted.

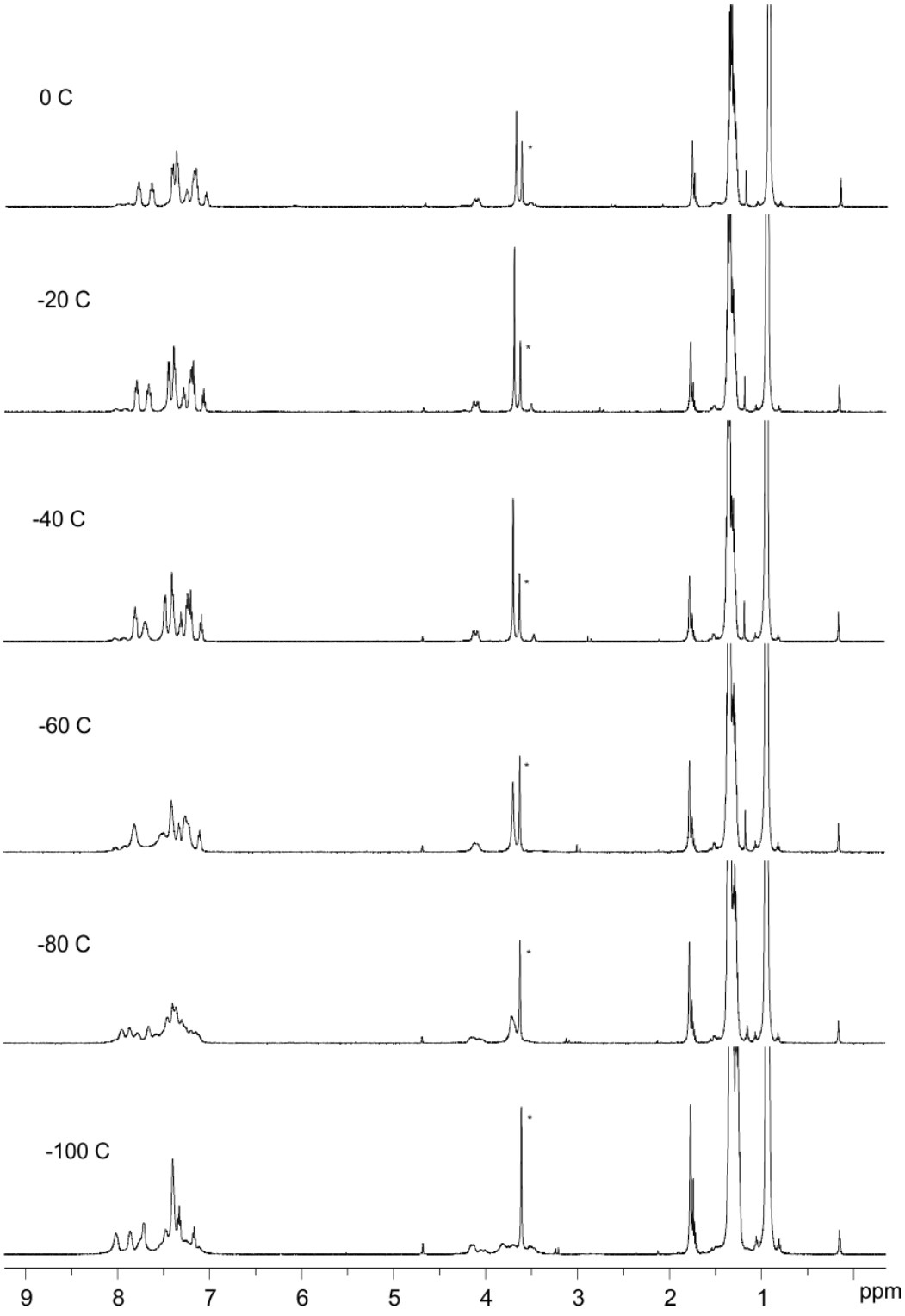


Figure S7. Variable-temperature ^{1}H NMR spectra of the monolithiated species **I** (0.05 M, THF-d_8).

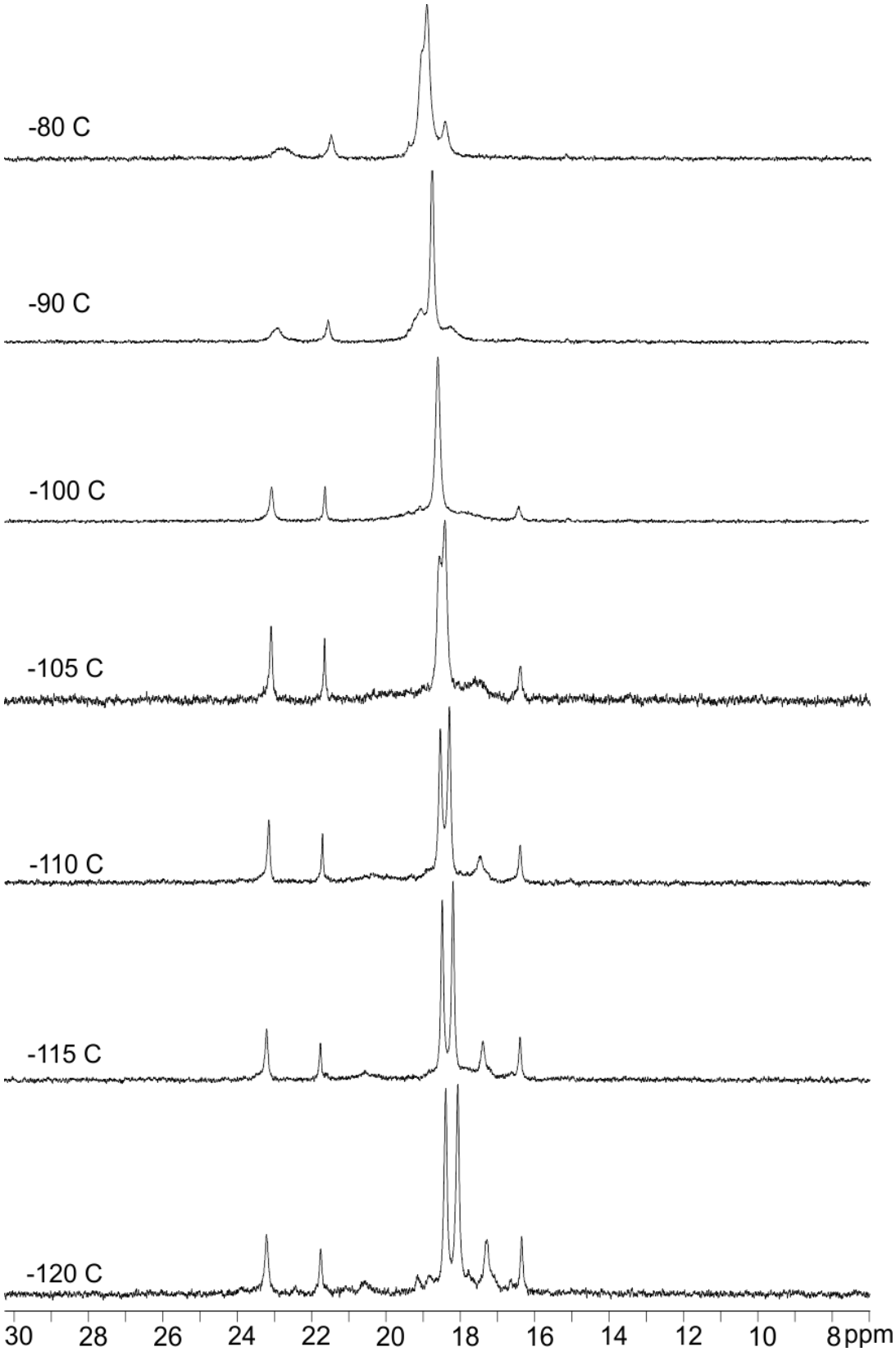


Figure S8. Variable-temperature ^{31}P NMR spectra of the monolithiated species **I** (0.05 M, THF-d_8).

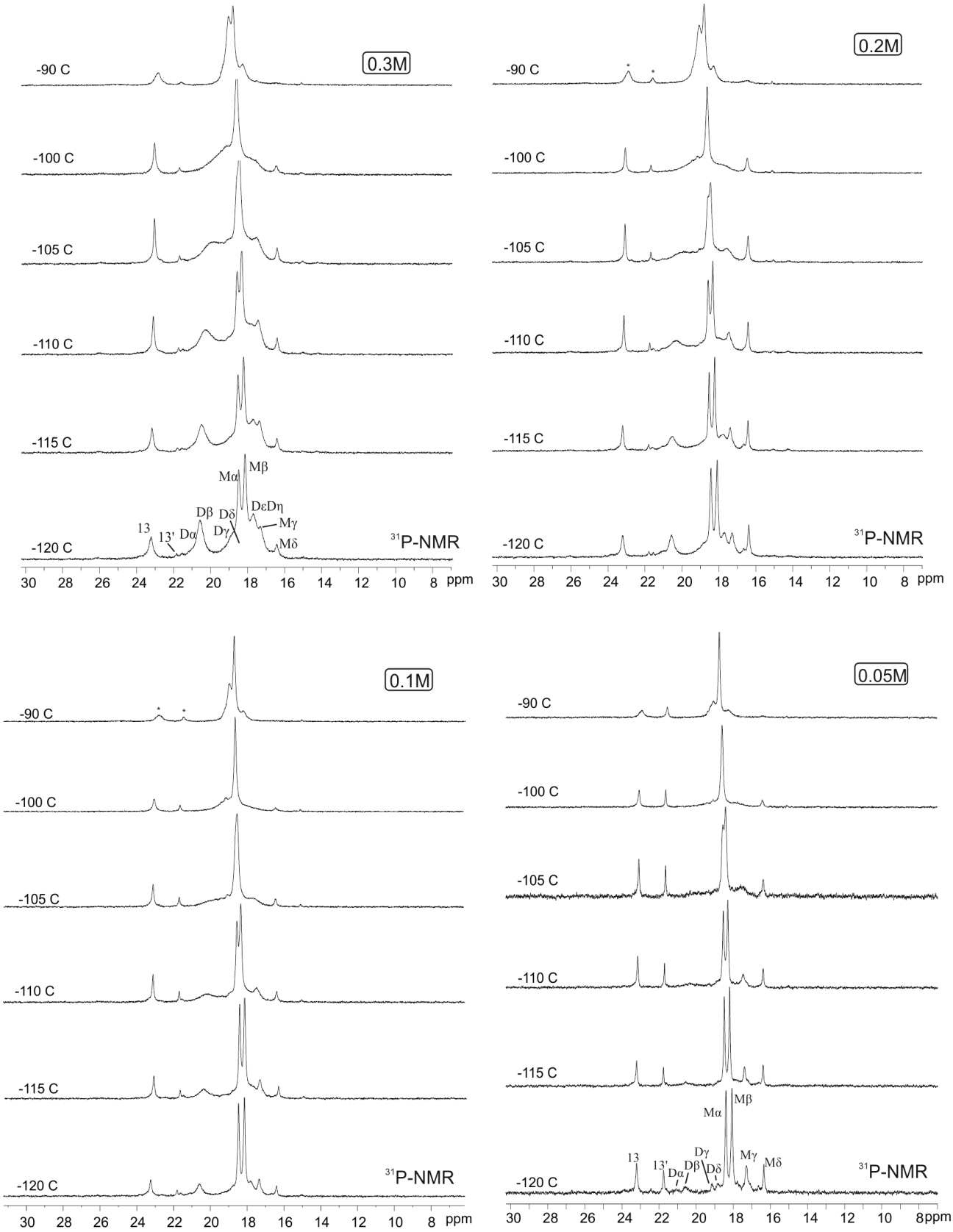


Figure S9. Variable-temperature and variable-concentration ^{31}P NMR spectra of the monolithiated species **I** (THF-d_8).

Monomer-Dimer equilibrium. Concentration and relative integrals obtained from ^{31}P NMR spectra of **I** measured in the concentration range of 0.05 M to 0.3 M at –120 ºC in THF-d_8 are shown below. The ^{31}P NMR spectra were acquired using the inverse-gated pulse sequence, with a pulse width of 15º and a recovery delay of 3 s. See the main text for the assignment of monomers ($\mathbf{M}_{\alpha,\beta}$), mixed monomers-LiBr ($\mathbf{M}_{\gamma,\delta}$) and dimers ($\mathbf{D}_{\alpha\text{-}\delta}$). Concentration values were obtained through integration of the corresponding signals using the deconvolution algorithm present in MNOVA (MestReNova, ver. 8.1.1)

Sample	[D][a]	[M][b]	[M·LiBr][c]	[M+M·LiBr]	log[D]	log[M]	log[M+M·LiBr]
0.3 M	0.12475	0.13638	0.03888	0.17525	-0.9040	-0.8653	-0.7563
0.2 M	0.06998	0.09633	0.03369	0.13002	-1.1550	-1.0162	-0.8860
0.1 M	0.03079	0.05839	0.01081	0.0692086	-1.5116	-1.2336	-1.1598
0.05 M	0.01059	0.02827	0.01114	0.03941	-1.9752	-1.5487	-1.4044

a. $D = (D_\alpha + D_\beta + D_\gamma + D_\delta + D_\varepsilon + D_\zeta)$

b. $M = (M_\alpha + M_\beta)$

c. $M{\cdot}LiBr = (M_\gamma + M_\delta)$

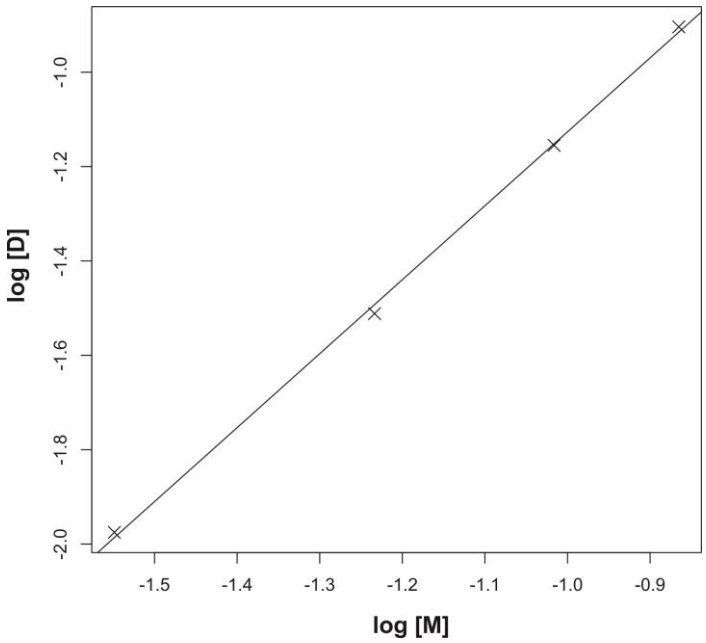


Figure S10. Monomer-dimer linear fit of species **I** ($y = 1.5671x + 0.4407$; $R^2 = 0.999$). The magnitude of K_{app} calculated from the linear regression equation is 2.76.

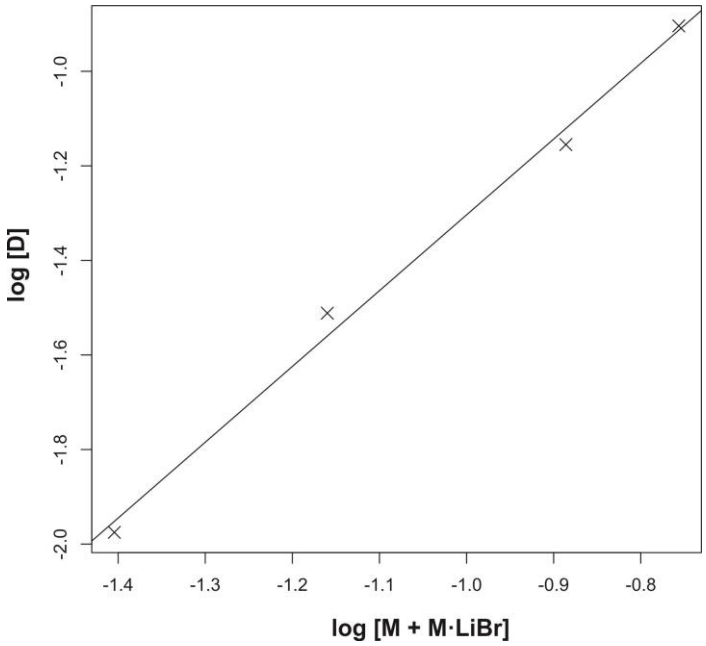


Figure S11. Monomer-dimer linear fit of species **I** including the concentration of mixed monomer-LiBr aggregates (y = 1.6032x + 0.2995; R^2 = 0.9936). The magnitude of K_{app} calculated from the linear regression equation is 1.99.

Since the concentration of THF has not been taken into account into the calculation, the constants obtained from the log-log plots are apparent equilibrium constants, K_{app}. The equilibrium constant can be obtained by including the concentration of neat THF into the equilibrium D + 2 THF ⇆ 2 M:

$$K = \frac{[M]^2}{[D][THF]^2}; \quad K_{app} = K[THF]^2 = \frac{[M]^2}{[D]}; \quad K = K_{app}/[THF]^2$$

$\Delta G = -RT\ln K$; R= 1.987 cal/mol·K; T= 153 K

$[THF]_{neat}$ = 12.34 mol/L

For a K_{app} of 2.76 the corresponding K is 0.018, that leads to a ΔG = 1.2 kcal/mol. Analogously, for a K_{app} of 1.99 the corresponding K is 0.013, from which one obtain a ΔG = 1.3 kcal/mol. Given that K < 1, the equilibrium will be shifted to the left. The dimer is stabilized by ≈ 1.2 kcal/mol as compared to the monomer. However, according to the Le Châtelier principle, the equilibrium will shift to the right at high THF concentrations, i.e., in diluted samples the monomer will predominate.

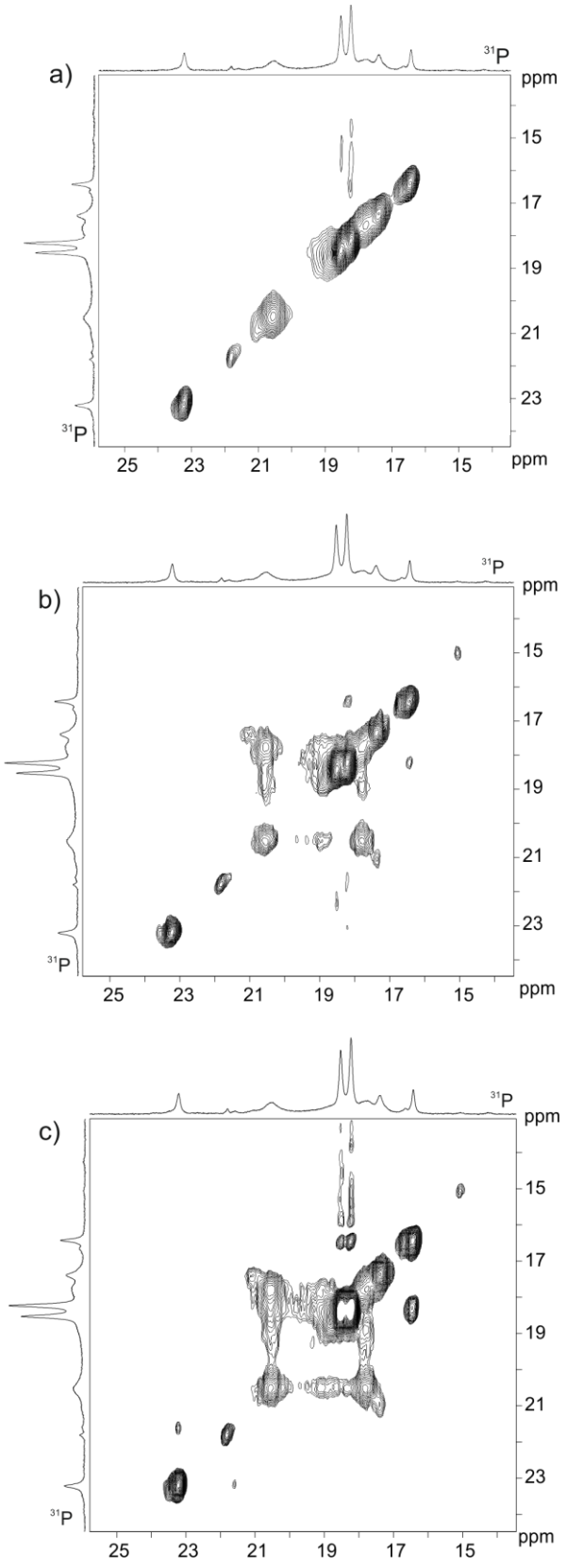


Figure S12. ^{31}P,^{31}P{^{1}H} EXSY NMR experiments of the monolithiated species **I** (0.2 M, THF-d_8) measured at -115 ºC. Different mixing times (τ_m) have been used in order to unravel the mechanism of exchange among the aggregates. (a) τ_m 0.1 ms; b) τ_m 50 ms; c) 100 ms.

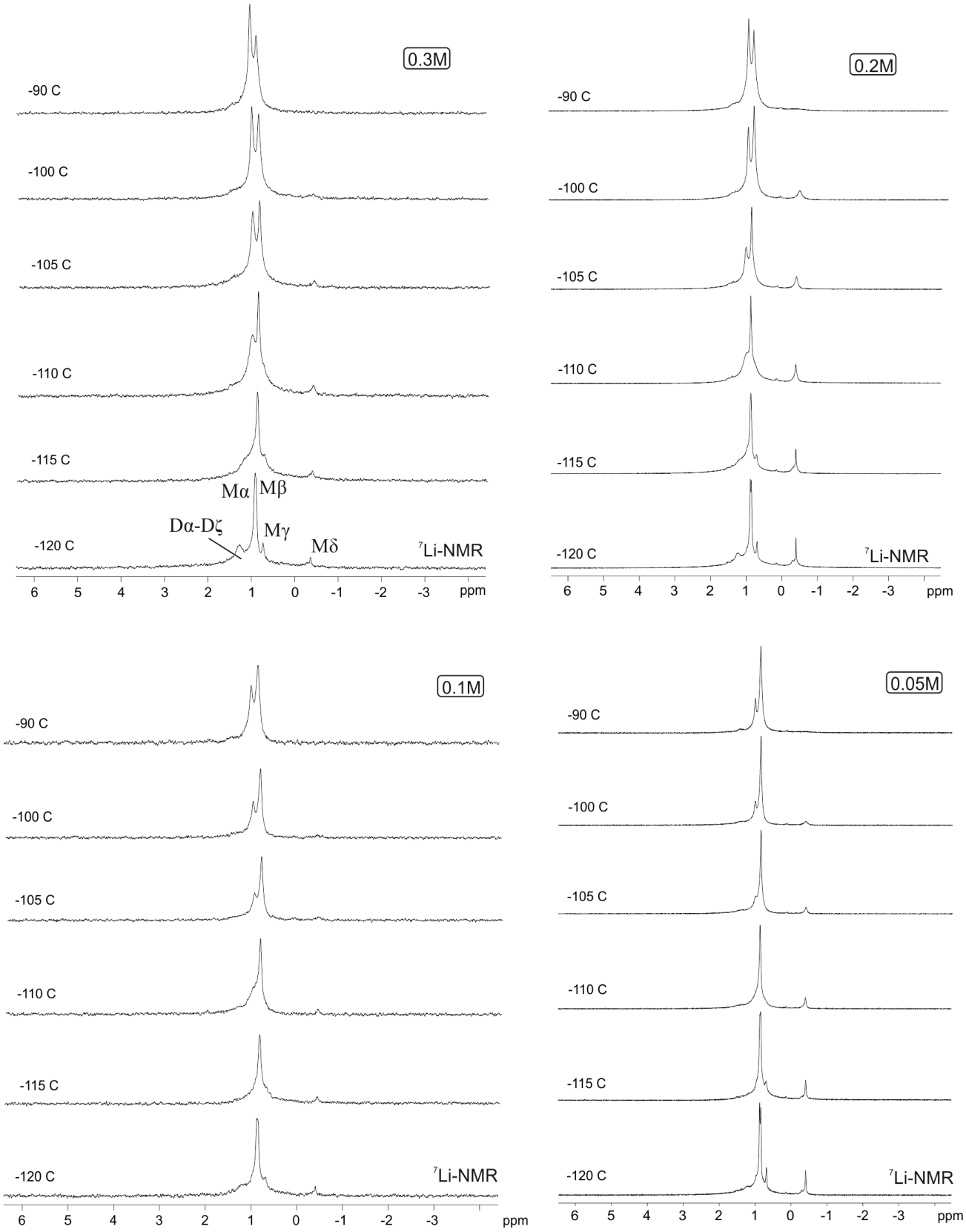


Figure S13. Variable-temperature and variable-concentration ^{7}Li NMR spectra of the monolithiated species **I** (THF-d_8).

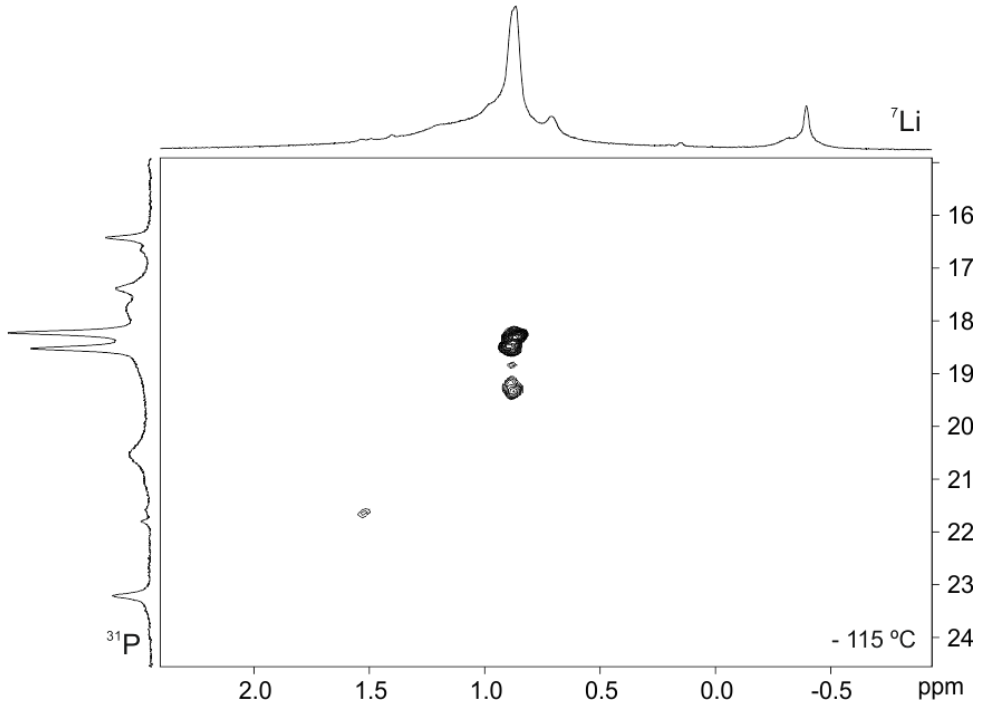
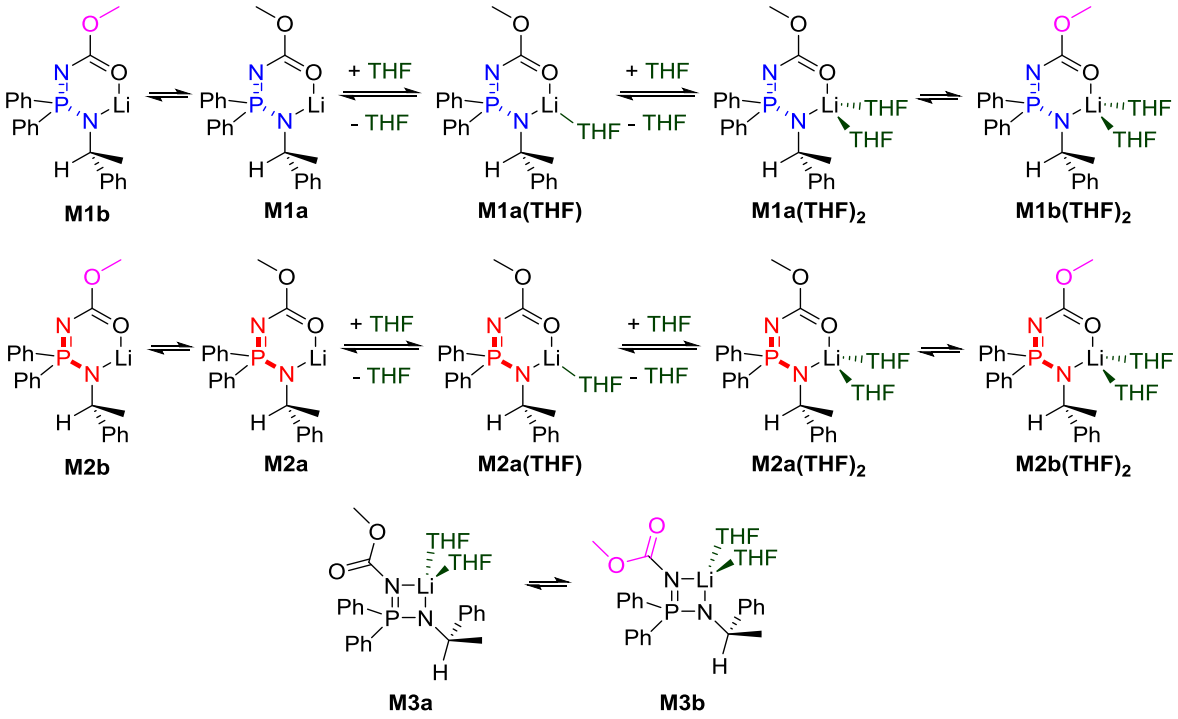


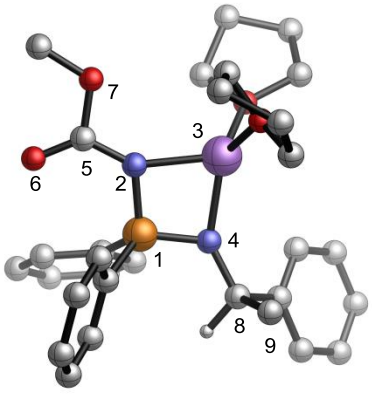
Figure S14. ^{7}Li,^{31}P{^{1}H} HMQC NMR spectrum of the monolithiated species **I** measured at -115 ºC (0.2 M, THF-d_8).

Table S2. Relative energies (kcal/mol) of (*O*,*N*-chelates)·$(THF)_n$ (n = 0, 1 and 2) and (*N*,*N*-chelates)·$(THF)_2$.



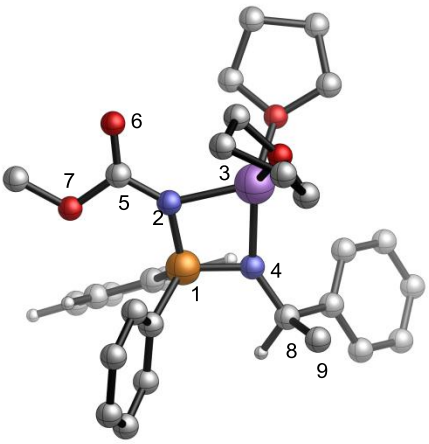
	ΔE_{solv}	ΔH_{solv}	ΔG_{solv}
M1a + 2THF	30.4	28.3	13.6
M1b + 2THF	31.4	29.3	14.5
M2a + 2THF	30.6	28.4	13.5
M2b + 2THF	31.5	29.2	14.2
M2a(THF) +THF	13.3	12.6	5.5
M1a(THF) + THF	14.4	13.7	5.6
$M1a(THF)_2$	1.4	1.7	0.7
$M1b(THF)_2$	2.6	2.8	1.6
$M2a(THF)_2$	0.0	0.0	0.0
$M2b(THF)_2$	2.4	2.5	2.7
$M3a(THF)_2$	4.9	4.8	3.5
$M3b(THF)_2$	5.3	5.3	5.0

Table S3. Selected structural parameters of **M3a(THF)$_2$** and **M3b(THF)$_2$** (distances in Å, angles in º). Free energies and enthalpies (in parentheses) are given in kcal/mol with respect to **M2a(THF)$_2$**.



M3a(THF)$_2$

3.5 (4.8)

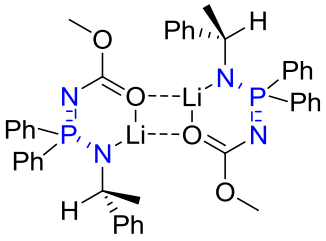


M3b(THF)$_2$

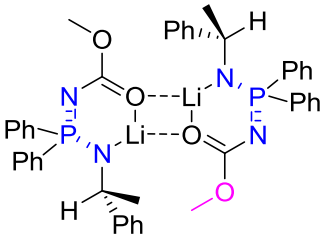
5.0 (5.3)

Parameter	**M3a(THF)$_2$**	**M3b(THF)$_2$**
P1-N2	1.6505	1.6428
P1-N4	1.6104	1.6101
N2-Li3	2.0329	2.0238
Li3-N4	2.0342	2.0412
N2-C5	1.3470	1.3431
C5-O6	1.2298	1.2337
P1-N4-Li3	91.82	91.84
P1-N4-C8	123.30	123.54
C8-N4-Li3	143.99	144.16
P1-N2-Li3-N4	1.27	-1.14
P1-N2-C5-O6	5.91	173.87
P1-N4-C8-C9	-108.04	108.58

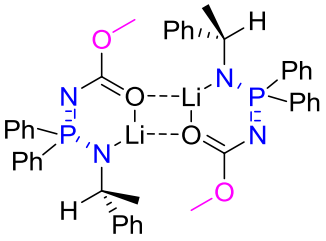
Table S4. Relative energies (kcal/mol) of unsolvated dimer *O,N*-chelates with O-Li bridges.



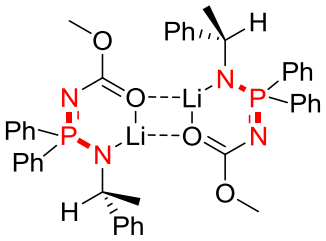
D1a



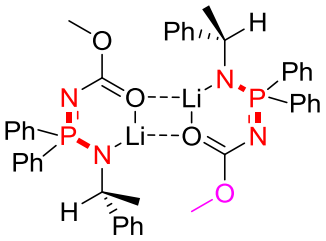
D1b



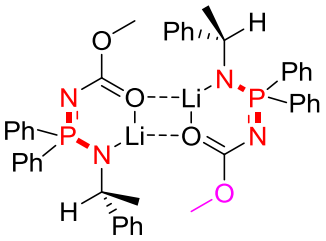
D1c



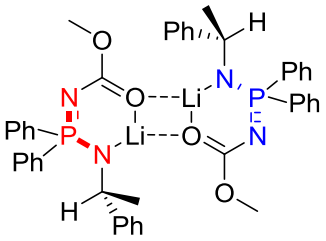
D2a



D2b



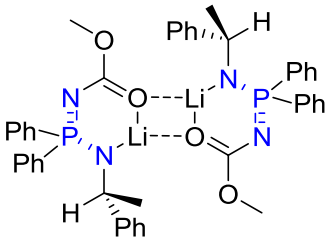
D2c



D3a

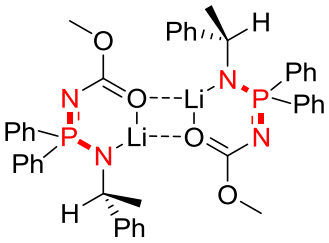
	ΔE_{solv}	ΔH_{solv}	ΔG_{solv}
D1a	3.3	3.7	3.4
D1b	4.5	4.4	3.7
D1c	4.9	4.8	5.1
D2a	0.0	0.0	0.0
D2b	2.7	2.6	3.1
D2c	5.2	4.8	6.9
D3a	0.7	0.8	0.4

Table S5. Relative energies (kcal/mol) of unsolvated *O,N*-chelate dimer with N-Li bridges. Dimers **D5a** and **D5a'** show different arrangement of the chiral side arms.



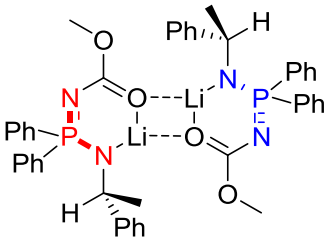
D1a

ΔG^{183}_{solv} = 3.4 kcal/mol



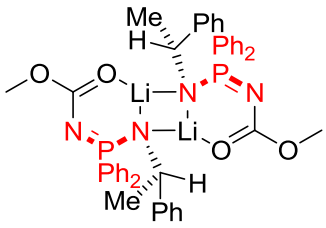
D2a

ΔG^{183}_{solv} = 0.0 kcal/mol



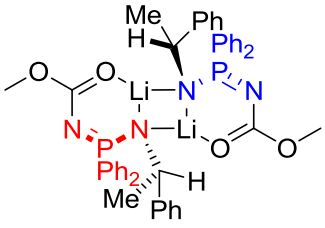
D3a

ΔG^{183}_{solv} = 0.4 kcal/mol



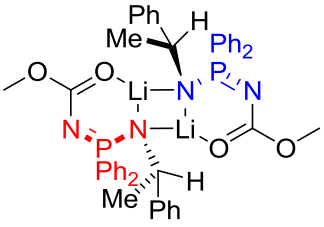
D4a

ΔG^{183}_{solv} = 6.3 kcal/mol



D5a

ΔG^{183}_{solv} = 3.7 kcal/mol



D5a'

ΔG^{183}_{solv} = 4.5 kcal/mol

	ΔE_{solv}	ΔH_{solv}	ΔG_{solv}
D1a	3.3	3.7	3.4
D2a	0.0	0.0	0.0
D3a	0.7	0.8	0.4
D4a	3.4	3.8	6.3
D5a	0.8	1.4	3.7
D5a'	1.4	2.0	4.5

Figure S15. Relative energies (kcal/mol) of solvated (L = THF) dimer *O,N*-chelates with O-Li bridges. The labels "d" and "u" are abbreviations of "down" and "up", respectively. They indicate the position of the THF molecule relative to the Li_2O_2 plane (structures viewed from left to right).

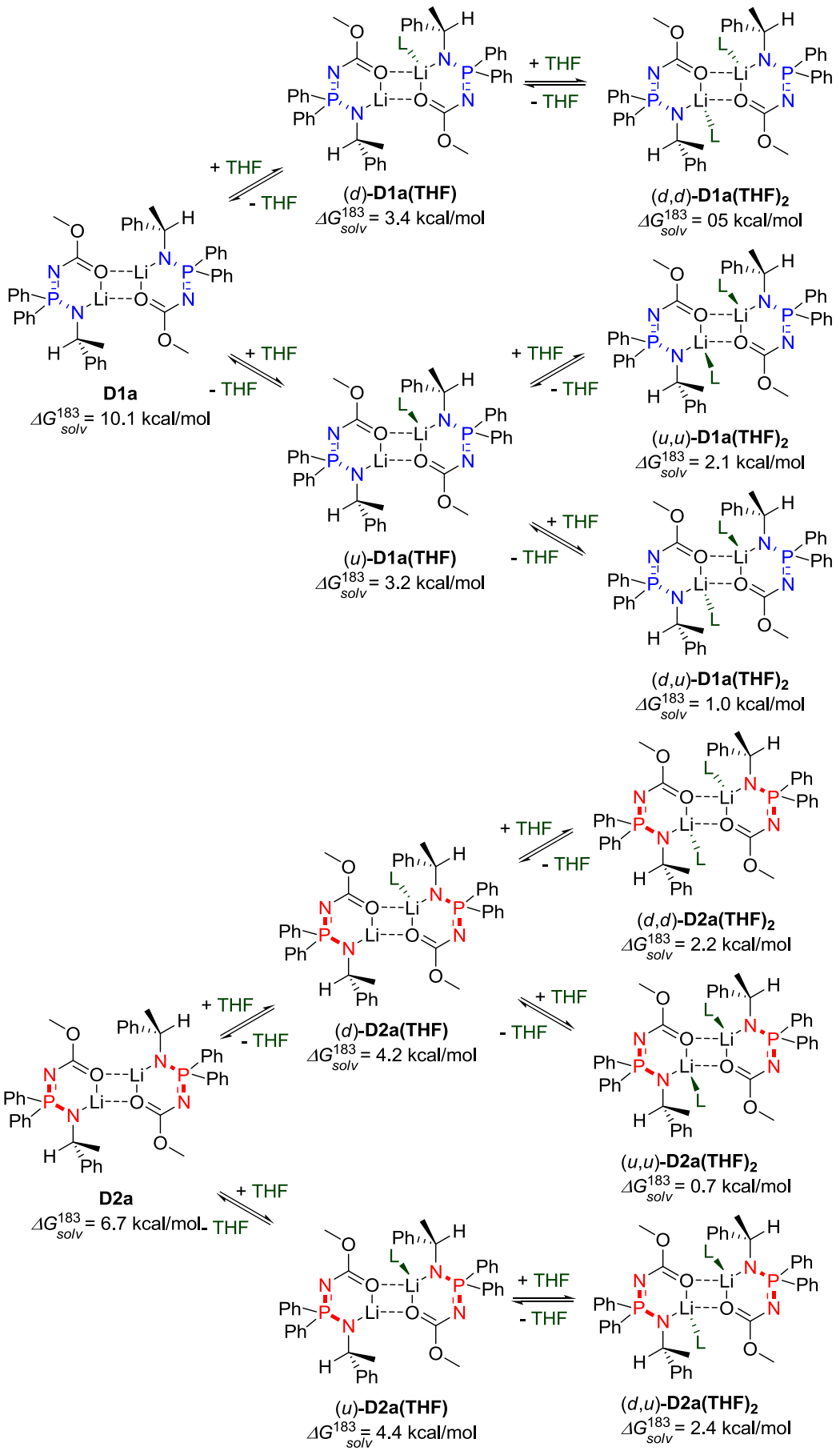
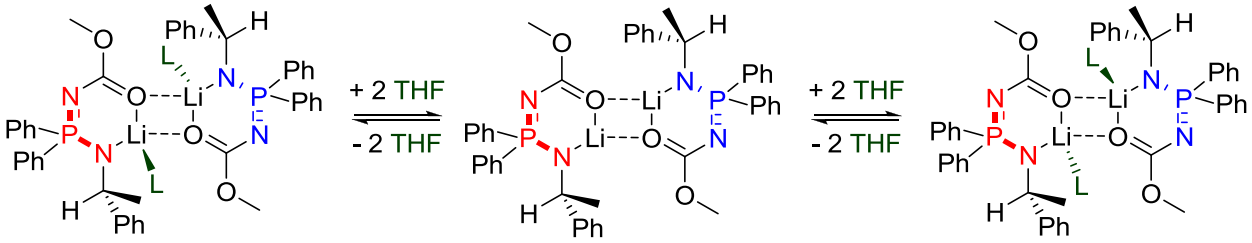


Figure S16. Relative energies (kcal/mol) of unsolvated **D3a** and dissolvated (L = THF) **(*d,u*)-D3a(THF)$_2$** dimers containing mixed twist-boat conformers of the six-membered rings. The labels "d" and "u" are the abbreviation of "down" and "up", respectively. They indicate the position of the THF molecule relative to the Li_2O_2 plane (structures viewed from left to right).



(*u,d*)-**D3a(THF)$_2$**
ΔG^{183}_{solv} = 3.0 kcal/mol

D3a
ΔG^{183}_{solv} = 7.1 kcal/mol

(*d,u*)-**D3a(THF)$_2$**
ΔG^{183}_{solv} = 0.0 kcal/mol

Table S6. Relative energies (kcal/mol) of solvated *O,N*-chelate dimers with O-Li bridges. The labels "d" and "u" are the abbreviation of "down" and "up", respectively. They indicate the position of the THF molecule relative to the Li_2O_2 plane (structures viewed from left to right).

	ΔE_{solv}	ΔH_{solv}	ΔG_{solv}
D1a + 2THF	28.1	26.3	10.1
D2a + 2THF	24.7	22.6	6.7
D3a + 2THF	25.4	23.4	7.1
(*d*)-**D1a(THF) + THF**	12.9	12.1	3.4
(*u*)-**D1a(THF) + THF**	12.2	11.3	3.2
(*d*)-**D2a(THF) + THF**	13.9	12.8	4.2
(*u*)-**D2a(THF) + THF**	12.9	12.0	4.4
(*d,d*)-**D1a(THF)$_2$**	1.8	1.8	0.5
(*u,u*)-**D1a(THF)$_2$**	2.7	2.7	2.1
(*d,u*)-**D1a(THF)$_2$**	1.3	1.4	1.0
(*d,d*)-**D2a(THF)$_2$**	3.5	3.2	2.2
(*u,u*)-**D2a(THF)$_2$**	1.4	1.2	0.7
(*d,u*)-**D2a(THF)$_2$**	1.9	2.1	2.4
(*d,u*)-**D3a(THF)$_2$**	0.0	0.0	0.0
(*u,d*)-**D3a(THF)$_2$**	3.7	3.8	3.0

Table S7. The Cartesian coordinates (Å), SCF energies, enthalpies at 183K, and Gibbs free energies at 183K for the optimized structures**.**

M1a

B3LYP SCF energy: -1460.52220320 a.u.
B3LYP enthalpy: -1460.11277200 a.u.
B3LYP free energy: -1460.15421400 a.u.
M06-2X SCF energy in solution: -1460.37991636 a.u.
M06-2X enthalpy in solution: -1459.97048516 a.u.
M06-2X free energy in solution: -1460.01192716 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	-0.79451200	-0.11392700	0.10346600
C	-0.30963500	-1.09841200	-1.35888800
C	-1.07950400	-2.18629500	-1.79289900
C	0.84735800	-0.74529100	-2.07114700
C	-0.69803200	-2.90829500	-2.92462900
H	-1.96793200	-2.45512700	-1.23209000
C	1.22581700	-1.46983900	-3.20087600
H	1.45893700	0.08644800	-1.73346600
C	0.45249000	-2.55106400	-3.63004100
H	-1.29945300	-3.75137200	-3.25475600
H	2.12552300	-1.19215900	-3.74332700
H	0.74808500	-3.11473000	-4.51120800
C	-1.43996400	1.48937100	-0.50900200
C	-0.57950300	2.58346500	-0.68480600
C	-2.79605400	1.62462500	-0.84165400
C	-1.06965600	3.79287200	-1.17980000
H	0.46885300	2.48016400	-0.42376700
C	-3.28336000	2.83425300	-1.33646000
H	-3.46546900	0.78170500	-0.70135700
C	-2.42134500	3.91979900	-1.50605100
H	-0.39611800	4.63608600	-1.30970700
H	-4.33665400	2.93042600	-1.58616500
H	-2.80241900	4.86243200	-1.89030400
N	0.46817600	0.27280300	1.04404700
N	-2.07882800	-0.95899800	0.72067700
Li	-0.46623500	0.86561700	2.63655300
C	-2.54615400	-0.65313100	1.92726100
O	-2.13127100	0.22187700	2.74543600
O	-3.60819700	-1.36300100	2.38250000
C	-4.14841800	-2.38238000	1.54200300
H	-4.98035100	-2.81078800	2.10544400
H	-3.40228600	-3.15310500	1.32633600
H	-4.50928400	-1.96670800	0.59615000
C	1.56359000	-0.67311100	1.29664800
H	1.44233400	-1.59927500	0.71465900
C	1.58043700	-1.08847500	2.78582500
H	1.72312700	-0.20467100	3.42732000
H	2.40421200	-1.77525800	3.01032500
H	0.63897800	-1.58150600	3.05903700
C	2.92786800	-0.09246100	0.91481000
C	3.98753800	-0.95416400	0.59918500
C	3.16994500	1.28622500	0.91161000
C	5.25439000	-0.45565500	0.29412300
H	3.81551900	-2.02904200	0.58610400
C	4.43712300	1.79022100	0.60977800
H	2.34938900	1.96124400	1.13444300
C	5.48473700	0.92169800	0.30019400
H	6.05969800	-1.14239200	0.04526900
H	4.60432300	2.86473600	0.61170500
H	6.46967700	1.31355500	0.06004400

M1b

B3LYP SCF energy: -1460.52170540 a.u.
B3LYP enthalpy: -1460.11234900 a.u.
B3LYP free energy: -1460.15395700 a.u.
M06-2X SCF energy in solution: -1460.37833238 a.u.
M06-2X enthalpy in solution: -1459.96897598 a.u.
M06-2X free energy in solution: -1460.01058398 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	0.77635800	0.03804700	0.21582500
C	0.09543500	1.29007200	1.35900300
C	0.74710900	1.60375200	2.55979900
C	-1.09282200	1.95711200	1.02186700
C	0.21468600	2.57384400	3.41057300
H	1.66243400	1.07801600	2.81018500
C	-1.62039500	2.92570700	1.87481500
H	-1.61059700	1.71050400	0.09919600
C	-0.96613700	3.23585900	3.06963100
H	0.72344000	2.81210400	4.34105300
H	-2.54250000	3.43527600	1.60836300
H	-1.37798000	3.99147200	3.73381700
C	1.42038300	0.92877000	-1.25291600
C	0.60877600	1.14067400	-2.37728100
C	2.72909300	1.43530100	-1.24611400
C	1.10094000	1.84284900	-3.47878200
H	-0.40230600	0.74591800	-2.38223900
C	3.21762300	2.13755500	-2.34785800
H	3.35922800	1.26825600	-0.37787000
C	2.40495700	2.34185400	-3.46532100
H	0.46629000	1.99995000	-4.34723700
H	4.23361300	2.52327700	-2.33510900
H	2.78740000	2.88827900	-4.32364200
N	-0.36043200	-0.96557600	-0.36451300
N	2.08291200	-0.54698200	1.03593400
Li	0.76223400	-2.37675600	-1.05593200
C	2.70490700	-1.64128300	0.62504100
O	2.41068700	-2.42316100	-0.33638400
O	3.80017400	-1.93499200	1.36998700
C	4.51991000	-3.11711600	1.01667900
H	5.35128300	-3.16960800	1.72257100
H	4.90003800	-3.06075300	-0.00773100
H	3.89218100	-4.00869900	1.11172300
C	-1.47799600	-1.43074700	0.46663100
H	-1.46761200	-0.95786500	1.46004700
C	-1.37134200	-2.95505400	0.70345800
H	-1.39390700	-3.49262000	-0.25777100
H	-2.20886400	-3.33840100	1.29687500

H	-0.43957300	-3.19799500	1.22994900
C	-2.83901500	-1.10839600	-0.15642800
C	-3.97178800	-1.00665200	0.66317800
C	-3.00333600	-0.95431300	-1.53795400
C	-5.23386400	-0.76408600	0.12038800
H	-3.86159600	-1.11164200	1.74112200
C	-4.26525500	-0.71472200	-2.08666000
H	-2.12775100	-1.00923100	-2.17748200
C	-5.38578300	-0.61899700	-1.26028000
H	-6.09728200	-0.68146100	0.77594400
H	-4.37171900	-0.59709400	-3.16251300
H	-6.36704000	-0.42688400	-1.68641700

M2a

B3LYP SCF energy: -1460.52064990 a.u.
B3LYP enthalpy: -1460.11135300 a.u.
B3LYP free energy: -1460.15315400 a.u.
M06-2X SCF energy in solution: -1460.37964921 a.u.
M06-2X enthalpy in solution: -1459.97035231 a.u.
M06-2X free energy in solution: -1460.01215331 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	-0.77970600	-0.15871900	-0.19920900
C	-1.74529600	1.27814100	0.43234100
C	-2.35097100	1.24699500	1.69833600
C	-1.95046500	2.39391000	-0.39054200
C	-3.14080100	2.31133300	2.13066800
H	-2.20276500	0.38786000	2.34612900
C	-2.73985600	3.46110600	0.04306900
H	-1.49254700	2.42041700	-1.37500800
C	-3.33498000	3.42136200	1.30422600
H	-3.60545200	2.27556800	3.11256500
H	-2.88907400	4.32161500	-0.60391600
H	-3.94948400	4.25127300	1.64326000
C	0.18197600	-0.72262400	1.25833200
C	0.88157000	0.19160400	2.06016500
C	0.28811900	-2.09228800	1.53633900
C	1.67316800	-0.25607100	3.11762800
H	0.80277200	1.25832000	1.86873700
C	1.08061000	-2.53913200	2.59383400
H	-0.26628600	-2.79798700	0.92607200
C	1.77465100	-1.62235700	3.38558300
H	2.20947600	0.46201000	3.73212700
H	1.15157100	-3.60341000	2.80300300
H	2.39027600	-1.97067800	4.21083100
N	0.12718500	0.26355000	-1.48059500
N	-1.83801800	-1.37009300	-0.46894500
Li	-0.61180700	-0.48149900	-3.04719400
C	-2.34763400	-1.80474500	-1.61373800
O	-2.04745300	-1.49622800	-2.80175700
O	-3.32737200	-2.73892300	-1.52678500
C	-3.77827700	-3.13164700	-0.23026000
H	-4.58584800	-3.84474300	-0.41059100
H	-4.14973600	-2.27297100	0.33621000
H	-2.97645200	-3.60884200	0.34141600
C	1.20623300	1.25177100	-1.40391800
H	0.96769100	2.05323300	-0.68424000
C	1.33862200	1.93068300	-2.78362300
H	1.59627300	1.18296500	-3.54740300
H	2.13265300	2.68498600	-2.78829900
H	0.39624500	2.41557100	-3.06730100
C	2.57287500	0.68578400	-0.99900700
C	3.52287600	1.53071900	-0.40921100
C	2.93417200	-0.63975600	-1.26161500
C	4.80095600	1.06882500	-0.09457300
H	3.25666900	2.56411300	-0.19154600
C	4.21207700	-1.10717200	-0.94908600
H	2.19743600	-1.31028200	-1.69402300
C	5.15122200	-0.25536800	-0.36590200
H	5.52042600	1.74031700	0.36767200
H	4.47205000	-2.14240100	-1.15641900
H	6.14447100	-0.62107900	-0.11872600

M2b

B3LYP SCF energy: -1460.51992090 a.u.
B3LYP enthalpy: -1460.11073800 a.u.
B3LYP free energy: -1460.15255800 a.u.
M06-2X SCF energy in solution: -1460.37829028 a.u.
M06-2X enthalpy in solution: -1459.96910738 a.u.
M06-2X free energy in solution: -1460.01092738 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	-0.76675400	-0.10875300	0.07221900
C	-1.68745600	1.46075100	-0.22088100
C	-2.22580800	2.18819500	0.85233900
C	-1.91857600	1.90770200	-1.52839000
C	-2.97609300	3.33944300	0.61915500
H	-2.05876000	1.84946800	1.87071400
C	-2.66790400	3.06301200	-1.76222700
H	-1.51147700	1.34404300	-2.36279800
C	-3.19656700	3.78009800	-0.68883100
H	-3.39035000	3.89346700	1.45742900
H	-2.83727400	3.40147900	-2.78119600
H	-3.78008400	4.67930700	-0.86875100
C	0.32662100	0.28393400	1.49034500
C	1.13192300	1.43247400	1.48238200
C	0.40566400	-0.59934800	2.57553800
C	2.00875500	1.68775900	2.53617300
H	1.06978600	2.13857800	0.65852800
C	1.28380800	-0.34222700	3.62897100
H	-0.24053900	-1.47123000	2.59014100
C	2.08767000	0.79888300	3.61016100
H	2.62822300	2.58048000	2.51946300
H	1.33440800	-1.03044400	4.46880100
H	2.76971800	0.99895600	4.43253700
N	0.01214700	-0.58852300	-1.27459400
N	-1.81503000	-1.19350900	0.68048400
Li	-0.95566000	-2.00754100	-2.04077700
C	-2.48308700	-2.15128400	0.06311500
O	-2.38739900	-2.57111000	-1.13178500
O	-3.37845100	-2.76138100	0.88055900
C	-4.12941800	-3.83822100	0.31814400

H	-4.77966200	-4.18627800	1.12329700
H	-3.47452500	-4.65071300	-0.01198300
H	-4.73132600	-3.50242000	-0.53158700
C	1.12618900	0.15175500	-1.86989600
H	1.00203900	1.24083600	-1.74397400
C	1.12381700	-0.11226400	-3.39082800
H	1.25933300	-1.18589300	-3.58489300
H	1.94092000	0.41410200	-3.89565400
H	0.17473000	0.21088000	-3.83663400
C	2.50903300	-0.20447100	-1.30872400
C	3.56398300	0.70912800	-1.43962800
C	2.77349800	-1.44590300	-0.72180700
C	4.85001900	0.39091900	-1.00353500
H	3.37403700	1.68379500	-1.88694700
C	4.05940600	-1.77011400	-0.28455400
H	1.95612000	-2.14841100	-0.59013700
C	5.10303100	-0.85444500	-0.42441100
H	5.65252400	1.11687300	-1.10952000
H	4.24363300	-2.73856600	0.17418100
H	6.10274500	-1.10488300	-0.07905100

M1a(THF)

B3LYP SCF energy: -1693.00392040 a.u.
B3LYP enthalpy: -1692.47182500 a.u.
B3LYP free energy: -1692.52179800 a.u.
M06-2X SCF energy in solution: -1692.81875656 a.u.
M06-2X enthalpy in solution: -1692.28666116 a.u.
M06-2X free energy in solution: -1692.33663416 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	-1.10111700	-0.50876900	-0.13830200
C	-2.77970300	0.13556600	0.20639800
C	-3.91091400	-0.38681100	-0.43420200
C	-2.93478100	1.18386900	1.12739800
C	-5.17750300	0.13081600	-0.15600200
H	-3.78043100	-1.19631300	-1.14400200
C	-4.20077100	1.69879500	1.40369800
H	-2.06227300	1.59885100	1.62509800
C	-5.32458200	1.17191900	0.76189800
H	-6.05011200	-0.28026600	-0.65700200
H	-4.31105400	2.50959800	2.11909800
H	-6.31157300	1.57294000	0.97759800
C	-0.51043300	-1.27758200	1.42249800
C	0.26708300	-0.53819800	2.32589800
C	-0.85816100	-2.59867500	1.74049800
C	0.69297000	-1.11350700	3.52549800
H	0.53760400	0.48219600	2.07049800
C	-0.43267300	-3.17138300	2.93919800
H	-1.45387300	-3.17546200	1.03939800
C	0.34354300	-2.43020000	3.83329800
H	1.29338300	-0.53222000	4.22109800
H	-0.70459400	-4.19707800	3.17469800
H	0.67363400	-2.87720700	4.76759800
N	-0.02739200	0.65790800	-0.44790200
N	-1.38024200	-1.73016400	-1.22360200
Li	1.53728400	-0.44822500	-0.97230200
C	-0.32085500	-2.30668600	-1.78600200
O	0.90565100	-2.05901200	-1.60510200
O	-0.55557500	-3.30088100	-2.68320200
C	-1.91108300	-3.64915300	-2.96050200
H	-1.85880000	-4.46305400	-3.68760200
H	-2.45906500	-2.80174100	-3.38400200
H	-2.42809000	-3.98484200	-2.05620200
C	-0.37336700	1.85761500	-1.22840200
H	-1.43526200	2.11303800	-1.09490200
C	-0.15647100	1.66341100	-2.74330200
H	0.88832300	1.41378900	-2.96980200
H	-0.40795200	2.57371600	-3.30140200
H	-0.78348900	0.84372400	-3.11040200
C	0.42495800	3.04709900	-0.69710200
C	-0.22422000	4.10841200	-0.05640200
C	1.82055900	3.10836900	-0.82550200
C	0.49220300	5.19769700	0.44629800
H	-1.30662100	4.07973500	0.05159800
C	2.54218200	4.19195400	-0.32520200
H	2.35194200	2.30285800	-1.32740200
C	1.87980400	5.24316800	0.31449800
H	-0.03578000	6.01040800	0.93929800
H	3.62328200	4.22083200	-0.44070200
H	2.44102100	6.08945600	0.70219800
O	3.44828500	-0.44166500	-0.77950200
C	4.13649500	0.06972100	0.37659800
C	4.10005800	-1.68737800	-1.13750200
C	4.39196900	-1.16898500	1.23699800
H	3.49301100	0.82463400	0.83379800
H	5.07470500	0.54500100	0.05549800
C	4.62394600	-2.28838900	0.18799800
H	4.91896300	-1.46049600	-1.83160200
H	3.34974600	-2.29776300	-1.64190200
H	5.24197200	-1.03700200	1.91309800
H	3.50616500	-1.38606600	1.84219800
H	5.68384000	-2.54671200	0.10219800
H	4.08132700	-3.19887800	0.45509800

M2a(THF)

B3LYP SCF energy: -1693.00566460 a.u.
B3LYP enthalpy: -1692.47351700 a.u.
B3LYP free energy: -1692.52194000 a.u.
M06-2X SCF energy in solution: -1692.82054869 a.u.
M06-2X enthalpy in solution: -1692.28840109 a.u.
M06-2X free energy in solution: -1692.33682409 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	1.37382100	0.04711400	0.09494100
C	1.81731500	1.71353500	-0.52717100
C	2.53899500	2.59818100	0.28848000
C	1.46875700	2.10849400	-1.82640600
C	2.90628700	3.85568700	-0.18889300
H	2.80037000	2.29979400	1.29932800
C	1.83412700	3.37016500	-2.30074900
H	0.90164300	1.42193600	-2.44726200
C	2.55410700	4.24360400	-1.48411100

H	3.46299200	4.53544500	0.45090600
H	1.55489900	3.67068200	-3.30750000
H	2.83869100	5.22537200	-1.85407900
C	2.87872200	-0.98553800	-0.07059500
C	3.51249500	-1.08818200	-1.31920000
C	3.39233200	-1.70439200	1.01710300
C	4.63731300	-1.89664000	-1.47685200
H	3.13083000	-0.52485700	-2.16667200
C	4.51546200	-2.51820700	0.85581300
H	2.90743900	-1.60644700	1.98229000
C	5.13890400	-2.61580600	-0.38892700
H	5.12390800	-1.96388100	-2.44637200
H	4.90588800	-3.07311100	1.70512800
H	6.01552100	-3.24669200	-0.51183300
N	0.15489400	-0.44610900	-0.84611300
N	1.18844700	0.14853200	1.74047500
Li	-1.35919100	0.66172500	-0.14757500
C	0.09236700	0.74944900	2.20040200
O	-0.87371900	1.23755200	1.55233900
O	-0.03604800	0.85732900	3.55163400
C	1.01685200	0.35072500	4.37004100
H	0.72300100	0.58101200	5.39703500
H	1.97108800	0.83108200	4.13384100
H	1.13055000	-0.73117400	4.24731800
C	-0.12377600	-1.87904400	-1.06594200
H	0.56480600	-2.51384300	-0.48421200
C	0.09836000	-2.23216100	-2.54253700
H	-0.51000800	-1.59312400	-3.19312800
H	-0.13936800	-3.28216800	-2.75416800
H	1.14768000	-2.06212400	-2.79921300
C	-1.53402900	-2.22168900	-0.56270000
C	-2.59006600	-2.58048500	-1.41167300
C	-1.79385200	-2.16094800	0.81746000
C	-3.86205500	-2.86573000	-0.90207500
H	-2.42415300	-2.65211700	-2.48190800
C	-3.05935200	-2.44352800	1.33040600
H	-0.98687500	-1.89150100	1.49458400
C	-4.10327000	-2.79646100	0.46961700
H	-4.66127000	-3.15061100	-1.58245300
H	-3.22810200	-2.39573600	2.40321800
H	-5.08893300	-3.02501700	0.86677000
O	-2.99365000	1.54146600	-0.65975700
C	-4.00855700	1.06758100	-1.57828100
C	-3.62581000	2.34315100	0.36592500
C	-5.37017400	1.31353500	-0.89105100
H	-3.80842700	0.00859500	-1.75918900
H	-3.91580600	1.61484100	-2.52361900
C	-4.98552100	1.67993000	0.55570000
H	-3.72521900	3.37716900	0.00552900
H	-2.96828400	2.31854500	1.23607700
H	-5.89620900	2.14676900	-1.36960400
H	-6.01916000	0.43496700	-0.94451500
H	-5.71538700	2.33719300	1.03792800
H	-4.87348500	0.77803500	1.16741200

M1a(THF)$_2$

B3LYP SCF energy:	-1925.47096160 a.u.
B3LYP enthalpy:	-1924.81690700 a.u.
B3LYP free energy:	-1924.87464200 a.u.
M06-2X SCF energy in solution:	-1925.25273836 a.u.
M06-2X enthalpy in solution:	-1924.59868376 a.u.
M06-2X free energy in solution:	-1924.65641876 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	1.44785100	-0.58812000	0.15338700
C	3.08337600	-0.22815700	0.90667500
C	3.59397400	-1.06547500	1.90850400
C	3.81265200	0.91244500	0.53657300
C	4.80669200	-0.76490500	2.53042200
H	3.03909900	-1.95813500	2.17722900
C	5.02494600	1.21166700	1.15894700
H	3.44161200	1.56247600	-0.25125500
C	5.52339900	0.37385600	2.15874900
H	5.19464700	-1.42403100	3.30296100
H	5.58235000	2.09540900	0.85934700
H	6.46917800	0.60553300	2.64188200
C	1.70538300	-0.34889700	-1.65530000
C	1.46227400	0.90651200	-2.23072400
C	2.18383400	-1.38878900	-2.46572600
C	1.69967500	1.12150800	-3.59035400
H	1.07713000	1.70679400	-1.60439000
C	2.41017800	-1.17727000	-3.82667400
H	2.36916700	-2.36282100	-2.02343500
C	2.17118800	0.07839500	-4.39072800
H	1.51524600	2.10131500	-4.02445100
H	2.77457200	-1.99200600	-4.44726800
H	2.35219100	0.24291400	-5.44997300
N	0.28094600	0.40928200	0.64095300
N	1.28218900	-2.21618900	0.40024300
Li	-1.50066700	-0.47747300	0.13264100
C	0.10494600	-2.78313000	0.16653900
O	-0.96714500	-2.25813400	-0.23795200
O	0.00799400	-4.12629700	0.39906100
C	1.17245000	-4.81495500	0.85030300
H	0.87946400	-5.86529700	0.92499200
H	1.49841900	-4.44749300	1.82880500
H	2.00077000	-4.70375500	0.14405600
C	0.44051500	1.37378300	1.73966500
H	1.50294800	1.60178600	1.90685500
C	-0.10215700	0.82957900	3.07462400
H	-1.15088000	0.52957100	2.98196700
H	-0.02060700	1.57789400	3.87351000
H	0.47387900	-0.05510800	3.36847200
C	-0.21692700	2.69768900	1.34830800
C	0.57180200	3.79819900	0.99012100
C	-1.61110000	2.84882000	1.31586800
C	-0.00606400	5.01020300	0.60420900
H	1.65567300	3.70416600	1.01904900
C	-2.19505400	4.05661800	0.93160900
H	-2.24488700	2.01312300	1.59959500
C	-1.39440900	5.14394800	0.57242000

H	0.62928500	5.85041200	0.33411400
H	-3.27852600	4.15310300	0.92010100
H	-1.84897200	6.08617500	0.27706000
O	-3.00448100	-0.67896100	1.51262300
C	-4.33937400	-0.14888100	1.33212600
C	-3.07254600	-1.94582300	2.20711900
C	-5.30881700	-1.19893700	1.90161600
H	-4.47928600	0.01975700	0.26038500
H	-4.41266200	0.81400300	1.85122800
C	-4.46497400	-2.48418600	1.89317800
H	-2.93894500	-1.77538400	3.28501200
H	-2.26001200	-2.56522900	1.82601400
H	-5.59624700	-0.94134800	2.92752900
H	-6.22492600	-1.27929400	1.30872000
H	-4.80534700	-3.22762800	2.62044800
H	-4.46892700	-2.94686500	0.89971500
O	-2.58346700	0.09511200	-1.47519200
C	-2.85922200	-0.94391800	-2.44123300
C	-2.33276200	1.34518800	-2.16637600
C	-2.10757100	-0.51084200	-3.69571700
H	-3.94404900	-0.99332000	-2.62045500
H	-2.51136300	-1.88290200	-2.00798800
C	-2.29864200	1.01576500	-3.67105600
H	-1.38151800	1.73273900	-1.79445200
H	-3.12415100	2.05811800	-1.90864500
H	-1.04782800	-0.76948300	-3.60367900
H	-2.50074800	-0.97639600	-4.60501600
H	-1.49594200	1.54921600	-4.18791400
H	-3.24672100	1.29074500	-4.14768700

M1b(THF)$_2$

B3LYP SCF energy:	-1925.46780620 a.u.
B3LYP enthalpy:	-1924.81370200 a.u.
B3LYP free energy:	-1924.87186200 a.u.
M06-2X SCF energy in solution:	-1925.25092885 a.u.
M06-2X enthalpy in solution:	-1924.59682465 a.u.
M06-2X free energy in solution:	-1924.65498465 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	1.47329500	-0.67596800	0.20238300
C	3.00517500	-0.51113200	1.20035900
C	3.35499500	-1.52922100	2.09907300
C	3.80897800	0.63657800	1.12415500
C	4.48051800	-1.39480500	2.91288500
H	2.75019200	-2.42980000	2.12965000
C	4.93365500	0.76961900	1.93968400
H	3.56942800	1.42257900	0.41272800
C	5.26942500	-0.24515300	2.83778300
H	4.74624200	-2.19297900	3.60139700
H	5.55044100	1.66182500	1.86833100
H	6.14755100	-0.14345600	3.47044500
C	1.97470200	-0.13354400	-1.49075700
C	1.79143800	1.20086200	-1.87988300
C	2.56162100	-1.03267100	-2.39427400
C	2.19605100	1.63342100	-3.14522600
H	1.31870300	1.89408400	-1.18878400
C	2.95404300	-0.60332700	-3.66321900
H	2.69900300	-2.06768500	-2.09570100
C	2.77516900	0.73044400	-4.03963600
H	2.05662700	2.67279600	-3.43318000
H	3.40204500	-1.30913600	-4.35823300
H	3.08583700	1.06426800	-5.02654500
N	0.25223900	0.23464700	0.73398200
N	1.25881100	-2.30007700	0.12081100
Li	-1.45194000	-0.52669200	-0.05862100
C	0.11757300	-2.84416900	-0.27093800
O	-0.97447000	-2.29455300	-0.58793500
O	0.19458500	-4.20930600	-0.31663400
C	-0.97925100	-4.90043300	-0.72835600
H	-0.71294200	-5.96003700	-0.71601700
H	-1.28765100	-4.60723300	-1.73744900
H	-1.81518600	-4.72210800	-0.04291800
C	0.36532300	1.20685000	1.83044600
H	1.41647500	1.46504800	2.02188600
C	-0.18396700	0.64003200	3.15305600
H	-1.23349400	0.34640500	3.04693600
H	-0.11221800	1.37593100	3.96433000
H	0.39103100	-0.24841900	3.43598100
C	-0.32759500	2.51594500	1.44831500
C	0.42966000	3.65894000	1.16126400
C	-1.72534800	2.61372600	1.36483400
C	-0.18035000	4.86099800	0.79285600
H	1.51444900	3.60787700	1.23383400
C	-2.34017200	3.81248700	1.00079000
H	-2.33640100	1.74300700	1.58796600
C	-1.57045400	4.94228700	0.71069900
H	0.43122800	5.73400000	0.57758200
H	-3.42541700	3.86827900	0.94953000
H	-2.05055600	5.87640500	0.43040200
O	-3.07185500	-0.74052300	1.16621800
C	-4.41072600	-0.62487600	0.66250500
C	-3.08452600	-1.88008600	2.04557500
C	-5.31175200	-0.90010500	1.87688400
H	-4.56801400	-1.37083700	-0.13052700
H	-4.51543600	0.37205300	0.23191600
C	-4.43572100	-1.80852900	2.78482700
H	-2.20960800	-1.80039800	2.69260000
H	-2.99734700	-2.79401500	1.44354400
H	-5.55800600	0.03417900	2.39029200
H	-6.25231500	-1.37556300	1.58311300
H	-4.31770700	-1.36593700	3.77800500
H	-4.86649500	-2.80546600	2.91724400
O	-2.33085300	0.26130100	-1.71572500
C	-2.49266200	-0.62827300	-2.84045000
C	-1.99986200	1.58878400	-2.19856200
C	-1.57466200	-0.05737500	-3.91676500
H	-3.54485900	-0.61979100	-3.16426000
H	-2.21854300	-1.62675000	-2.49686500
C	-1.75079000	1.45785700	-3.71379500
H	-1.11652100	1.91738800	-1.64746800
H	-2.82733900	2.26863900	-1.96652700
H	-0.53945400	-0.35519400	-3.72062100

H	-1.84632700	-0.38875700	-4.92404500
H	-0.87467900	2.02819600	-4.03427700
H	-2.61588100	1.82206000	-4.27990600

M2a(THF)$_2$

B3LYP SCF energy:	-1925.46850250 a.u.
B3LYP enthalpy:	-1924.81482400 a.u.
B3LYP free energy:	-1924.87102900 a.u.
M06-2X SCF energy in solution:	-1925.25499562 a.u.
M06-2X enthalpy in solution:	-1924.60131712 a.u.
M06-2X free energy in solution:	-1924.65752212 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	-0.82733500	0.80310600	-0.45165500
C	-0.66758900	2.51844000	0.21818200
C	-1.29113000	3.60628000	-0.41298500
C	0.13114400	2.75502900	1.34412800
C	-1.11834000	4.90131900	0.07331500
H	-1.91436200	3.43683900	-1.28680000
C	0.30041300	4.05187000	1.83555300
H	0.62263300	1.91617900	1.82834000
C	-0.32331500	5.12613800	1.20085700
H	-1.60443900	5.73610600	-0.42527200
H	0.91792700	4.22194200	2.71421100
H	-0.19232600	6.13587500	1.58170300
C	-2.62582400	0.66076500	-0.79739500
C	-3.57607500	1.05645500	0.15565200
C	-3.06719600	0.09514300	-2.00169400
C	-4.93883600	0.88688500	-0.08852300
H	-3.25536900	1.51104900	1.08920000
C	-4.43047400	-0.07268300	-2.24595600
H	-2.33179300	-0.19314300	-2.74533900
C	-5.36863500	0.32123600	-1.29014800
H	-5.66422100	1.19833300	0.65850600
H	-4.76097000	-0.50703800	-3.18623600
H	-6.43074800	0.19139700	-1.48182700
N	-0.21863700	-0.29731900	0.56456200
N	-0.16099000	0.77021900	-1.95505700
Li	1.77710700	-0.45543100	0.23314000
C	1.15397700	0.74332900	-2.13216100
O	2.07632600	0.64132000	-1.28255100
O	1.59599300	0.81275600	-3.42548200
C	0.62865700	1.00045100	-4.45780300
H	1.20418300	1.09781800	-5.38188800
H	0.03520100	1.90273800	-4.28501000
H	-0.05038900	0.14456900	-4.52854100
C	-0.87622800	-0.61596300	1.83662300
H	-1.33189500	0.27865900	2.29807900
C	0.18962900	-1.11477500	2.83482600
H	0.67892700	-2.01382500	2.43994000
H	-0.25975900	-1.37196700	3.80055800
H	0.95393600	-0.34621900	2.99418700
C	-1.98848700	-1.66949600	1.74600000
C	-2.99499200	-1.70338700	2.72097500
C	-1.99850700	-2.65057300	0.74955600
C	-3.98045300	-2.69066200	2.70685100
H	-3.00803700	-0.94244400	3.50008600
C	-2.98178500	-3.64161000	0.73034900
H	-1.23569900	-2.61448400	-0.02074500
C	-3.97638400	-3.66769500	1.70915300
H	-4.75519700	-2.69311000	3.47004400
H	-2.97474700	-4.39274800	-0.05633300
H	-4.74497500	-4.43629400	1.69128700
O	3.19102400	0.17276000	1.52499000
C	4.01270000	-0.67858700	2.35679300
C	3.89916800	1.39609100	1.22174900
C	5.36327800	0.04216600	2.51651200
H	4.10794700	-1.64342300	1.84797800
H	3.50366000	-0.84073100	3.31323700
C	5.37450000	1.02110600	1.32982600
H	3.62802400	2.16486500	1.95968900
H	3.57425900	1.71418000	0.23032600
H	5.39403500	0.59492400	3.46246000
H	6.20678800	-0.65457500	2.51054200
H	6.02138200	1.88831700	1.49357400
H	5.70279500	0.51735000	0.41311300
O	2.52465700	-2.24631100	-0.39572900
C	3.72474500	-2.10042200	-1.19402200
C	1.56600000	-3.08031600	-1.09851900
C	3.33340100	-2.52856200	-2.60664100
H	4.50667300	-2.74921700	-0.77428800
H	4.03869100	-1.05669300	-1.13337200
C	2.29889400	-3.62977400	-2.32593600
H	0.71338300	-2.45243900	-1.37819000
H	1.21917300	-3.85752300	-0.41053900
H	2.87382900	-1.68489700	-3.13233100
H	4.19024700	-2.87892200	-3.19052200
H	1.61974800	-3.80989300	-3.16473300
H	2.80002400	-4.57554200	-2.08674000

M2b(THF)$_2$

B3LYP SCF energy:	-1925.46723770 a.u.
B3LYP enthalpy:	-1924.81344700 a.u.
B3LYP free energy:	-1924.86932600 a.u.
M06-2X SCF energy in solution:	-1925.25109493 a.u.
M06-2X enthalpy in solution:	-1924.59730423 a.u.
M06-2X free energy in solution:	-1924.65318323 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	1.13086700	-0.94670400	-0.32749600
C	0.58227100	-2.66821600	0.04394800
C	0.64151600	-3.66470300	-0.94300600
C	0.13266000	-3.00598400	1.32686700
C	0.26064100	-4.97379800	-0.64794500
H	0.97911900	-3.40356400	-1.94166000
C	-0.24364500	-4.31845700	1.62401500
H	0.06329400	-2.22612000	2.07979800
C	-0.17991900	-5.30369100	0.63670600

H	0.30733500	-5.73776100	-1.41998300
H	-0.58789000	-4.57073500	2.62428400
H	-0.47318100	-6.32519300	0.86616200
C	2.95854600	-1.02183900	-0.23993800
C	3.59845900	-1.58921100	0.87281300
C	3.73479900	-0.46876800	-1.26755500
C	4.99082000	-1.59528100	0.96059200
H	3.00961500	-2.04383400	1.66559100
C	5.12742100	-0.47766600	-1.17805500
H	3.23347400	-0.05476900	-2.13613800
C	5.75721500	-1.03716800	-0.06475600
H	5.47646400	-2.04050600	1.82514200
H	5.72156600	-0.05059700	-1.98191800
H	6.84225900	-1.04447600	0.00167100
N	0.46665400	0.06066200	0.74048200
N	0.83642000	-0.69986700	-1.92749100
Li	-1.48009900	0.26798700	0.18060400
C	-0.39071700	-0.42610600	-2.34166000
O	-1.44926000	-0.25458500	-1.66981000
O	-0.46142100	-0.32273500	-3.70357100
C	-1.73833900	-0.02780000	-4.25731500
H	-1.59637200	-0.03887000	-5.34058000
H	-2.09581500	0.96009800	-3.94505800
H	-2.48484700	-0.77632000	-3.97223600
C	1.20612100	0.90072900	1.67400900
H	2.17743200	0.44856300	1.93376400
C	0.40445000	0.98926600	2.99048900
H	-0.58616000	1.42238300	2.80717200
H	0.90741500	1.60330900	3.74530100
H	0.26236700	-0.01547600	3.40250600
C	1.54261000	2.30747000	1.14266800
C	2.24260200	3.21852100	1.95185500
C	1.20731900	2.71003800	-0.15510200
C	2.57642300	4.49079000	1.48983500
H	2.54466500	2.92597000	2.95510300
C	1.54091700	3.98499100	-0.62415800
H	0.69845000	2.00510000	-0.80344800
C	2.22143300	4.88374500	0.19666300
H	3.12049000	5.17437200	2.13739900
H	1.27936200	4.26756100	-1.64158800
H	2.48520600	5.87314600	-0.16846300
O	-2.90216700	-0.91076800	0.98523300
C	-3.81859300	-0.55500900	2.04148600
C	-3.39931800	-2.05699800	0.25888200
C	-4.97902100	-1.56055000	1.96340500
H	-4.14678000	0.47539500	1.86498800
H	-3.28883000	-0.59193100	2.99999700
C	-4.90589200	-2.04847300	0.50684600
H	-2.92846500	-2.96651400	0.65434400
H	-3.10311300	-1.92655100	-0.78312200
H	-4.80795600	-2.39783400	2.64981100
H	-5.94028800	-1.10649900	2.22237200
H	-5.36391900	-3.03119900	0.35854600
H	-5.39904600	-1.33560600	-0.16502000
O	-2.50835300	2.04217500	0.23084400
C	-3.31194400	2.30289700	-0.93259500
C	-2.23091200	3.30656800	0.87129100
C	-2.74456500	3.60657000	-1.49070500
H	-4.36691900	2.41635400	-0.63688600
H	-3.20208000	1.44204500	-1.59346100
C	-2.39681200	4.39988100	-0.21159300
H	-1.21672800	3.24960500	1.26851600
H	-2.93544600	3.44899900	1.70165700
H	-1.83941400	3.39198700	-2.06840100
H	-3.45035800	4.13253500	-2.14107200
H	-1.48279800	4.98725800	-0.33059300
H	-3.20602000	5.08750600	0.05569600

M3a(THF)$_2$

B3LYP SCF energy:	-1925.46372880 a.u.
B3LYP enthalpy:	-1924.81013200 a.u.
B3LYP free energy:	-1924.86844000 a.u.
M06-2X SCF energy in solution:	-1925.24723245 a.u.
M06-2X enthalpy in solution:	-1924.59363565 a.u.
M06-2X free energy in solution:	-1924.65194365 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	1.11106300	-0.27765900	-0.17734800
C	2.45421300	-1.14686800	0.73217300
C	2.19153500	-2.39296500	1.32044700
C	3.70438000	-0.54759700	0.94650900
C	3.15557700	-3.02546700	2.10393600
H	1.23148700	-2.86932900	1.14498000
C	4.66771100	-1.17784400	1.73673100
H	3.93579200	0.40728700	0.48283400
C	4.39551500	-2.41759800	2.31626700
H	2.94359700	-3.99721300	2.54287400
H	5.63291000	-0.70272100	1.89249900
H	5.14781100	-2.91163100	2.92577200
C	1.97709500	0.57732500	-1.55819600
C	1.64078500	1.90979800	-1.83885200
C	2.93333600	-0.07278500	-2.35722600
C	2.25268800	2.58573300	-2.89659800
H	0.90251800	2.41486900	-1.22349000
C	3.53909300	0.60573400	-3.41442000
H	3.17627600	-1.11155400	-2.16415300
C	3.20302500	1.93505300	-3.68430100
H	1.98899300	3.62052700	-3.10018100
H	4.27404000	0.09433000	-4.03094900
H	3.68094900	2.46084200	-4.50735900
N	0.22294200	0.70226000	0.74146000
N	-0.03914400	-1.33048600	-0.71844500
Li	-1.48127400	-0.31215200	0.28941900
C	0.24610800	-2.33844900	-1.56529200
O	1.32752700	-2.73033200	-2.00062100
O	-0.92811200	-2.98423000	-1.93830200
C	-0.74038900	-4.08870300	-2.82369900
H	-1.74055400	-4.48055500	-3.02434500
H	-0.11682900	-4.86329500	-2.36616100
H	-0.26509800	-3.77195400	-3.75705100
C	0.79673700	1.70611300	1.62727200
H	1.88026600	1.83378700	1.46124700

C	0.63236600	1.27332100	3.10250600
H	-0.43246800	1.15997700	3.33677800
H	1.05745200	2.00729600	3.79761800
H	1.12891600	0.31054700	3.26299100
C	0.17555400	3.09573400	1.43205300
C	0.78496500	4.21569500	2.01857800
C	-1.00187300	3.29296800	0.70158000
C	0.23263500	5.48938700	1.89126000
H	1.70972900	4.08827700	2.57862500
C	-1.56044900	4.56852400	0.57328400
H	-1.46390700	2.43951800	0.21553300
C	-0.94910500	5.67157500	1.16839600
H	0.72781500	6.34154100	2.35078800
H	-2.47443300	4.70006300	-0.00209200
H	-1.38157700	6.66354400	1.06493100
O	-2.87763900	0.42497000	-0.91829200
C	-4.20273600	0.87573900	-0.56278000
C	-2.79110300	0.17973600	-2.34435600
C	-4.95563800	1.05916000	-1.88620800
H	-4.11240900	1.80111900	0.01592200
H	-4.66628500	0.11159300	0.07268700
C	-4.24081600	0.06118400	-2.81134100
H	-2.19262800	-0.72178200	-2.48604100
H	-2.28156600	1.02900900	-2.81803900
H	-6.02812700	0.86813000	-1.78410400
H	-4.82867800	2.08139500	-2.26125600
H	-4.61347000	-0.95591800	-2.64101300
H	-4.35995300	0.29485500	-3.87355700
O	-2.58760900	-1.40543800	1.54856400
C	-2.88906600	-2.73586900	1.05709800
C	-2.35456500	-1.44367700	2.97842600
C	-2.40280700	-3.68553000	2.14977000
H	-2.38069900	-2.86277300	0.09841600
H	-3.97532000	-2.81887600	0.91058400
C	-2.68270300	-2.87330200	3.42390600
H	-2.98744000	-0.68604500	3.45214800
H	-1.30539500	-1.18765300	3.15908700
H	-2.91905700	-4.65007400	2.12839900
H	-1.32790900	-3.86908200	2.03845600
H	-3.73935500	-2.95789200	3.70418400
H	-2.07984400	-3.18771400	4.28097500

M3b(THF)$_2$

B3LYP SCF energy:	-1925.46388670 a.u.
B3LYP enthalpy:	-1924.81025900 a.u.
B3LYP free energy:	-1924.86693500 a.u.
M06-2X SCF energy in solution:	-1925.24650041 a.u.
M06-2X enthalpy in solution:	-1924.59287271 a.u.
M06-2X free energy in solution:	-1924.64954871 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	1.09071700	0.10941000	-0.10150700
C	2.58030200	-0.32816500	0.89026200
C	2.71575700	-1.63200100	1.39002400
C	3.53029400	0.63772500	1.25736000
C	3.77428200	-1.96317500	2.23531500
H	1.99093900	-2.38719400	1.10097800
C	4.58769100	0.30758700	2.10725000
H	3.45555800	1.64923100	0.86767200
C	4.71174500	-0.99313100	2.59779100
H	3.87206600	-2.98024700	2.60671700
H	5.31678500	1.06584200	2.38121000
H	5.53748800	-1.25136500	3.25576200
C	1.73358800	1.23765000	-1.40934900
C	0.92949100	2.31561700	-1.80751800
C	2.96881200	1.03664900	-2.04682600
C	1.35023300	3.17600900	-2.82343000
H	-0.02149200	2.48062500	-1.31072300
C	3.38711000	1.89747600	-3.06096700
H	3.59733200	0.20278400	-1.75348100
C	2.57906600	2.96862700	-3.45108900
H	0.71977900	4.01087000	-3.11841800
H	4.34517200	1.73277300	-3.54770800
H	2.90876200	3.63984700	-4.24020000
N	-0.11002100	0.74561700	0.76231000
N	0.35119400	-1.22509400	-0.71057300
Li	-1.38988200	-0.74214600	0.20112600
C	0.79694500	-2.13784700	-1.58937000
O	0.11618900	-3.05052300	-2.06442500
O	2.12756300	-2.01083500	-1.93494000
C	2.60564700	-2.96506200	-2.88461000
H	3.65707200	-2.71821300	-3.04790400
H	2.05084400	-2.89622000	-3.82505100
H	2.51238900	-3.98470100	-2.49899200
C	0.05483800	1.88932700	1.64889400
H	1.04302300	2.36633600	1.52949800
C	-0.03496300	1.43726800	3.12461900
H	-1.00796400	0.96670000	3.30748200
H	0.07357600	2.27752500	3.82078700
H	0.75101500	0.70476800	3.33677700
C	-0.97580600	2.99634100	1.38679200
C	-0.81246100	4.25169900	1.99297700
C	-2.09517200	2.80041700	0.56994100
C	-1.74034300	5.27430100	1.80133000
H	0.05917200	4.43300600	2.61936500
C	-3.02956000	3.82282200	0.37647200
H	-2.21679000	1.84610000	0.06763400
C	-2.85955500	5.06227700	0.99218400
H	-1.58699400	6.23943400	2.27835700
H	-3.89024000	3.64963800	-0.26604700
H	-3.58415700	5.85790800	0.83838800
O	-2.89928000	-0.53361600	-1.07458200
C	-4.29255800	-0.54900900	-0.68937700
C	-2.74441100	-1.04032900	-2.42702800
C	-5.07474200	-0.98453300	-1.93510900
H	-4.56769300	0.44979100	-0.33383100
H	-4.40617400	-1.25872600	0.13850900
C	-4.03313300	-1.81076700	-2.70620500
H	-1.84084400	-1.65309400	-2.45267900
H	-2.63003500	-0.18765400	-3.10973400
H	-5.97754100	-1.54838200	-1.68121600
H	-5.37791400	-0.11075900	-2.52388200

H	-3.96368500	-2.82514700	-2.29602500
H	-4.25001000	-1.89038900	-3.77569600
O	-2.09431100	-2.21708000	1.35884700
C	-1.90336800	-3.53447100	0.77551100
C	-1.84997600	-2.26348000	2.78558600
C	-1.12253800	-4.32518900	1.82286400
H	-1.37499200	-3.41390300	-0.17387600
H	-2.89134800	-3.98073200	0.59429000
C	-1.66805600	-3.74413900	3.13668700
H	-2.69873600	-1.79699900	3.29664700
H	-0.94803900	-1.67865000	2.99729100
H	-1.27285200	-5.40496200	1.72991700
H	-0.05019700	-4.11943800	1.72691300
H	-2.63223100	-4.20374300	3.38464700
H	-0.99661000	-3.88756000	3.98860300

D1a

B3LYP SCF energy:	-2921.11433900 a.u.
B3LYP enthalpy:	-2920.29335100 a.u.
B3LYP free energy:	-2920.36367300 a.u.
M06-2X SCF energy in solution:	-2920.80910474 a.u.
M06-2X enthalpy in solution:	-2919.98811674 a.u.
M06-2X free energy in solution:	-2920.05843874 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	3.57906100	-0.95220500	0.28934500
C	5.20064200	-1.34638900	1.03809900
C	5.26412100	-2.06127500	2.24228500
C	6.38789100	-0.88143000	0.45254600
C	6.49565900	-2.30380700	2.85178100
H	4.34635300	-2.43643400	2.68326000
C	7.61809000	-1.12509100	1.06427000
H	6.35251400	-0.33727200	-0.48738000
C	7.67307400	-1.83553200	2.26521200
H	6.53635900	-2.86311500	3.78283100
H	8.53277000	-0.76573200	0.60029300
H	8.63173300	-2.02790300	2.73988900
C	3.81229600	-1.16812500	-1.52104800
C	3.89144400	-0.04039600	-2.34891300
C	3.92800900	-2.44749100	-2.08825400
C	4.08577700	-0.18883600	-3.72471300
H	3.79414500	0.94883500	-1.91080800
C	4.12117200	-2.59272900	-3.46097800
H	3.85802700	-3.32510100	-1.45227200
C	4.20048900	-1.46314300	-4.28082800
H	4.14381300	0.69168800	-4.35910700
H	4.20622800	-3.58628300	-3.89356700
H	4.34878300	-1.57875100	-5.35146800
N	3.04808100	0.52418100	0.63626400
N	2.61299200	-2.21787200	0.77561300
Li	1.15480300	0.62648000	0.19200500
C	1.31470100	-2.16360700	0.59918000
O	0.61615000	-1.21953400	0.09736800
O	0.56252700	-3.22578900	0.99320800
C	1.23928500	-4.35056400	1.56252700
H	0.45794500	-5.08501900	1.76671800
H	1.74878000	-4.07133300	2.48913400
H	1.97450600	-4.75814100	0.86341300
C	3.81566000	1.56848200	1.33059300
H	4.75523900	1.16043700	1.72874900
C	3.01094800	2.09561600	2.53272000
H	2.04553100	2.50600100	2.21289900
H	3.55809500	2.88869000	3.05694100
H	2.81653600	1.27867600	3.23633700
C	4.19980800	2.70500200	0.38126800
C	5.54571900	2.98543600	0.11749400
C	3.22222200	3.48744100	-0.25389900
C	5.91261600	4.00977100	-0.75985900
H	6.31699800	2.39128600	0.60362400
C	3.58345700	4.50947200	-1.13142200
H	2.16818300	3.30552800	-0.05539300
C	4.93154100	4.77438000	-1.38997000
H	6.96487400	4.20779800	-0.94949900
H	2.81048200	5.10445000	-1.61203100
H	5.21175300	5.57150300	-2.07378900
O	-0.61521300	1.21896100	0.09477200
Li	-1.15372900	-0.62660000	0.19480100
C	-1.31370200	2.16408600	0.59465600
N	-3.04694600	-0.52325100	0.63862800
N	-2.61189500	2.21863300	0.77150300
O	-0.56151600	3.22730100	0.98591300
P	-3.57873700	0.95225100	0.28897200
C	-3.81540100	-1.56755400	1.33200100
C	-1.23818600	4.35334600	1.55281200
C	-5.19923700	1.34774500	1.03945600
C	-3.81495400	1.16542200	-1.52139000
H	-4.75514700	-1.15934400	1.72960500
C	-3.01161400	-2.09493100	2.53465400
C	-4.19916800	-2.70405500	0.38250000
H	-0.45682600	5.08830700	1.75510200
H	-1.74743400	4.07623600	2.48018900
H	-1.97360300	4.75927700	0.85294600
C	-5.26074600	2.06299800	2.24352400
C	-6.38752200	0.88335500	0.45555800
C	-3.89405400	0.03658100	-2.34773200
C	-3.93261900	2.44396100	-2.09007100
H	-2.04604100	-2.50545600	2.21548900
H	-3.55928400	-2.88793500	3.05842900
H	-2.81756800	-1.27804100	3.23842700
C	-5.54495900	-2.98449600	0.11814500
C	-3.22130100	-3.48655600	-0.25217700
C	-6.49134900	2.30648300	2.85451800
H	-4.34219700	2.43770300	2.68326400
C	-7.61679100	1.12794300	1.06878800
H	-6.35368900	0.33891800	-0.48426500
C	-4.09032500	0.18309900	-3.72346900
H	-3.79520800	-0.95203000	-1.90860400
C	-4.12768500	2.58728300	-3.46272400
H	-3.86264000	3.32245000	-1.45530200
C	-5.91146800	-4.00888800	-0.75931300
H	-6.31645100	-2.39030900	0.60389200
C	-3.58213900	-4.50864000	-1.12978900

H	-2.16735800	-3.30463200	-0.05316300
C	-7.66980500	1.83876700	2.26959000
H	-6.53050600	2.86610100	3.78544800
H	-8.53228500	0.76900100	0.60609400
C	-4.20698100	1.45658600	-4.28104400
H	-4.14833200	-0.69828700	-4.35666600
H	-4.21424000	3.58021000	-3.89645600
C	-4.93011800	-4.77354200	-1.38892800
H	-6.96364200	-4.20691100	-0.94942300
H	-2.80896400	-5.10366800	-1.61001100
H	-8.62773800	2.03186700	2.74543500
H	-4.35676800	1.57069900	-5.35163700
H	-5.21002700	-5.57070900	-2.07282000

D1b

B3LYP SCF energy:	-2921.10701700 a.u.
B3LYP enthalpy:	-2920.28659900 a.u.
B3LYP free energy:	-2920.35770700 a.u.
M06-2X SCF energy in solution:	-2920.80733973 a.u.
M06-2X enthalpy in solution:	-2919.98692173 a.u.
M06-2X free energy in solution:	-2920.05802973 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	3.41302800	-1.17960200	-0.05341600
C	5.14420900	-1.75650700	0.07132700
C	5.43829000	-3.05129100	0.51936700
C	6.19455600	-0.88889100	-0.26781100
C	6.76589600	-3.46847300	0.63247600
H	4.61886500	-3.71972500	0.76162300
C	7.51903700	-1.31018000	-0.15522300
H	5.97914100	0.11654500	-0.61935800
C	7.80615600	-2.60077200	0.29652600
H	6.98649400	-4.47466300	0.97937400
H	8.32584900	-0.63291200	-0.42260100
H	8.83884300	-2.92917000	0.38228900
C	3.16751200	-0.67987100	-1.80301000
C	3.23378200	0.67426000	-2.15846300
C	2.95245100	-1.64471200	-2.79992900
C	3.08945600	1.05823700	-3.49363200
H	3.39010200	1.41771800	-1.38186500
C	2.80840600	-1.25781600	-4.13181300
H	2.89516000	-2.69364500	-2.52459000
C	2.87791500	0.09391600	-4.48005000
H	3.14127900	2.11045600	-3.76140600
H	2.64126000	-2.01009400	-4.89841200
H	2.76624900	0.39362100	-5.51908700
N	3.07871600	0.08523300	0.88267300
N	2.54560700	-2.57556300	0.14614500
Li	1.14094200	0.19305300	0.90648200
C	1.25144700	-2.58299300	0.34449900
O	0.45066800	-1.58462700	0.45857400
O	0.73635100	-3.83568600	0.44304000
C	-0.65536900	-3.97281100	0.71166700
H	-0.83776200	-5.04748700	0.76807500
H	-1.26796700	-3.54613700	-0.08998400
H	-0.92872700	-3.50759500	1.66469400
C	3.93694100	0.59665200	1.95698300
H	4.81244100	-0.05107400	2.10476800
C	3.16554400	0.61674700	3.29153800
H	2.27684800	1.25717200	3.21743900
H	3.78724000	1.00780600	4.10581200
H	2.84261700	-0.39769000	3.55352200
C	4.47183100	1.99265200	1.63034400
C	5.83605400	2.27938800	1.75798800
C	3.61246000	3.02157500	1.21567600
C	6.33513000	3.55474900	1.47860300
H	6.51751000	1.49231400	2.07457800
C	4.10595200	4.29587800	0.93703700
H	2.54867800	2.82298900	1.11068000
C	5.47088300	4.56822700	1.06587400
H	7.39949200	3.75265800	1.58055000
H	3.42345900	5.08010900	0.61767400
H	5.85491900	5.56096900	0.84533800
O	-0.54015800	0.95880100	0.82999400
Li	-1.24815100	-0.77829400	0.42074900
C	-1.21452400	2.01685700	1.07105100
N	-3.23201400	-0.46499400	0.41873700
N	-2.46931900	2.26432600	0.76612900
O	-0.50138900	2.96430100	1.72685700
P	-3.32529500	1.07674800	-0.04288300
C	-4.02125100	-0.95413800	1.55808800
C	-1.16160400	4.19091300	2.05507600
C	-5.03252700	1.72994000	-0.02385600
C	-2.74922200	1.10626400	-1.78107400
H	-4.81706500	-0.24047400	1.82359400
C	-3.14114900	-1.11418800	2.81858900
C	-4.72743000	-2.27540100	1.23686200
H	-0.41532900	4.78818200	2.58184900
H	-2.02670700	4.00730200	2.69798600
H	-1.49392600	4.70922500	1.15089800
C	-5.32356200	3.02500700	0.42642000
C	-6.07371800	0.91437200	-0.49521300
C	-2.91255500	-0.02148900	-2.59920400
C	-2.17696700	2.26726500	-2.32218900
H	-2.33391500	-1.83590900	2.63735200
H	-3.71933100	-1.48033600	3.67438600
H	-2.69103700	-0.15346300	3.09215600
C	-5.72843300	-2.75146800	2.09764600
C	-4.40600100	-3.04273700	0.11214900
C	-6.63670600	3.49721400	0.40158700
H	-4.51583000	3.64658400	0.79670800
C	-7.38442000	1.38926100	-0.51712700
H	-5.85911100	-0.09666200	-0.83028400
C	-2.49941700	0.00839300	-3.93204700
H	-3.35855800	-0.91840800	-2.18174400
C	-1.76747300	2.29529600	-3.65504700
H	-2.04809500	3.14304100	-1.69380900
C	-6.37761900	-3.96013000	1.85045500
H	-6.00996800	-2.16321400	2.96913300
C	-5.05094300	-4.25752900	-0.13835800
H	-3.65374100	-2.66841500	-0.57421800
C	-7.66707000	2.68218700	-0.07039000

H	-6.85509700	4.50219600	0.75328500
H	-8.18447500	0.74922800	-0.87906100
C	-1.92645800	1.16598500	-4.46112800
H	-2.62486500	-0.87260000	-4.55594100
H	-1.32044600	3.19768300	-4.06341500
C	-6.03774600	-4.72270700	0.73003700
H	-7.15333800	-4.30483200	2.52980300
H	-4.78502600	-4.83638600	-1.01984200
H	-8.68900300	3.05197200	-0.08804100
H	-1.60352900	1.18831200	-5.49855100
H	-6.54315000	-5.66475700	0.53412300

D1c

B3LYP SCF energy:	-2921.10085450 a.u.
B3LYP enthalpy:	-2920.28064400 a.u.
B3LYP free energy:	-2920.35008500 a.u.
M06-2X SCF energy in solution:	-2920.80660664 a.u.
M06-2X enthalpy in solution:	-2919.98639614 a.u.
M06-2X free energy in solution:	-2920.05583714 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	3.35087800	-1.06949000	-0.28246400
C	5.06855700	-1.69236100	-0.30982500
C	5.35130200	-3.06331100	-0.22995700
C	6.12401100	-0.77467100	-0.42987700
C	6.67355300	-3.50766700	-0.27519700
H	4.52889700	-3.76268200	-0.12471700
C	7.44330600	-1.22350600	-0.47400700
H	5.91374100	0.29034800	-0.47097100
C	7.71912800	-2.59087100	-0.39911600
H	6.88674300	-4.57150500	-0.21079100
H	8.25498700	-0.50633100	-0.56176400
H	8.74796800	-2.94005800	-0.43355100
C	2.90436900	-0.59763400	-1.99647600
C	3.11273800	0.71237300	-2.45280300
C	2.38478800	-1.55643000	-2.87967500
C	2.79872300	1.05944100	-3.76777700
H	3.51622200	1.45252700	-1.76958400
C	2.07323600	-1.20701700	-4.19378500
H	2.22329200	-2.57163200	-2.53012900
C	2.27876400	0.10055500	-4.63907500
H	2.96180500	2.07763000	-4.11148000
H	1.66794000	-1.95557600	-4.86929400
H	2.03540400	0.37110200	-5.66326500
N	3.17945400	0.27984200	0.58835800
N	2.48064700	-2.43471600	0.07708400
Li	1.20638300	0.49002600	0.54271300
C	1.20960300	-2.36522300	0.39394200
O	0.46823500	-1.32058800	0.49796200
O	0.65328800	-3.57656600	0.63859100
C	-0.72093100	-3.62468900	1.01469700
H	-0.94533900	-4.68220200	1.16397200
H	-1.36835400	-3.22413600	0.22758300
H	-0.90268500	-3.08000500	1.94705700
C	3.84528000	0.40604100	1.89417900
H	4.55625800	-0.41818100	2.06203900
C	2.81611700	0.33462400	3.04510300
H	2.08335400	1.14851100	2.95789600
H	3.29471000	0.43411100	4.02573900
H	2.28152500	-0.62191100	3.01894900
C	4.66135800	1.69826300	2.00444100
C	5.59543100	1.83993200	3.04187200
C	4.50144600	2.76250200	1.11075400
C	6.33686100	3.01137600	3.18935300
H	5.75027800	1.01771700	3.73817300
C	5.23927300	3.94082700	1.25622600
H	3.80177900	2.64822400	0.28960400
C	6.15877500	4.07133400	2.29654800
H	7.05884600	3.09508700	3.99794400
H	5.09977400	4.75470300	0.54837600
H	6.73710700	4.98482600	2.40784400
O	-0.46798300	1.32019800	0.49775900
Li	-1.20621100	-0.49040500	0.54229900
C	-1.20922700	2.36495500	0.39416400
N	-3.17924400	-0.27995600	0.58821500
N	-2.48034200	2.43469600	0.07767000
O	-0.65266100	3.57617400	0.63888500
P	-3.35091400	1.06973100	-0.28198800
C	-3.84495900	-0.40695500	1.89400100
C	0.72173300	3.62403000	1.01438000
C	-5.06854000	1.69281000	-0.30826100
C	-2.90531000	0.59860300	-1.99643900
H	-4.55618900	0.41697000	2.06223900
C	-2.81578500	-0.33570100	3.04492700
C	-4.66065700	-1.69946800	2.00372800
H	0.94635700	4.68148200	1.16376500
H	1.36873000	3.22353100	0.22688700
H	0.90384400	3.07915200	1.94655800
C	-5.35108900	3.06373500	-0.22729100
C	-6.12415700	0.77533800	-0.42856400
C	-3.11395800	-0.71120700	-2.45320400
C	-2.38618000	1.55775700	-2.87951400
H	-2.08275100	-1.14930400	2.95735500
H	-3.29431400	-0.43576300	4.02553600
H	-2.28151100	0.62102100	3.01916200
C	-5.59452700	-1.84193100	3.04123500
C	-4.50062700	-2.76319700	1.10945600
C	-6.67330400	3.50828700	-0.27167600
H	-4.52855200	3.76292900	-0.12190100
C	-7.44341400	1.22436700	-0.47183900
H	-5.91404500	-0.28967900	-0.47054200
C	-2.80066600	-1.05772900	-3.76849500
H	-3.51709700	-1.45163500	-1.77008200
C	-2.07535600	1.20889100	-4.19394300
H	-2.22446300	2.57280300	-2.52961800
C	-6.33564500	-3.01363800	3.18820800
H	-5.74948000	-1.02013100	3.73800200
C	-5.23813700	-3.94178400	1.25441500
H	-3.80110300	-2.64832500	0.28827100
C	-7.71904100	2.59171100	-0.39584000
H	-6.88633600	4.57210500	-0.20641800
H	-8.25521800	0.50735400	-0.55980300

C	-2.28116200	-0.09848700	-4.63967300
H	-2.96395800	-2.07576900	-4.11253900
H	-1.67041600	1.95772700	-4.86935900
C	-6.15744500	-4.07307400	2.29481000
H	-7.05747600	-3.09795600	3.99687400
H	-5.09854300	-4.75524800	0.54611000
H	-8.74785100	2.94104700	-0.42961400
H	-2.03837800	-0.36860600	-5.66411300
H	-6.73553300	-4.98676900	2.40571000

D2a

B3LYP SCF energy:	-2921.11664810 a.u.
B3LYP enthalpy:	-2920.29617800 a.u.
B3LYP free energy:	-2920.36612700 a.u.
M06-2X SCF energy in solution:	-2920.81444177 a.u.
M06-2X enthalpy in solution:	-2919.99397167 a.u.
M06-2X free energy in solution:	-2920.06392067 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	3.51244800	0.59342000	0.16703500
C	2.94348300	2.33305000	0.23610100
C	2.56449800	3.00096000	-0.93623400
C	2.92367700	3.02342300	1.45759200
C	2.16665700	4.33834200	-0.88636100
H	2.57341100	2.45684400	-1.87559100
C	2.53149700	4.36067800	1.50351500
H	3.20977900	2.50801700	2.36958400
C	2.15192700	5.01958600	0.33146700
H	1.86584800	4.84604100	-1.79901600
H	2.51889700	4.88777900	2.45399100
H	1.84444300	6.06155400	0.36881100
C	5.34115200	0.63764300	0.24750300
C	6.04859800	0.03586100	1.29648700
C	6.05134700	1.27680600	-0.78123000
C	7.44430700	0.07165200	1.31420900
H	5.49228500	-0.45085000	2.08997600
C	7.44470600	1.31303700	-0.76025300
H	5.51116700	1.74856900	-1.59770900
C	8.14339700	0.70912900	0.28826600
H	7.98560400	-0.39798500	2.13155600
H	7.98522700	1.81209600	-1.56015300
H	9.22986500	0.73746000	0.30489000
N	2.95890400	0.00069800	-1.22479800
N	3.10821500	-0.10098400	1.63325100
Li	1.00862600	-0.32925600	-0.86932200
C	1.84593700	-0.40035500	1.84917700
O	0.85559400	-0.26034300	1.05790900
O	1.50217400	-0.93170400	3.05197500
C	2.54187000	-1.13145700	4.01347100
H	2.04570100	-1.53998200	4.89612500
H	3.03596000	-0.18704600	4.25856900
H	3.28965700	-1.83611300	3.63847100
C	3.64275300	-1.09262000	-1.94265200
H	4.66795800	-1.23209600	-1.56893800
C	3.75658900	-0.72429300	-3.43091000
H	2.76897400	-0.52361700	-3.86102600
H	4.22602000	-1.53237500	-4.00485300
H	4.35996500	0.18267700	-3.54393900
C	2.91950700	-2.42510300	-1.74410500
C	3.52464400	-3.46595600	-1.02902300
C	1.62247900	-2.62960800	-2.24235700
C	2.85763600	-4.67328200	-0.81004600
H	4.53067300	-3.32668200	-0.63840200
C	0.94692100	-3.83008100	-2.01508800
H	1.12659600	-1.85492300	-2.82393300
C	1.56376200	-4.85825700	-1.29941900
H	3.34936400	-5.46817100	-0.25434900
H	-0.06131800	-3.95672400	-2.39970800
H	1.03980100	-5.79439100	-1.12577600
O	-0.85621600	-0.26137900	-1.05537400
Li	-1.00952500	-0.32748100	0.87239400
C	-1.84606900	-0.40295800	-1.84692900
N	-2.96067400	0.00091600	1.22610200
N	-3.10863500	-0.10392700	-1.63205800
O	-1.50143500	-0.93568000	-3.04887500
P	-3.51382300	0.59178400	-0.16674400
C	-3.64315700	-1.09404800	1.94288300
C	-2.54058000	-1.13754200	-4.01051600
C	-2.94576000	2.33162500	-0.23717200
C	-5.34253100	0.63485000	-0.24802700
H	-4.66765100	-1.23552900	1.56795400
C	-3.75951800	-0.72630700	3.43108700
C	-2.91688300	-2.42494400	1.74474300
H	-2.04386000	-1.54771700	-4.89209500
H	-3.03470400	-0.19370700	-4.25778200
H	-3.28843700	-1.84157600	-3.63450500
C	-2.92510400	3.02048800	-1.45949600
C	-2.56836700	3.00119100	0.93473200
C	-6.05354900	1.27319600	0.78065200
C	-6.04916800	0.03311700	-1.29758100
H	-2.77284800	-0.52356500	3.86240200
H	-4.22786500	-1.53552500	4.00431200
H	-4.36498800	0.17932500	3.54359000
C	-3.51831800	-3.46628300	1.02722900
C	-1.62046100	-2.62726200	2.24545300
C	-2.53362800	4.35790600	-1.50667400
H	-3.20995200	2.50375000	-2.37112700
C	-2.17124100	4.33873800	0.88360600
H	-2.57799800	2.45825600	1.87476200
C	-7.44691300	1.30869500	0.75903200
H	-5.51398200	1.74481700	1.59761600
C	-7.44489100	0.06817300	-1.31594600
H	-5.49222200	-0.45302000	-2.09097600
C	-2.84830900	-4.67194600	0.80833100
H	-4.52378300	-3.32866400	0.63458200
C	-0.94187100	-3.82604100	2.01825300
H	-1.12740400	-1.85211300	2.82879900
C	-2.15565000	5.01848000	-0.33505300
H	-2.52035000	4.88383900	-2.45778700
H	-1.87167500	4.84774900	1.79593900
C	-8.14479500	0.70485600	-0.29006900
H	-7.98808500	1.80710900	1.55889600

H	-7.98555700	-0.40143300	-2.13372900
C	-1.55504800	-4.85472100	1.30018100
H	-3.33719000	-5.46726300	0.25073700
H	0.06586600	-3.95090900	2.40475000
H	-1.84873200	6.06058000	-0.37336800
H	-9.23127000	0.73260800	-0.30717700
H	-1.02869400	-5.78950200	1.12652400

D2b

B3LYP SCF energy:	-2921.10900790 a.u.
B3LYP enthalpy:	-2920.28866200 a.u.
B3LYP free energy:	-2920.35784500 a.u.
M06-2X SCF energy in solution:	-2920.81012903 a.u.
M06-2X enthalpy in solution:	-2919.98978313 a.u.
M06-2X free energy in solution:	-2920.05896613 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	3.25955100	-0.82563600	-0.14369000
C	2.54490400	-2.51197800	-0.13834000
C	2.21702500	-3.13953400	1.07168600
C	2.37183100	-3.21022200	-1.34334800
C	1.71977200	-4.44427400	1.07625800
H	2.34728100	-2.59139000	1.99998100
C	1.87935900	-4.51428000	-1.33530300
H	2.61922400	-2.72577500	-2.28310000
C	1.55317900	-5.13289100	-0.12582300
H	1.46154900	-4.92057500	2.01835200
H	1.74795800	-5.04776700	-2.27301700
H	1.16865600	-6.14943700	-0.12155300
C	5.06879600	-1.04047800	-0.31245600
C	5.78633900	-0.40921500	-1.33701600
C	5.75730000	-1.82344300	0.62754000
C	7.17211900	-0.55953700	-1.41855400
H	5.24602500	0.18834200	-2.06288100
C	7.14087300	-1.97253300	0.54314300
H	5.20881700	-2.32123000	1.42295200
C	7.85033600	-1.33957200	-0.48059400
H	7.72171500	-0.06853200	-2.21748400
H	7.66484800	-2.58323600	1.27350800
H	8.92885500	-1.45682900	-0.54719700
N	2.82622300	-0.14482000	1.25799700
N	2.83639000	-0.11933200	-1.59512700
Li	0.85428400	0.13751300	1.00854200
C	1.59968100	0.30547200	-1.73346300
O	0.64565500	0.23906000	-0.88789000
O	1.24084100	0.89289100	-2.90234000
C	2.24458800	1.03295500	-3.91254400
H	1.73991600	1.50387700	-4.75828000
H	2.64549100	0.05802700	-4.20325500
H	3.06476900	1.66453100	-3.55976600
C	3.70396500	0.84115100	1.91804100
H	4.75747000	0.54916500	1.79718700
C	3.42024800	0.82648000	3.42851200
H	2.38564300	1.11933600	3.63975800
H	4.08132800	1.52205600	3.95830400
H	3.57448600	-0.18179700	3.82748500
C	3.58653800	2.25679900	1.34730300
C	4.70059500	2.88191800	0.77399600
C	2.37855300	2.96838300	1.38284800
C	4.61475900	4.17441400	0.25037600
H	5.64656500	2.34632100	0.73219800
C	2.28460000	4.25874500	0.86234600
H	1.49462400	2.51706600	1.82879700
C	3.40564400	4.86818400	0.29254200
H	5.49439700	4.63740400	-0.19026900
H	1.33481900	4.78517800	0.90209100
H	3.33562700	5.87440900	-0.11254300
O	-0.98045300	0.45699800	1.34218700
Li	-1.15274800	0.65252500	-0.62524900
C	-2.02642300	0.37784600	2.08246100
N	-3.06289800	0.33201700	-1.08522000
N	-3.24737200	0.03797700	1.74792800
O	-1.90826400	0.68597200	3.40068600
P	-3.63797700	-0.43720100	0.20897100
C	-3.71314100	1.53770200	-1.63388600
C	-0.64265300	1.13170400	3.87510900
C	-3.09628200	-2.17881200	0.04075300
C	-5.46766400	-0.46352100	0.26653400
H	-4.72265500	1.67117000	-1.21747700
C	-3.87267400	1.38131200	-3.15475500
C	-2.92275300	2.79693600	-1.27257400
H	-0.78976100	1.35227400	4.93427300
H	-0.31657100	2.03808100	3.35417600
H	0.12370500	0.35509600	3.77225400
C	-3.10987000	-3.02804100	1.15820500
C	-2.71108300	-2.68820400	-1.20671300
C	-6.18014800	-0.90806800	-0.85849200
C	-6.17176500	-0.03852700	1.40121800
H	-2.90516100	1.18961200	-3.63168200
H	-4.31002300	2.28118800	-3.60427700
H	-4.52501700	0.52909400	-3.37242100
C	-3.44648700	3.73204600	-0.37013300
C	-1.64125600	3.02986900	-1.80027900
C	-2.74898000	-4.36846400	1.02531700
H	-3.40105900	-2.63281500	2.12692300
C	-2.34403900	-4.02908300	-1.33458300
H	-2.69178700	-2.02029200	-2.06231700
C	-7.57403400	-0.92638500	-0.84897500
H	-5.64173000	-1.24243200	-1.74137000
C	-7.56800900	-0.05561100	1.40657100
H	-5.61162800	0.29619400	2.26787400
C	-2.72054500	4.86721900	-0.00518500
H	-4.43601500	3.56617800	0.05015000
C	-0.90798100	4.16078300	-1.43145700
H	-1.20873000	2.33454900	-2.51742600
C	-2.36592600	-4.87020600	-0.22112100
H	-2.76516400	-5.02109900	1.89441000
H	-2.03951700	-4.41517000	-2.30388100
C	-8.27007000	-0.49865600	0.28460500
H	-8.11692100	-1.27403200	-1.72398900
H	-8.10730900	0.27594200	2.29020100
C	-1.44732500	5.08587700	-0.53497800

H	-3.15075400	5.58148300	0.69251000
H	0.08269700	4.31779300	-1.84944100
H	-2.08436500	-5.91524000	-0.32284900
H	-9.35699100	-0.51300100	0.29230500
H	-0.88353600	5.97289700	-0.25723700

D2c

B3LYP SCF energy:	-2921.10160490 a.u.
B3LYP enthalpy:	-2920.28181000 a.u.
B3LYP free energy:	-2920.34839600 a.u.
M06-2X SCF energy in solution:	-2920.80613178 a.u.
M06-2X enthalpy in solution:	-2919.98633688 a.u.
M06-2X free energy in solution:	-2920.05292288 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	-3.37699900	-0.68582400	0.13706800
C	-2.70588000	-2.33456700	-0.29194300
C	-2.48381400	-2.68330700	-1.63173500
C	-2.47941000	-3.28623100	0.71428000
C	-2.04213200	-3.96601000	-1.96084200
H	-2.65522300	-1.93862100	-2.40301400
C	-2.04274100	-4.56795800	0.38144600
H	-2.64599500	-3.01524400	1.75248600
C	-1.82539100	-4.90966000	-0.95551100
H	-1.86922200	-4.22783700	-3.00155800
H	-1.86937800	-5.29957100	1.16598500
H	-1.48683200	-5.91008600	-1.21274700
C	-5.18479400	-0.90537700	0.33314300
C	-5.81778900	-0.66970300	1.56098400
C	-5.95287500	-1.30710000	-0.77112700
C	-7.20029000	-0.82819300	1.67817500
H	-5.21303600	-0.37149800	2.41090300
C	-7.33256200	-1.46580300	-0.65027500
H	-5.46962200	-1.49799700	-1.72575100
C	-7.95837600	-1.22478300	0.57557900
H	-7.68437300	-0.64382600	2.63375900
H	-7.91893900	-1.77816500	-1.51035200
H	-9.03409600	-1.34911200	0.66998300
N	-2.99421400	0.28487000	-1.09906700
N	-2.89233400	-0.35443500	1.68426500
Li	-1.06138300	0.63700100	-0.76138700
C	-1.71676100	0.15629900	1.96388900
O	-0.77787800	0.50029600	1.16130900
O	-1.51882700	0.32695800	3.29600900
C	-0.30258800	0.93644700	3.71948900
H	-0.36859200	0.98919800	4.80806400
H	-0.20256700	1.94711000	3.30925200
H	0.57145700	0.33862100	3.43766400
C	-3.84308300	1.44161600	-1.45081900
H	-4.85544400	1.31791000	-1.04004200
C	-3.99602000	1.50841000	-2.97819800
H	-3.02121100	1.57486200	-3.47482700
H	-4.59597500	2.37487400	-3.28130800
H	-4.48702500	0.59858000	-3.33869900
C	-3.30243300	2.74725700	-0.86431400
C	-3.91558800	3.32284900	0.25671600
C	-2.17808800	3.39045900	-1.40365300
C	-3.42348100	4.49911000	0.82456300
H	-4.79152300	2.84228400	0.68713600
C	-1.68032600	4.56728200	-0.84015400
H	-1.69678600	2.98569800	-2.29111200
C	-2.30272100	5.12670300	0.27744600
H	-3.91999000	4.92830000	1.69126900
H	-0.80984700	5.04758700	-1.27842100
H	-1.92388700	6.04821300	0.71219500
O	0.77766500	0.50007400	-1.16092100
Li	1.06122600	0.63645600	0.76178600
C	1.71652400	0.15626200	-1.96359900
N	2.99412200	0.28463200	1.09930500
N	2.89219100	-0.35433000	-1.68410400
O	1.51843600	0.32697500	-3.29569000
P	3.37700000	-0.68582500	-0.13697900
C	3.84280900	1.44147300	1.45116200
C	0.30198800	0.93616600	-3.71900900
C	2.70618100	-2.33474500	0.29184500
C	5.18482300	-0.90501100	-0.33317900
H	4.85527400	1.31777900	1.04063700
C	3.99538100	1.50842300	2.97857300
C	3.30225600	2.74703300	0.86438700
H	0.36780700	0.98887300	-4.80759800
H	0.20180400	1.94683700	-3.30882300
H	-0.57187700	0.33816800	-3.43699700
C	2.47987400	-3.28633700	-0.71448200
C	2.48418800	-2.68367700	1.63160000
C	5.95304800	-1.30670400	0.77100200
C	5.81770100	-0.66906200	-1.56102600
H	3.02045800	1.57493600	3.47496800
H	4.59526600	2.37491800	3.28173700
H	4.48629300	0.59862900	3.33928500
C	3.91565700	3.32251600	-0.25656500
C	2.17778200	3.39026900	1.40340200
C	2.04343800	-4.56818000	-0.38178800
H	2.64640400	-3.01519900	-1.75265700
C	2.04273300	-3.96649400	1.96056700
H	2.65547100	-1.93904600	2.40296000
C	7.33276100	-1.46510900	0.65005500
H	5.46988700	-1.49780900	1.72563100
C	7.20022900	-0.82725100	-1.67831200
H	5.21284300	-0.37088400	-2.41087900
C	3.42364700	4.49869500	-0.82466000
H	4.79170100	2.84192000	-0.68673100
C	1.68011100	4.56701100	0.83965300
H	1.69628300	2.98559100	2.29078900
C	1.82615900	-4.91007300	0.95513100
H	1.87020600	-5.29973700	-1.16640800
H	1.86987900	-4.22846900	3.00125500
C	7.95845800	-1.22381400	-0.57580500
H	7.91925000	-1.77745100	1.51006300
H	7.68422100	-0.64266900	-2.63390100
C	2.30274100	5.12631700	-0.27787200
H	3.92033400	4.92779600	-1.69130900
H	0.80951600	5.04733700	1.27766300

H	1.48778700	-5.91059000	1.21225700
H	9.03419800	-1.34790500	-0.67028100
H	1.92397700	6.04776400	-0.71281600

D3a

B3LYP SCF energy:	-2921.11593990 a.u.
B3LYP enthalpy:	-2920.29528600 a.u.
B3LYP free energy:	-2920.36581800 a.u.
M06-2X SCF energy in solution:	-2920.81334198 a.u.
M06-2X enthalpy in solution:	-2919.99268808 a.u.
M06-2X free energy in solution:	-2920.06322008 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	3.30177400	0.84754500	0.43769600
C	4.97798800	1.54254700	0.20457000
C	5.17481900	2.93023900	0.20453600
C	6.07043500	0.69443900	-0.03389900
C	6.44360500	3.46050500	-0.03348900
H	4.33161000	3.58206800	0.40761300
C	7.33775200	1.22733000	-0.27109900
H	5.93388700	-0.38365400	-0.02788100
C	7.52560000	2.61123600	-0.27218000
H	6.58797300	4.53778300	-0.02758000
H	8.17841800	0.56213800	-0.44966600
H	8.51376700	3.02582500	-0.45397000
C	3.51544600	-0.54636000	1.61970400
C	3.47080900	-1.86624600	1.15241700
C	3.73537700	-0.30862700	2.98629400
C	3.64797100	-2.93381800	2.03658500
H	3.28831100	-2.05209100	0.09818000
C	3.90804300	-1.37531200	3.86772100
H	3.76241500	0.71247000	3.35505900
C	3.86570600	-2.69022300	3.39316100
H	3.61318800	-3.95395800	1.66315500
H	4.07616000	-1.18296600	4.92429500
H	4.00269600	-3.52058400	4.08127200
N	2.61126300	0.34789400	-0.92550100
N	2.50882600	2.03682700	1.28663800
Li	0.70084500	0.14791000	-0.61070600
C	1.20982800	1.96812400	1.47033900
O	0.39221300	1.09549500	1.02783900
O	0.61183400	2.92995100	2.21879600
C	1.43794000	3.95934200	2.76824700
H	0.76434600	4.59023200	3.35153200
H	1.91237200	4.54462900	1.97517700
H	2.21663100	3.53767400	3.40998800
C	3.26147500	0.28931600	-2.24069800
H	4.20269300	0.85715800	-2.23789300
C	2.34992800	0.94291600	-3.29645900
H	1.38522800	0.42345700	-3.35654400
H	2.80957600	0.90903900	-4.29147700
H	2.15958000	1.98862700	-3.03068900
C	3.61552800	-1.14287400	-2.64869500
C	4.92616200	-1.47360800	-3.01274500
C	2.64232700	-2.15420300	-2.68050500
C	5.26392800	-2.77491500	-3.39517000
H	5.69314400	-0.70196700	-2.99412300
C	2.97504100	-3.45416200	-3.06090600
H	1.61461000	-1.92645000	-2.40702200
C	4.28860400	-3.77100800	-3.41924800
H	6.28948400	-3.00797100	-3.67147800
H	2.20605200	-4.22277500	-3.07905500
H	4.54664400	-4.78487600	-3.71431400
O	-1.10380600	-0.22014600	-0.83063000
Li	-1.41056100	0.59189400	0.91169300
C	-1.96300400	-0.90569900	-1.47766200
N	-3.39836000	0.41931300	1.17239400
N	-3.27452900	-0.85095600	-1.39477200
O	-1.40168200	-1.78357700	-2.34782700
P	-3.94766800	0.25202500	-0.33352300
C	-3.76462800	-0.54221800	2.23354700
C	-2.27752600	-2.60627200	-3.12294200
C	-3.76849400	1.90568900	-1.09934500
C	-5.72485100	-0.18290800	-0.39829800
H	-4.65764500	-1.12176000	1.95416800
C	-4.11803400	0.23245100	3.51234400
C	-2.64046100	-1.55416600	2.46359300
H	-1.62349700	-3.21534500	-3.74999700
H	-2.93902500	-1.99648000	-3.74496600
H	-2.88606000	-3.24444400	-2.47601900
C	-3.66518000	3.05225300	-0.29893200
C	-3.75729300	2.03944400	-2.49602600
C	-6.63470800	0.58078400	0.35021400
C	-6.19908100	-1.25756700	-1.16223700
H	-3.29041100	0.88130100	3.82011600
H	-4.34980200	-0.44974100	4.33913000
H	-4.98894900	0.87042800	3.32931000
C	-2.79448100	-2.89119900	2.07547400
C	-1.40985800	-1.16335300	3.01576200
C	-3.54493200	4.31250800	-0.88813000
H	-3.66573100	2.94157800	0.78093700
C	-3.64247600	3.29996900	-3.08129600
H	-3.82884800	1.15352300	-3.11982900
C	-7.99462700	0.27493000	0.33362900
H	-6.27581700	1.41590300	0.94570300
C	-7.56122600	-1.56384500	-1.17468600
H	-5.49087200	-1.84083400	-1.74023700
C	-1.75216800	-3.80877100	2.22083700
H	-3.74193800	-3.21411400	1.64895600
C	-0.35960700	-2.07390900	3.15324800
H	-1.26605000	-0.13784500	3.35122900
C	-3.53480400	4.43804000	-2.27814900
H	-3.45767000	5.19515100	-0.25989800
H	-3.63198500	3.39399300	-4.16398600
C	-8.45975200	-0.79940300	-0.42901300
H	-8.69098100	0.87340200	0.91499600
H	-7.92053600	-2.40019000	-1.76885500
C	-0.52821000	-3.40148200	2.75456300
H	-1.89559800	-4.84145700	1.91212900
H	0.58950400	-1.74679400	3.56899000
H	-3.44140300	5.41951700	-2.73581800
H	-9.52004800	-1.03836500	-0.44170400

H	0.28978600	-4.10900000	2.85893500

D4a

B3LYP SCF energy:	-2921.08401160 a.u.
B3LYP enthalpy:	-2920.26280700 a.u.
B3LYP free energy:	-2920.32877700 a.u.
M06-2X SCF energy in solution:	-2920.80906761 a.u.
M06-2X enthalpy in solution:	-2919.98786301 a.u.
M06-2X free energy in solution:	-2920.05383301 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	-2.70220000	0.85820500	0.36340300
C	-4.45930100	0.39780600	0.11650300
C	-5.39660000	1.34660700	-0.31419700
C	-4.88120200	-0.91589400	0.37040300
C	-6.73100000	0.98190800	-0.50269700
H	-5.06909900	2.36590600	-0.48489700
C	-6.21450200	-1.27569300	0.18700300
H	-4.16940200	-1.66309400	0.70630300
C	-7.14160100	-0.32789200	-0.25279700
H	-7.45040000	1.72470800	-0.83799700
H	-6.52820300	-2.29709300	0.38320300
H	-8.18160100	-0.61009100	-0.39579700
C	-2.31360100	0.35280400	2.08030300
C	-1.90810200	-0.95489600	2.39050300
C	-2.50850000	1.27170400	3.12240300
C	-1.69540200	-1.33189600	3.71730300
H	-1.76260200	-1.68889600	1.60350300
C	-2.29700000	0.89160400	4.44740300
H	-2.82739900	2.28210500	2.88720300
C	-1.89050100	-0.41009600	4.74670300
H	-1.37560300	-2.34569600	3.94090300
H	-2.45020000	1.61280400	5.24590300
H	-1.72650200	-0.70569600	5.77960300
N	-1.63250100	0.04750400	-0.57829700
N	-2.75599900	2.50560500	0.28940300
Li	0.12870000	1.20190200	-0.18739700
C	-1.64209900	3.23260400	0.26830300
O	-0.43849900	2.85080300	0.28560300
O	-1.78739700	4.58120400	0.21920300
C	-3.10839700	5.12250500	0.19650300
H	-2.97619600	6.20670500	0.19980300
H	-3.64619700	4.81420500	-0.70539700
H	-3.68169700	4.80860500	1.07370300
C	-1.87400100	-0.15619600	-2.04179700
O	0.43909700	-2.85159800	0.28040300
Li	-0.12810200	-1.20259700	-0.19189700
C	1.64269700	-3.23339900	0.26240300
N	1.63289900	-0.04689900	-0.57909700
N	2.75649700	-2.50640000	0.28480300
O	1.78799500	-4.58189900	0.21130300
P	2.70229800	-0.85910000	0.36180300
C	1.87549900	0.15970100	-2.04209700
C	3.10899500	-5.12310000	0.18780300
C	4.45939900	-0.39790100	0.11700300
C	2.31229900	-0.35679900	2.07940300
H	2.97689400	-6.20730000	0.18950300
H	3.64689500	-4.81350000	-0.71359700
H	3.68219500	-4.81040000	1.06550300
C	5.39719800	-1.34580200	-0.31499700
C	4.88110000	0.91529900	0.37350300
C	1.90700000	0.95040100	2.39160300
C	2.50579800	-1.27779900	3.12000300
C	6.73159800	-0.98070300	-0.50199700
H	5.06979700	-2.36490100	-0.48779700
C	6.21440000	1.27559800	0.19160300
H	4.16900000	1.66179900	0.71060300
C	1.69300000	1.32500100	3.71900300
H	1.76260000	1.68600100	1.60600300
C	2.29299800	-0.90019900	4.44540300
H	2.82459700	-2.28790000	2.88320300
C	7.14189900	0.32879700	-0.24949700
H	7.45129800	-1.72270300	-0.83829700
H	6.52800100	2.29669700	0.38990300
C	1.88669900	0.40110100	4.74680300
H	1.37330100	2.33840100	3.94420300
H	2.44509800	-1.62289900	5.24270300
H	8.18189900	0.61139600	-0.39139700
H	1.72160000	0.69480100	5.78010300
H	0.90929900	0.52190200	-2.42679700
H	-0.90770100	-0.51789700	-2.42669700
C	-2.16030000	1.14220400	-2.81379700
H	-2.18860000	0.95700400	-3.89359700
H	-3.11120000	1.59640500	-2.51849700
H	-1.37340000	1.87750400	-2.61449700
C	-2.85680200	-1.29519500	-2.35429700
C	-4.04840200	-1.10289400	-3.06199700
C	-2.53190300	-2.60229600	-1.95449700
C	-4.89810300	-2.17519400	-3.34819700
H	-4.33220100	-0.10869400	-3.39089700
C	-3.37600400	-3.67489500	-2.23729700
H	-1.60690300	-2.79929600	-1.41549700
C	-4.56750400	-3.46469400	-2.93619700
H	-5.82050300	-1.99609300	-3.89479700
H	-3.09630500	-4.67599500	-1.91899700
H	-5.22590400	-4.29959400	-3.16189700
C	2.85810000	1.29960000	-2.35169700
C	4.05000000	1.10929900	-3.05939700
C	2.53250100	2.60580100	-1.94919700
C	4.89920100	2.18249900	-3.34309700
H	4.33419900	0.11599900	-3.39029700
C	3.37620200	3.67930000	-2.22949700
H	1.60720100	2.80120100	-1.41009700
C	4.56800200	3.47109900	-2.92849700
H	5.82190100	2.00499800	-3.88979700
H	3.09590300	4.67960000	-1.90919700
H	5.22610200	4.30669800	-3.15229700
C	2.16279800	-1.13719900	-2.81629700
H	1.37619800	-1.87309900	-2.61869700
H	2.19159800	-0.94999900	-3.89569700
H	3.11379800	-1.59150000	-2.52129700

D5a

B3LYP SCF energy:	-2921.08729130 a.u.
B3LYP enthalpy:	-2920.26595600 a.u.
B3LYP free energy:	-2920.33216200 a.u.
M06-2X SCF energy in solution:	-2920.81310722 a.u.
M06-2X enthalpy in solution:	-2919.99177192 a.u.
M06-2X free energy in solution:	-2920.05797792 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	2.61200000	0.79230600	0.27290100
C	1.79649600	2.17360400	1.17580100
C	1.68489300	3.43350400	0.57190100
C	1.30829700	2.00460300	2.48370100
C	1.08339000	4.49500200	1.25130100
H	2.07149300	3.57650500	-0.43189900
C	0.71129400	3.06730100	3.16380100
H	1.40869900	1.04740300	2.99090100
C	0.59499100	4.31470100	2.54620100
H	0.99618800	5.46330200	0.76610100
H	0.34069500	2.91860000	4.17430100
H	0.12848900	5.14220000	3.07380100
C	4.25860100	0.63241100	1.06940100
C	4.36090200	0.19921100	2.40070100
C	5.42640000	0.97211400	0.37310100
C	5.60630200	0.10041400	3.02050100
H	3.46910200	-0.07259100	2.95710100
C	6.67190000	0.87211700	0.99460100
H	5.34059900	1.30441400	-0.65489900
C	6.76540100	0.43631700	2.31720100
H	5.67080300	-0.23898600	4.05090100
H	7.57099900	1.13481900	0.44310100
H	7.73630100	0.35942000	2.79980100
N	1.58490300	-0.45599600	0.49610100
N	2.98919900	1.30700700	-1.24159900
Li	0.01150200	0.06230000	-0.86359900
C	2.09399900	1.28390500	-2.22559900
O	0.86960000	0.97970200	-2.18359900
O	2.52789800	1.64260600	-3.45979900
C	3.91449700	1.94041000	-3.62999900
H	4.02569600	2.20171000	-4.68479900
H	4.21999500	2.78161100	-3.00039900
H	4.53249900	1.07011100	-3.38999900
C	1.94040700	-1.89329500	0.24520100
O	-0.86089500	-1.18770300	2.90800100
Li	-0.08629700	-0.20540100	1.59370100
C	-2.06169400	-1.56890600	2.93990100
N	-1.67189900	0.30649500	0.24320100
N	-2.98569400	-1.53820800	1.98320100
O	-2.44119200	-2.08000700	4.14060100
P	-2.70209500	-0.94390800	0.47450100
C	-2.04520200	1.72109400	0.57120100
C	-3.78569100	-2.53271000	4.29470100
C	-4.40069600	-0.71631200	-0.18379900
C	-1.97619200	-2.28930600	-0.54679900
H	-1.08100400	2.24139700	0.65190100
H	-3.84569000	-2.91791100	5.31510100
H	-4.49719300	-1.71161200	4.16260100
H	-4.02408900	-3.32521100	3.57880100
C	-5.51739500	-1.07481500	0.58530100
C	-4.59639700	-0.22721300	-1.48459900
C	-1.57139200	-2.05020500	-1.87199900
C	-1.86318800	-3.58570500	-0.02699900
C	-6.80499500	-0.94191800	0.06340100
H	-5.35969400	-1.45961500	1.58620100
C	-5.88299800	-0.10171600	-2.00549900
H	-3.74889800	0.08109000	-2.08699900
C	-1.05519000	-3.08530300	-2.65329900
H	-1.67559500	-1.05880500	-2.30689900
C	-1.33988600	-4.61850400	-0.80779900
H	-2.18978800	-3.77860600	0.98980100
C	-6.98999700	-0.45881900	-1.23269900
H	-7.66319500	-1.22062100	0.66940100
H	-6.01939900	0.28608400	-3.01109900
C	-0.93518600	-4.37100300	-2.12039900
H	-0.75059000	-2.88580200	-3.67709900
H	-1.25038300	-5.61740400	-0.38959900
H	-7.99299700	-0.35852200	-1.63949900
H	-0.52938400	-5.17570200	-2.72719900
H	1.02620800	-2.34149800	-0.16919900
C	-2.78390400	2.43339200	-0.57249900
C	-2.14150500	2.57049400	-1.81499900
C	-4.06000600	2.98988900	-0.42819900
C	-2.76440600	3.22199200	-2.87899900
H	-1.14040300	2.17109600	-1.95699900
C	-4.68650700	3.64598700	-1.49209900
H	-4.58680500	2.91108700	0.51710100
C	-4.04440800	3.76198900	-2.72329900
H	-2.24240700	3.31629400	-3.82809900
H	-5.68050800	4.06398500	-1.35259900
H	-4.52960900	4.27378800	-3.55049900
C	-2.72850300	1.88509200	1.93860100
H	-2.85750600	2.94579200	2.18070100
H	-3.71290100	1.40639000	1.97040100
H	-2.11520200	1.43109400	2.72280100
C	2.20290900	-2.63259500	1.56710100
H	3.09140800	-2.25139200	2.07890100
H	1.34710900	-2.50479700	2.23770100
H	2.34551200	-3.70519400	1.38760100
C	3.02220800	-2.13539300	-0.81329900
C	4.36420800	-2.37568900	-0.48919900
C	2.66480800	-2.13419300	-2.17039900
C	5.31890900	-2.58558600	-1.48689900
H	4.67690900	-2.39708800	0.54940100
C	3.61340800	-2.34009100	-3.17089900
H	1.62680700	-1.97009600	-2.44659900
C	4.94960900	-2.56508700	-2.83159900
H	6.35371000	-2.76818400	-1.20809900
H	3.30770800	-2.33189200	-4.21419900
H	5.69230900	-2.73228500	-3.60759900

D5a'

B3LYP SCF energy:	-2921.08877110 a.u.
B3LYP enthalpy:	-2920.26737400 a.u.
B3LYP free energy:	-2920.33338000 a.u.
M06-2X SCF energy in solution:	-2920.81215295 a.u.
M06-2X enthalpy in solution:	-2919.99075585 a.u.
M06-2X free energy in solution:	-2920.05676185 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	2.62599700	-1.16890000	0.10970600
C	1.92509700	-1.89670000	-1.41959400
C	1.60259600	-3.26009900	-1.46799400
C	1.75999700	-1.11469900	-2.57599400
C	1.10699600	-3.82709900	-2.64339400
H	1.74239600	-3.87039900	-0.58159400
C	1.26829700	-1.68449900	-3.75109400
H	2.03269700	-0.06180000	-2.56989400
C	0.93869600	-3.04139900	-3.78499400
H	0.85209600	-4.88299900	-2.66619400
H	1.14529700	-1.06819900	-4.63739400
H	0.55469600	-3.48489900	-4.69969400
C	4.41719700	-0.97310100	-0.22989400
C	4.85899800	0.01159900	-1.12719400
C	5.35749700	-1.82890100	0.36230600
C	6.21509800	0.13589900	-1.42659400
H	4.15049800	0.69920000	-1.57679400
C	6.71419700	-1.70010200	0.06270600
H	5.00989600	-2.58750100	1.05410600
C	7.14489700	-0.72010200	-0.83299400
H	6.54439800	0.90809900	-2.11619400
H	7.43449700	-2.36720200	0.52920600
H	8.20189700	-0.62110200	-1.06619400
N	1.83899800	0.25360000	0.31760600
N	2.61459700	-2.30630000	1.29870600
Li	-0.07110300	-0.47089900	1.16800600
C	1.56629600	-2.51329900	2.09220600
O	0.43849700	-1.95019900	2.09340600
O	1.70209600	-3.46589900	3.05000600
C	2.94619600	-4.15880000	3.15060600
H	2.81639600	-4.86720000	3.97180600
H	3.17859600	-4.69460000	2.22530600
H	3.76519600	-3.46890000	3.37580600
C	2.51469800	1.18920000	1.27460600
O	-0.27830200	2.23440100	-1.80159400
Li	0.30139800	0.76080100	-0.91669400
C	-1.44830100	2.70320200	-1.85349400
N	-1.53610300	-0.14899800	-0.20879400
N	-2.53580200	2.34300200	-1.18169400
O	-1.58440100	3.72330200	-2.74109400
P	-2.56070200	1.12230200	-0.07619400
C	-1.80960300	-1.26539800	-1.17449400
C	-2.87010100	4.32170200	-2.90039400
C	-4.34880200	0.70400300	0.00060600
C	-2.18820200	1.83860200	1.57180600
H	-0.84300300	-1.77449800	-1.27749400
H	-2.72570000	5.12880200	-3.62209400
H	-3.59620100	3.60020300	-3.28829400
H	-3.24330100	4.72420300	-1.95409400
C	-5.26940200	1.35560300	-0.83259400
C	-4.81840300	-0.24039700	0.92640600
C	-2.04120200	1.01070200	2.69780600
C	-2.10880100	3.22870200	1.73520600
C	-6.63130200	1.06180400	-0.74629400
H	-4.90400200	2.09530300	-1.53549400
C	-6.17900300	-0.52759600	1.01500600
H	-4.12360300	-0.77319700	1.56620600
C	-1.80930200	1.56310200	3.95800600
H	-2.11610300	-0.06949800	2.59720600
C	-1.87120100	3.77910200	2.99590600
H	-2.23370100	3.87130200	0.86960600
C	-7.08880200	0.12240400	0.17840600
H	-7.33460200	1.57260400	-1.39899400
H	-6.52560300	-1.26709600	1.73130600
C	-1.72140100	2.94870200	4.10810600
H	-1.69570200	0.90990200	4.81890600
H	-1.80300000	4.85780200	3.10850600
H	-8.14980300	-0.10349500	0.24760600
H	-1.53820100	3.37930200	5.08880600
H	3.29249800	0.65460000	1.83990600
C	-2.76060300	-2.33809800	-0.61899400
C	-2.42590400	-2.99309800	0.57860600
C	-3.93070400	-2.73289700	-1.27809400
C	-3.24520400	-3.99049700	1.10630600
H	-1.51210400	-2.72829800	1.10390600
C	-4.75360400	-3.73349700	-0.75269400
H	-4.22150300	-2.25489700	-2.20759400
C	-4.41770400	-4.36439700	0.44340600
H	-2.96030400	-4.48239800	2.03320600
H	-5.66030400	-4.01469600	-1.28289400
H	-5.05580500	-5.14389700	0.85220600
C	-2.18500300	-0.78679800	-2.58719400
H	-2.21010300	-1.62959800	-3.28649400
H	-3.16340300	-0.29509700	-2.61229400
H	-1.44420300	-0.06859800	-2.95069400
C	1.51179800	1.70160100	2.31990600
H	0.68679800	2.24360100	1.84510600
H	1.10259800	0.87030100	2.90660600
H	1.99909900	2.39180000	3.01760600
C	3.21979900	2.37230000	0.60870600
C	2.62839900	3.12420000	-0.41589400
C	4.48159900	2.76469900	1.07590600
C	3.28809900	4.22880000	-0.96009400
H	1.64969900	2.86230100	-0.80519400
C	5.14119900	3.87079900	0.53760600
H	4.95959800	2.18939900	1.86640600
C	4.54599900	4.60759900	-0.48709400
H	2.81010000	4.79450000	-1.75589400
H	6.12229900	4.14989900	0.91410600
H	5.05720000	5.46709900	-0.91339400

(*d*,*d*)-**D1a(THF)$_2$**

B3LYP SCF energy:	-3386.04327930 a.u.
B3LYP enthalpy:	-3384.97860800 a.u.
B3LYP free energy:	-3385.06349100 a.u.
M06-2X SCF energy in solution:	-3385.67756034 a.u.
M06-2X enthalpy in solution:	-3384.61288904 a.u.
M06-2X free energy in solution:	-3384.69777204 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	3.27940700	-1.15248400	-0.67700700
C	4.25751200	-2.68578100	-0.42860700
C	3.64291600	-3.93708300	-0.57760700
C	5.59881200	-2.62927600	-0.02130700
C	4.35542000	-5.10888000	-0.32030700
H	2.61101600	-3.98438600	-0.91050700
C	6.31061600	-3.80227400	0.23459300
H	6.09260900	-1.66757400	0.08649300
C	5.68942000	-5.04377600	0.08679300
H	3.86972300	-6.07358200	-0.44240700
H	7.35101600	-3.74597000	0.54409300
H	6.24442300	-5.95737400	0.28399300
C	4.45750300	0.01972000	-1.47540700
C	5.08540000	0.99802200	-0.69170700
C	4.75730300	-0.05737900	-2.84470700
C	6.00379700	1.88062500	-1.26640700
H	4.83950000	1.07052100	0.36349300
C	5.66820000	0.83002400	-3.41870700
H	4.26810600	-0.80968100	-3.45600700
C	6.29439700	1.79902600	-2.62960700
H	6.48859400	2.63272700	-0.64900700
H	5.89130100	0.76552500	-4.48080700
H	7.00639500	2.48802900	-3.07740700
N	2.67180500	-0.54418600	0.67379300
N	2.21710800	-1.57428700	-1.87860700
Li	1.25490000	0.86160900	0.16099300
C	1.07510600	-0.95789100	-2.07350700
O	0.56840300	0.03790700	-1.47320700
O	0.27380800	-1.43519400	-3.08050700
C	0.73271200	-2.56629200	-3.82470700
H	-0.05228800	-2.76979500	-4.55640700
H	0.87521500	-3.43389200	-3.17470700
H	1.67751100	-2.34648900	-4.33000700
C	2.98870700	-1.03968500	2.02109300
H	3.58861000	-1.95928300	1.96629300
C	1.69850800	-1.40358900	2.77649300
H	1.03710500	-0.53629100	2.86859300
H	1.92510900	-1.77058800	3.78549300
H	1.15791000	-2.18429100	2.23079300
C	3.82770300	-0.02888200	2.80719300
C	5.14610400	-0.33207800	3.16929300
C	3.31149900	1.22311600	3.17759300
C	5.93470100	0.58402500	3.87149300
H	5.56150700	-1.30007600	2.89589300
C	4.09459600	2.14021900	3.87879300
H	2.28639800	1.47951300	2.92359300
C	5.41159700	1.82632300	4.22789300
H	6.95580200	0.32362800	4.14039300
H	3.67329300	3.10241700	4.16219300
H	6.01959500	2.54192500	4.77579300
O	-0.57270100	1.26110300	0.77799300
Li	-1.25779800	0.33680100	-0.80320700
C	-1.09460100	1.23300200	1.93349300
N	-2.67259400	-0.85740400	0.08989300
N	-2.24589900	0.74519800	2.33289300
O	-0.30190300	1.82000400	2.88859300
P	-3.29609700	-0.04460600	1.32079300
C	-2.98148900	-2.26140500	-0.21600700
C	-0.77620300	1.83720300	4.23699300
C	-4.28149300	-1.08100900	2.47149300
C	-4.47100100	1.25569000	0.74679300
H	-3.58528800	-2.71190700	0.58469300
C	-1.68538700	-3.08650000	-0.30280700
C	-3.80828900	-2.39100800	-1.49760700
H	-0.00050500	2.34940500	4.81059300
H	-0.91680000	0.82190200	4.61779300
H	-1.72490500	2.37599900	4.31269300
C	-3.67469100	-1.61940700	3.61499300
C	-5.61779200	-1.40451400	2.19319300
C	-5.09090100	1.11478800	-0.50240700
C	-4.77190500	2.37468900	1.53919300
H	-1.02438800	-2.69959800	-1.08480700
H	-1.90348300	-4.13820100	-0.52730700
H	-1.14928700	-3.03269900	0.65069300
C	-5.10878700	-2.90811200	-1.45300700
C	-3.29519000	-1.99660600	-2.74360700
C	-4.38998900	-2.46621000	4.46219300
H	-2.64609200	-1.35720400	3.84099300
C	-6.33278900	-2.25071600	3.04219300
H	-6.10669400	-0.98711500	1.31719300
C	-6.00300400	2.07418500	-0.94980700
H	-4.84229800	0.25968900	-1.12360700
C	-5.67710800	3.33578600	1.08779300
H	-4.28690500	2.48989100	2.50379300
C	-5.88298700	-3.02441500	-2.61130700
H	-5.52168600	-3.22331300	-0.49680700
C	-4.06409000	-2.11110800	-3.90200700
H	-2.76350100	1.09499600	-3.91020700
C	-5.71968800	-2.78351400	4.17779300
H	-3.91008700	-2.87450800	5.34799300
H	-7.36948900	-2.48892000	2.81909300
C	-6.29540800	3.18558400	-0.15690700
H	-6.48150300	1.95358300	-1.91850700
H	-5.90141100	4.20138500	1.70609300
C	-5.36328800	-2.62431300	-3.84170700
H	-6.89048500	-3.42911800	-2.54950700
H	-3.64549100	-1.80580700	-4.85870700
H	-6.27738500	-3.44021600	4.84049300
H	-7.00241000	3.93378200	-0.50650700
H	-5.96038800	-2.71421500	-4.74580700
O	1.99429400	2.69461200	-0.26950700
C	2.18489200	3.18831200	-1.61220700
C	1.86849000	3.79341100	0.66169300
C	2.48848700	4.68091300	-1.46180700
H	1.26259300	3.01600900	-2.18220700

H	2.99539400	2.61981500	-2.07420700
C	1.68928600	5.04501100	-0.20050700
H	2.78559000	3.84531400	1.26239300
H	1.02379100	3.57950900	1.32059300
H	3.56068700	4.83541700	-1.29260700
H	2.19728500	5.25891300	-2.34450700
H	2.04938300	5.95101200	0.29659300
H	0.63078600	5.19120700	-0.44790700
O	-1.99070300	1.71339900	-2.08950700
C	-2.16390700	3.10499800	-1.74760700
C	-1.84740200	1.55609900	-3.51930700
C	-2.44651000	3.82009700	-3.07070700
H	-1.24030900	3.46630100	-1.27700700
H	-2.97980800	3.18039500	-1.02480700
C	-1.64870700	2.96960000	-4.07170700
H	-2.28279200	-1.60750200	-2.80980700
H	-1.00500000	0.88460200	-3.70080700
H	-3.51721000	3.77989300	-3.30300700
H	-2.14221300	4.87139800	-3.05270700
H	-1.99890700	3.06899800	-5.10380700
H	-0.58720800	3.24450300	-4.04560700

(*u*,*u*)-**D1a(THF)$_2$**

B3LYP SCF energy:	-3386.04004100 a.u.
B3LYP enthalpy:	-3384.97545000 a.u.
B3LYP free energy:	-3385.05906500 a.u.
M06-2X SCF energy in solution:	-3385.67609920 a.u.
M06-2X enthalpy in solution:	-3384.61150820 a.u.
M06-2X free energy in solution:	-3384.69512320 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	3.36458300	-0.24457400	0.58910900
C	2.92961000	-1.93208700	1.19606600
C	2.14550900	-2.79018800	0.41715200
C	3.38357500	-2.36988800	2.45228200
C	1.82806400	-4.07038000	0.88039900
H	1.78570900	-2.45738500	-0.55009400
C	3.06304800	-3.64504800	2.91429500
H	3.99064500	-1.70954900	3.06548700
C	2.28536600	-4.49971700	2.12550700
H	1.22669100	-4.72974600	0.26058400
H	3.42186200	-3.97559800	3.88591900
H	2.03928100	-5.49619200	2.48372600
C	5.20073000	-0.23778200	0.65717900
C	5.87962300	0.90820400	1.09555500
C	5.94512100	-1.33290000	0.19310900
C	7.27346200	0.95797300	1.07095200
H	5.30448200	1.74705300	1.47490100
C	7.34005900	-1.28077100	0.16480300
H	5.43617300	-2.23567200	-0.13423300
C	8.00624700	-0.13541500	0.60333000
H	7.78912600	1.84802400	1.42289300
H	7.90513600	-2.13690600	-0.19449000
H	9.09241700	-0.09665500	0.58595900
N	2.78671800	0.14817300	-0.85767500
N	2.94375500	0.78019700	1.82040100
Li	1.13821200	1.32863400	-0.73842300
C	1.72608900	1.25348200	1.96793800
O	0.73193800	1.16605600	1.18824000
O	1.47026800	1.97346800	3.10402400
C	2.50725600	2.06574100	4.08370400
H	2.07292400	2.62651400	4.91453700
H	2.81931400	1.07301000	4.41883400
H	3.38033500	2.59227900	3.68670200
C	3.47701800	-0.17261900	-2.11382600
H	4.54143500	-0.39072100	-1.93816400
C	3.43896200	1.05019000	-3.05189900
H	2.40446700	1.31729300	-3.29659600
H	3.91357000	1.90985000	-2.56690200
H	3.96261400	0.83688200	-3.99148700
C	2.89920900	-1.38625300	-2.84625900
C	1.51507500	-1.55716000	-2.99753400
C	3.75235700	-2.33391800	-3.42444000
C	1.00180900	-2.64471700	-3.70524800
H	0.83494000	-0.84459400	-2.53829200
C	3.24398600	-3.42375600	-4.13577700
H	4.82938100	-2.21746100	-3.31551400
C	1.86553900	-3.58245700	-4.27835900
H	-0.07433600	-2.76439400	-3.79922400
H	3.92570200	-4.15039700	-4.57173500
H	1.46585000	-4.43181100	-4.82690000
O	-0.73183300	1.16579800	-1.18821600
Li	-1.13823900	1.32836200	0.73849100
C	-1.72585700	1.25259200	-1.96813800
N	-2.78672800	0.14777300	0.85762800
N	-2.94337600	0.77892500	-1.82069100
O	-1.47005300	1.97215400	-3.10447800
P	-3.36446500	-0.24535600	-0.58913500
C	-3.47703500	-0.17348800	2.11365500
C	-2.50693100	2.06374400	-4.08434800
C	-2.92969100	-1.93308900	-1.19564500
C	-5.20061800	-0.23827200	-0.65735700
H	-4.54127000	-0.39233000	1.93781300
C	-3.44006200	1.04937300	3.05172900
C	-2.89856500	-1.38668800	2.84629400
H	-2.07268800	2.62445600	-4.91526600
H	-2.81853500	1.07079100	-4.41924300
H	-3.38027500	2.59004100	-3.68761600
C	-2.14518400	-2.79086000	-0.41678100
C	-3.38394300	-2.37126400	-2.45163100
C	-5.94528800	-1.33330000	-0.19352700
C	-5.87923400	0.90794500	-1.09556600
H	-2.40582100	1.31721700	3.29667000
H	-3.91514500	1.90869600	2.56660000
H	-3.96379500	0.83570700	3.99119000
C	-3.75124600	-2.33470300	3.42460700
C	-1.51435800	-1.55682000	2.99769300
C	-1.82759800	-4.07108700	-0.87984800
H	-1.78517600	-2.45780100	0.55030100
C	-3.06327500	-3.64645000	-2.91346600
H	-3.99133300	-1.71118900	-3.06480200
C	-7.34022000	-1.28085500	-0.16528800

H	-5.43656500	-2.23625100	0.13366700
C	-7.27306000	0.95803300	-1.07103300
H	-5.30389200	1.74673400	-1.47474300
C	-3.24234000	-3.42411700	4.13619600
H	-4.82832400	-2.21884800	3.31557500
C	-1.00055300	-2.64396200	3.70566600
H	-1.90902800	3.82407700	3.09269800
C	-2.28516700	-4.50078300	-2.12473100
H	-1.22590000	-4.73018300	-0.26006300
H	-3.42230100	-3.97728500	-3.88491400
C	-8.00612200	-0.13527200	-0.60364300
H	-7.90550900	-2.13692500	0.19382500
H	-7.78850100	1.84826200	-1.42285000
C	-1.86381200	-3.58204500	4.27890700
H	-3.92369100	-4.15104100	4.57225500
H	0.07564900	-2.76303700	3.79972900
H	-2.03897700	-5.49728000	-2.48281700
H	-9.09228300	-0.09626500	-0.58632000
H	-1.46370700	-4.43107600	4.82764500
O	1.62067800	3.26485200	-1.10692300
C	2.52303200	4.02316800	-0.27269800
C	1.23422600	4.04461000	-2.25273700
C	2.64321100	5.41430600	-0.92038800
H	2.08670400	4.06669700	0.73145400
H	3.48032400	3.49561500	-0.21174100
C	1.38253800	5.49472100	-1.79870600
H	1.90985900	3.82463100	-3.09248100
H	0.22244700	3.74140500	-2.52724800
H	3.54133200	5.47066600	-1.54611400
H	2.70465300	6.21486300	-0.17696000
H	1.48388600	6.19403200	-2.63447200
H	0.51295300	5.79587400	-1.20207300
O	-1.62167700	3.26434100	1.10693500
C	-2.52365000	4.02238100	0.27207600
C	-1.23462600	4.04475900	2.25217600
C	-2.64605000	5.41278400	0.92070400
H	-2.08606400	4.06735500	-0.73149800
H	-3.48022600	3.49376100	0.20939700
C	-1.38498400	5.49471000	1.79827100
H	-0.83455800	-0.84398800	2.53836900
H	-0.22221400	3.74269100	2.52560700
H	-3.54387300	5.46704100	1.54705200
H	-2.70940000	6.21372800	0.17785000
H	-1.48665600	6.19383000	2.63415700
H	-0.51616000	5.79701400	1.20110200

(*d*,*u*)-**D1a(THF)$_2$**

B3LYP SCF energy:	-3386.04102700 a.u.
B3LYP enthalpy:	-3384.97608900 a.u.
B3LYP free energy:	-3385.05960500 a.u.
M06-2X SCF energy in solution:	-3385.67838275 a.u.
M06-2X enthalpy in solution:	-3384.61344475 a.u.
M06-2X free energy in solution:	-3384.69696075 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	3.75771600	0.27679900	0.65982400
C	5.39255300	1.10159800	0.82226200
C	5.47673500	2.37333500	1.40849100
C	6.55164900	0.52899500	0.27640200
C	6.69096400	3.05875300	1.44396300
H	4.58695700	2.80619200	1.85531000
C	7.76600400	1.21789200	0.30771700
H	6.51374800	-0.46675500	-0.15727900
C	7.83740900	2.48409000	0.88980100
H	6.74506900	4.03911800	1.91072300
H	8.65653200	0.76162500	-0.11673200
H	8.78363400	3.01818800	0.91832300
C	4.13910600	-1.48449900	1.06955900
C	3.73724200	-2.51719900	0.21419800
C	4.81795000	-1.80711500	2.25719000
C	4.01947000	-3.84982900	0.53284300
H	3.21078900	-2.27617800	-0.70276700
C	5.09256400	-3.13519500	2.57732100
H	5.13354700	-1.01393400	2.92946900
C	4.69632200	-4.16029800	1.71236400
H	3.71710300	-4.64075700	-0.14887800
H	5.61886900	-3.37264300	3.49839700
H	4.91844300	-5.19568000	1.95827000
N	3.07143700	0.52682000	-0.77041300
N	2.91424500	0.84902100	1.95672000
Li	1.15674200	1.10735800	-0.59802000
C	1.60258300	0.79924100	2.08102700
O	0.72726000	0.49595500	1.22020300
O	1.07932100	1.14512100	3.29298000
C	1.98477900	1.45349700	4.35437300
H	1.35451000	1.64660200	5.22525900
H	2.58432400	2.33804200	4.11880600
H	2.66014000	0.61627900	4.55192100
C	3.79944600	0.47265000	-2.04786800
H	4.88795000	0.53100000	-1.89213600
C	3.41668200	1.69248700	-2.90928300
H	2.33546400	1.71566400	-3.08888700
H	3.92234500	1.65890300	-3.88188000
H	3.70389500	2.61706800	-2.39777800
C	3.54111900	-0.81148000	-2.84014700
C	4.60852200	-1.52829700	-3.39333100
C	2.23651300	-1.28082700	-3.06263800
C	4.39056200	-2.68507800	-4.14675100
H	5.62633900	-1.17758700	-3.23136900
C	2.01543800	-2.43489800	-3.81571100
H	1.39084500	-0.74543800	-2.63959500
C	3.09093300	-3.14342900	-4.36010200
H	5.23667200	-3.22751000	-4.56199000
H	0.99748600	-2.78005500	-3.98167300
H	2.91556200	-4.04277400	-4.94523400
O	-0.53007100	0.36838600	-1.25811900
Li	-0.97616900	-0.18788100	0.57481200
C	-1.28343000	1.02068000	-2.04676100
N	-2.95236600	0.39968400	0.64264900
N	-2.58357400	1.20999200	-2.00066800
O	-0.59969100	1.60347800	-3.07489400
P	-3.54717900	0.51597800	-0.84338000

C	-3.66171200	0.84514300	1.84807000
C	-1.33848700	2.35957600	-4.03413600
C	-5.09251000	1.50255700	-0.94732600
C	-4.01366600	-1.12398900	-1.55063500
H	-4.49307300	1.51709400	1.58855100
C	-2.70990300	1.65920000	2.74658100
C	-4.27818200	-0.29631100	2.66331200
H	-0.60417200	2.68683900	-4.77322300
H	-1.81674000	3.22727600	-3.56947300
H	-2.10946800	1.74739000	-4.51067500
C	-5.06809700	2.80292100	-1.46919000
C	-6.30349100	0.98598000	-0.46086000
C	-4.35540700	-2.18328100	-0.69808700
C	-4.06243000	-1.32396800	-2.93955900
H	-1.82256400	1.07605500	3.01688200
H	-3.21180900	1.96757300	3.67167800
H	-2.37617500	2.55639900	2.21497600
C	-5.51951500	-0.11781100	3.28857800
C	-3.61205200	-1.51586500	2.84980000
C	-6.23169900	3.57292400	-1.50270700
H	-4.13539900	3.19356700	-1.86227700
C	-7.46552900	1.75731200	-0.49378700
H	-6.34353400	-0.02296900	-0.05927500
C	-4.74263400	-3.41853600	-1.22444500
H	-4.30607600	-2.04253000	0.37719200
C	-4.44218000	-2.55976000	-3.46331300
H	-3.79409500	-0.50818700	-3.60352000
C	-6.08089900	-1.12064500	4.08224500
H	-6.05440900	0.82008100	3.15006500
C	-4.16919800	-2.52055400	3.64338600
H	-2.66621000	-1.68326600	2.34335500
C	-7.43159500	3.05245300	-1.01498100
H	-6.20203900	4.57834300	-1.91510000
H	-8.39762800	1.34472600	-0.11668500
C	-4.78472200	-3.60901400	-2.60646900
H	-5.00820900	-4.23107100	-0.55274600
H	-4.47091000	-2.70476300	-4.54032500
C	-5.40541800	-2.32776500	4.26477700
H	-7.04798600	-0.95977200	4.55290700
H	-3.63718700	-3.46030400	3.77492000
H	-8.33812200	3.65155100	-1.04432700
H	-5.08235400	-4.57116500	-3.01579100
H	-5.83925500	-3.11214700	4.87979600
O	0.91829000	3.12827200	-0.40889200
C	1.97849000	4.10871300	-0.40526700
C	-0.21583800	3.61619000	0.34869500
C	1.57420700	5.15566900	0.63550500
H	2.05278400	4.54768700	-1.40894200
H	2.91569400	3.59609700	-0.17631200
C	0.04070900	5.10939000	0.55535900
H	-0.25609600	3.07437600	1.29960100
H	-1.12387200	3.39442700	-0.21845100
H	1.91089300	4.85225900	1.63408100
H	1.99391300	6.14305800	0.41973100
H	-0.45374000	5.49659800	1.45142100
H	-0.31454900	5.68670500	-0.30686400
O	-0.72209500	-2.18822000	0.85034100
C	-0.67540900	-3.07735900	-0.27955800
C	0.11340400	-2.74803900	1.88723700
C	-0.67699700	-4.46814000	0.35161200
H	0.24001600	-2.89394300	-0.85991700
H	-1.54589000	-2.86112300	-0.90058300
C	0.20371100	-4.26752100	1.60497000
H	-0.36279600	-2.50923300	2.84238600
H	1.09742900	-2.27016100	1.85387600
H	-1.69964700	-4.74254300	0.63267100
H	-0.29023300	-5.23858000	-0.32260400
H	-0.14450900	-4.86548500	2.45236800
H	1.24130700	-4.55011800	1.40399100

(*d*,*d*)-**D2a(THF)$_2$**

B3LYP SCF energy:	-3386.03826110 a.u.
B3LYP enthalpy:	-3384.97405000 a.u.
B3LYP free energy:	-3385.05849800 a.u.
M06-2X SCF energy in solution:	-3385.67483075 a.u.
M06-2X enthalpy in solution:	-3384.61061965 a.u.
M06-2X free energy in solution:	-3384.69506765 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	3.14984800	-0.65273600	-1.17349400
C	3.12844200	-2.41255500	-1.72737700
C	2.08977700	-3.23693200	-1.26812900
C	4.05046100	-2.93377800	-2.64559900
C	1.97900100	-4.55428700	-1.71351200
H	1.37008500	-2.83664700	-0.55918000
C	3.93882600	-4.25161400	-3.09202200
H	4.85789300	-2.30928400	-3.01517600
C	2.90448200	-5.06487400	-2.62586800
H	1.17096600	-5.18352200	-1.34855600
H	4.66095900	-4.64276800	-3.80418500
H	2.81949100	-6.09155100	-2.97258400
C	4.89139100	-0.10909500	-1.45259800
C	5.95441800	-0.76407700	-0.81054300
C	5.17035500	1.01958700	-2.23673200
C	7.26250900	-0.30088000	-0.94888200
H	5.76609300	-1.63783100	-0.19411700
C	6.47933500	1.48684200	-2.37067800
H	4.35360300	1.51617300	-2.75047500
C	7.52797900	0.82757000	-1.72770100
H	8.07302700	-0.81873500	-0.44311500
H	6.68022200	2.36118700	-2.98504000
H	8.54761900	1.18923400	-1.83365500
N	2.59685200	-0.49190500	0.32684600
N	2.32467500	0.16868200	-2.33286200
Li	1.22276800	0.96915400	0.59294100
C	1.19263500	0.82391900	-2.22996900
O	0.53631600	1.16541100	-1.20283200
O	0.61736400	1.24991000	-3.39718000
C	1.23209000	0.86671400	-4.62995000
H	0.57565100	1.25387500	-5.41252000
H	1.31498100	-0.22051700	-4.70626100
H	2.23121400	1.30244300	-4.72575000

C	3.03650800	-1.35228400	1.43229300
H	3.28528300	-2.36452800	1.07173800
C	1.86918800	-1.52134000	2.42656900
H	1.56819800	-0.55202100	2.84092600
H	2.15630500	-2.16955500	3.26270400
H	1.00086300	-1.96137200	1.92384900
C	4.27221300	-0.85340300	2.19084500
C	5.14358100	-1.77819900	2.78257800
C	4.53716900	0.51132600	2.35863600
C	6.25007200	-1.35740100	3.52268700
H	4.95320600	-2.84351600	2.65982600
C	5.64201400	0.93582600	3.09896700
H	3.87555000	1.23485800	1.89227900
C	6.50378100	0.00561900	3.68401600
H	6.91512600	-2.09363500	3.96812400
H	5.83612300	2.00004600	3.21474800
H	7.36615800	0.33916900	4.25582100
O	-0.59799600	1.02829700	1.30427800
Li	-1.29060200	1.07608200	-0.50055000
C	-1.30161500	0.64177600	2.28317000
N	-2.71152900	-0.35476000	-0.42209000
N	-2.44496100	-0.00321900	2.30007400
O	-0.77479400	0.99907700	3.49432500
P	-3.19227700	-0.77227800	1.05441600
C	-3.24826700	-1.01492400	-1.61978600
C	-1.44822000	0.55994100	4.67693000
C	-2.94240300	-2.57470100	1.36877800
C	-4.97701300	-0.50505800	1.42253500
H	-3.53150700	-2.06061000	-1.40772100
C	-2.14257100	-1.07948500	-2.69363600
C	-4.49104600	-0.34621800	-2.21947500
H	-0.82413500	0.89828200	5.50717200
H	-1.54468100	-0.52871900	4.69286400
H	-2.44638000	1.00204700	4.75054500
C	-1.93368700	-3.24478400	0.66190200
C	-3.66711200	-3.27506700	2.34405000
C	-5.95968000	-1.27335000	0.77914500
C	-5.38082700	0.52524400	2.28301900
H	-1.80060800	-0.07313700	-2.96046600
H	-2.50830300	-1.56472700	-3.60605500
H	-1.27958300	-1.64214600	-2.32000300
C	-5.42005000	-1.11979100	-2.92853500
C	-4.70421800	1.03476700	-2.13199600
C	-1.65953100	-4.58909200	0.91960800
H	-1.36708000	-2.70237800	-0.08969600
C	-3.39124300	-4.61785600	2.60356400
H	-4.45030400	-2.76981000	2.90149000
C	-7.31385800	-1.01503400	0.98919000
H	-5.67177700	-2.08114100	0.11236400
C	-6.73623600	0.78526100	2.49166900
H	-4.62263400	1.10780200	2.79647700
C	-6.53291600	-0.53615900	-3.53572400
H	-5.27005600	-2.19601000	-3.00439000
C	-5.81622900	1.62224700	-2.73889100
H	-2.51404400	3.74049100	-2.73849100
C	-2.38827900	-5.27816700	1.89029800
H	-0.87814700	-5.09904300	0.36157200
H	-3.96054400	-5.14946700	3.36183100
C	-7.70523000	0.01632500	1.84512900
H	-8.06262900	-1.61741500	0.48181200
H	-7.03525800	1.58477200	3.16509500
C	-6.73578000	0.84171400	-3.44211900
H	-7.24337700	-1.15766500	-4.07589700
H	-5.96918500	2.69628500	-2.65700300
H	-2.17599000	-6.32516300	2.09099200
H	-8.76086200	0.21767000	2.00859300
H	-7.60343900	1.30131400	-3.90892700
O	2.06555200	2.70514500	1.22344800
C	2.67060100	3.62996700	0.29267500
C	1.70804500	3.38207800	2.44888900
C	2.84401400	4.94562300	1.06093800
H	1.99547200	3.73996500	-0.56471800
H	3.61475800	3.20165800	-0.05815500
C	1.71278400	4.86998400	2.09953600
H	2.46244200	3.14976600	3.21349700
H	0.74328800	2.98879300	2.77403700
H	3.81798800	4.97133800	1.56354300
H	2.77900000	5.82114300	0.40770200
H	1.88276000	5.50726600	2.97275600
H	0.75630200	5.15903800	1.64677600
O	-2.03850800	2.93334100	-0.88265700
C	-2.37068400	3.82145700	0.20868500
C	-1.65793000	3.69395100	-2.05070500
C	-2.29471700	5.24340100	-0.36332800
H	-1.64102500	3.65765800	1.00986700
H	-3.36564000	3.55844600	0.58234800
C	-1.29674800	5.08047800	-1.52154900
H	-3.99518200	1.64155300	-1.57706200
H	-0.83653700	3.16340000	-2.53538400
H	-3.27229100	5.55615000	-0.74847300
H	-1.97852700	5.97657400	0.38519400
H	-1.38666100	5.86035800	-2.28400300
H	-0.26652600	5.08534400	-1.14529100

(*u*,*u*)-**D2a(THF)$_2$**

B3LYP SCF energy:	-3386.04129208 a.u.
B3LYP enthalpy:	-3384.97692000 a.u.
B3LYP free energy:	-3385.06049400 a.u.
M06-2X SCF energy in solution:	-3385.67822791 a.u.
M06-2X enthalpy in solution:	-3384.61385583 a.u.
M06-2X free energy in solution:	-3384.69742983 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	-3.46722700	-0.10949700	-0.35937600
C	-4.51392600	-1.60058500	-0.56920800
C	-4.03124800	-2.69262200	-1.30416000
C	-5.76791500	-1.69714300	0.05185700
C	-4.78704600	-3.85972600	-1.41113000
H	-3.07092300	-2.61188400	-1.80317200
C	-6.52112700	-2.86764600	-0.05219100
H	-6.16798400	-0.85134000	0.60475300
C	-6.03123900	-3.95084100	-0.78329300

H	-4.40557300	-4.69855900	-1.98754000
H	-7.49280500	-2.92948100	0.43104300
H	-6.61918600	-4.86115300	-0.86822000
C	-4.67625100	1.28338200	-0.47085500
C	-4.90634400	2.09494400	0.64652300
C	-5.37563000	1.54400100	-1.66029200
C	-5.82446300	3.14738100	0.58127200
H	-4.34683500	1.90422400	1.55748500
C	-6.28873200	2.59529900	-1.72639500
H	-5.19743700	0.92311000	-2.53365800
C	-6.51610200	3.39809300	-0.60423700
H	-5.99820800	3.76944600	1.45604500
H	-6.82410900	2.79053200	-2.65221200
H	-7.23007300	4.21627600	-0.65660800
N	-2.62692300	-0.07257600	1.00789100
N	-2.60375400	-0.04387600	-1.76452200
Li	-1.10868600	1.27969500	0.88558800
C	-1.48362800	0.62770600	-1.90268500
O	-0.83014500	1.30809600	-1.05150400
O	-0.90274600	0.62274800	-3.13938300
C	-1.50643400	-0.17215000	-4.16434400
H	-0.91789100	0.02151900	-5.06378700
H	-1.45913300	-1.23425900	-3.90894400
H	-2.54967200	0.11494500	-4.31964400
C	-3.01146100	-0.84017000	2.19731100
H	-4.10017000	-1.00354600	2.24478300
C	-2.63691600	-0.04017600	3.46144400
H	-1.55811100	0.14763400	3.48704500
H	-3.15746500	0.92468600	3.46713300
H	-2.91032200	-0.59022100	4.36972000
C	-2.37300300	-2.23279000	2.26887800
C	-1.14073800	-2.51579300	1.66853300
C	-3.01066800	-3.25321500	2.98715700
C	-0.56146000	-3.78182700	1.78374600
H	-0.64641700	-1.73993900	1.09274100
C	-2.43623900	-4.51921000	3.10783700
H	-3.97640300	-3.05556600	3.44980900
C	-1.20604000	-4.78877800	2.50509000
H	0.38646900	-3.98318300	1.29073600
H	-2.95464100	-5.29763400	3.66292900
H	-0.75935300	-5.77651000	2.58842200
O	0.84733700	1.22040300	1.17868800
Li	1.12846500	1.30500100	-0.74715400
C	1.50948100	0.51857500	2.00222600
N	2.60286300	-0.10137700	-0.94571300
N	2.60532100	-0.18340100	1.82813300
O	0.96888700	0.52114500	3.25901300
P	3.43406000	-0.32096700	0.41058400
C	2.92959700	-0.81290600	-2.18770800
C	1.59598400	-0.27825200	4.26560100
C	4.24521500	-1.96303300	0.53870100
C	4.84482300	0.86255500	0.57404600
H	3.99609700	-1.08742400	-2.23314700
C	2.66828300	0.11639600	-3.39125900
C	2.14991500	-2.12044500	-2.37911600
H	1.01915500	-0.10067300	5.17583100
H	1.56072100	-1.33832900	4.00035900
H	2.63826100	0.01910800	4.40977900
C	3.58682500	-3.01088400	1.19815400
C	5.48097900	-2.21405900	-0.07493500
C	5.26207100	1.60358500	-0.53863400
C	5.52137400	1.02472500	1.79326800
H	1.61383800	0.41022200	-3.42041500
H	3.28013800	1.02272900	-3.31170700
H	2.91021400	-0.38574200	-4.33545400
C	0.91255800	-2.34508000	-1.76640400
C	2.66194400	-3.11456300	-3.22431300
C	4.15171000	-4.28511100	1.23790700
H	2.63959400	-2.81683100	1.69136700
C	6.04354300	-3.49111000	-0.03779200
H	6.01594200	-1.40858300	-0.57078600
C	6.34042500	2.48794400	-0.44016000
H	4.72735400	1.48988300	-1.47743900
C	6.59251100	1.91182800	1.89403900
H	5.19947800	0.45795600	2.66190400
C	0.20326100	-3.52716700	-1.99518600
H	0.51596600	-1.59233100	-1.09333200
C	1.95815100	-4.29619900	-3.45852500
H	1.62366100	3.29871100	-3.49647400
C	5.37919700	-4.52855800	0.61753400
H	3.63455900	-5.08846500	1.75615200
H	7.00324200	-3.67257200	-0.51481400
C	7.00549500	2.64341800	0.77661600
H	6.65893900	3.05403900	-1.31214100
H	7.10700800	2.03362100	2.84391500
C	0.72198500	-4.50689700	-2.84398000
H	-0.74663400	-3.68638800	-1.49100800
H	2.37965600	-5.05632100	-4.11223800
H	5.81851600	-5.52227700	0.64951500
H	7.84301600	3.33186300	0.85611900
H	0.17418800	-5.43004500	-3.01645800
O	-1.59509100	3.11349300	1.62247100
C	-1.72829500	4.21937900	0.70122200
C	-1.01124700	3.56274700	2.86774000
C	-1.46581700	5.48122600	1.52757100
H	-0.98950000	4.09298700	-0.09932700
H	-2.73032300	4.17862000	0.26531200
C	-0.48018500	4.97025400	2.59075900
H	-1.79673700	3.57559700	3.63535100
H	-0.24046900	2.84509700	3.15618900
H	-2.39108300	5.82960600	2.00194200
H	-1.06720400	6.30203700	0.92291000
H	-0.45040200	5.59215900	3.49083000
H	0.53488900	4.91854200	2.17911900
O	1.60443900	3.15893800	-1.42224000
C	2.39315000	4.17221700	-0.76235600
C	1.03898900	3.67657000	-2.64696100
C	2.45762200	5.35455900	-1.73653600
H	1.88945200	4.44527300	0.17389100
H	3.37254000	3.75092700	-0.51997700
C	1.15021700	5.19630300	-2.52916500
H	3.63033400	-2.96398100	-3.69904200
H	0.01939300	3.29561900	-2.72547400
H	3.32050700	5.25363600	-2.40563600
H	2.54239100	6.31590200	-1.22068800
H	1.17071400	5.69313800	-3.50397100

H	0.30407700	5.59958100	-1.95943000

(*d*,*u*)-**D2a(THF)$_2$**

B3LYP SCF energy:	-3386.04001740 a.u.
B3LYP enthalpy:	-3384.97503500 a.u.
B3LYP free energy:	-3385.05731400 a.u.
M06-2X SCF energy in solution:	-3385.67730675 a.u.
M06-2X enthalpy in solution:	-3384.61232435 a.u.
M06-2X free energy in solution:	-3384.69460335 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	-3.50075100	0.49288800	-0.58197100
C	-4.91372200	-0.64506400	-0.92871500
C	-4.97450500	-1.38968400	-2.11548300
C	-5.92848200	-0.81363500	0.02682800
C	-6.02027500	-2.28785000	-2.33838500
H	-4.19818100	-1.25089800	-2.86030400
C	-6.97490300	-1.70764600	-0.19760100
H	-5.90139700	-0.25606300	0.95759900
C	-7.02259800	-2.44834700	-1.38077200
H	-6.05350200	-2.85848800	-3.26328800
H	-7.74940900	-1.82940500	0.55498600
H	-7.83749100	-3.14658800	-1.55435800
C	-4.28059200	2.16924800	-0.59209700
C	-3.59588100	3.22753000	0.02523700
C	-5.48958500	2.43961600	-1.24789100
C	-4.10881700	4.52480400	-0.00948100
H	-2.66091200	3.02437400	0.53965300
C	-6.00195600	3.73783100	-1.28589400
H	-6.03423000	1.63410500	-1.73078600
C	-5.31431100	4.78238400	-0.66601700
H	-3.57187200	5.33281500	0.48125000
H	-6.94092700	3.93197400	-1.79802600
H	-5.71663700	5.79181100	-0.69206700
N	-2.68203500	0.22782100	0.77370300
N	-2.63308600	0.41108700	-1.97649500
Li	-0.79594500	-0.46265900	0.49547400
C	-1.32725300	0.41107300	-2.12895700
O	-0.40896200	0.22701000	-1.28390700
O	-0.85450900	0.61483700	-3.40133300
C	-1.80406600	0.84076700	-4.44564500
H	-1.20904200	1.04147000	-5.33953400
H	-2.43104500	-0.04186900	-4.60501100
H	-2.45022700	1.69230700	-4.21645700
C	-3.20774600	0.55839500	2.10731000
H	-3.98582200	1.33697700	2.04527200
C	-2.07108500	1.14171200	2.97210200
H	-1.25197400	0.42248600	3.07806500
H	-1.66426700	2.04704500	2.50731400
H	-2.43559600	1.39616300	3.97452600
C	-3.84022200	-0.62098600	2.85251200
C	-3.25791300	-1.89581900	2.84138600
C	-4.99293100	-0.42431500	3.62414300
C	-3.81953200	-2.94124100	3.57570100
H	-2.36454600	-2.06691400	2.24856900
C	-5.55910200	-1.46880900	4.35920200
H	-5.45462600	0.56187700	3.65042400
C	-4.97310300	-2.73448500	4.33640800
H	-3.35399000	-3.92414900	3.55430600
H	-6.45761200	-1.29266300	4.94601000
H	-5.41015300	-3.55193400	4.90437300
O	0.96668800	0.14915800	1.10467600
Li	1.35239000	0.80962200	-0.70918400
C	1.78525400	-0.40830300	1.89690600
N	3.31436000	0.20197300	-0.89556900
N	3.09612700	-0.50213300	1.82342600
O	1.17638100	-0.99747400	2.97129800
P	3.94729700	0.18766300	0.57758800
C	3.91899900	-0.44324400	-2.06916000
C	2.00415700	-1.60557800	3.96398100
C	5.57609100	-0.65159200	0.67826600
C	4.28618800	1.91427700	1.12987500
H	4.96615900	-0.71153500	-1.86861700
C	3.93844700	0.54586500	-3.24867800
C	3.22527300	-1.75162900	-2.46202300
H	1.31716600	-1.96685200	4.73222200
H	2.57716600	-2.43928700	3.54683600
H	2.70350500	-0.88102900	4.39095500
C	5.66884900	-1.95385300	1.18921500
C	6.73234800	-0.02945200	0.18400400
C	4.47783500	2.92302300	0.17669500
C	4.38858100	2.23462300	2.49250600
H	2.92777300	0.89805700	-3.48377500
H	4.54678900	1.42078500	-2.99325700
H	4.35729200	0.08113400	-4.14954300
C	1.94529000	-1.77244800	-3.03651900
C	3.88741100	-2.97289300	-2.27844500
C	6.89436900	-2.62136900	1.20228200
H	4.77774900	-2.42771500	1.58739500
C	7.95703000	-0.69812700	0.19701800
H	6.68011600	0.98549800	-0.20091800
C	4.77506800	4.22831100	0.57588700
H	4.36951100	2.67646000	-0.87502600
C	4.67822400	3.53984900	2.89154600
H	4.23247900	1.45771300	3.23457300
C	1.35908700	-2.97676000	-3.42940500
H	1.39419700	-0.84865600	-3.18415300
C	3.30090800	-4.18151400	-2.66199400
H	4.87979400	-2.97559600	-1.83237200
C	8.03966800	-1.99597500	0.70508200
H	6.95607700	-3.62877900	1.60601900
H	8.84646300	-0.20393000	-0.18495800
C	4.87443200	4.53833200	1.93369000
H	4.92468100	5.00291800	-0.17239100
H	4.75087300	3.77867200	3.94953400
C	2.03435000	-4.18743600	-3.24768200
H	0.37338900	-2.96594000	-3.88900900
H	3.83962200	-5.11472300	-2.51476000
H	8.99415700	-2.51581600	0.71816400
H	5.10265500	5.55443500	2.24562100
H	1.58030900	-5.12290300	-3.56570900
O	-0.79249200	-2.49542900	0.39533200

C	0.40270800	-3.30309400	0.49067600
C	-1.79718600	-3.19204100	-0.38311600
C	-0.07007500	-4.73563200	0.25555300
H	1.11853700	-2.98805500	-0.27756900
H	0.83270300	-3.12817300	1.47863300
C	-1.16819200	-4.52907500	-0.80034200
H	-2.67818100	-3.32544400	0.25337600
H	-2.07895500	-2.56720000	-1.23551800
H	-0.48980600	-5.15843800	1.17644700
H	0.73724800	-5.38846400	-0.08930500
H	-1.90261800	-5.33987000	-0.82749000
H	-0.71324100	-4.44458400	-1.79250200
O	1.17544100	2.82133600	-0.79882100
C	0.82694400	3.59991200	0.36759100
C	0.84124600	3.54099300	-2.00579400
C	0.54684000	5.01099700	-0.15286100
H	-0.05911000	3.15174800	0.83393800
H	1.66088500	3.54847600	1.07148800
C	-0.01158100	4.73085200	-1.55704400
H	1.77310700	3.87150600	-2.48418500
H	0.32253000	2.85363200	-2.67924300
H	1.47955100	5.58387800	-0.21741600
H	-0.14726900	5.56313000	0.48840600
H	0.07290000	5.58445700	-2.23682200
H	-1.06811500	4.44516400	-1.49773100

(*d,u*)-**D3a(THF)$_2$**

B3LYP SCF energy:	-3386.03823600 a.u.
B3LYP enthalpy:	-3384.97356000 a.u.
B3LYP free energy:	-3385.05633100 a.u.
M06-2X SCF energy in solution:	-3385.68041227 a.u.
M06-2X enthalpy in solution:	-3384.61573627 a.u.
M06-2X free energy in solution:	-3384.69850727 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	3.57881400	-0.26826700	-0.56729700
C	5.31018000	-0.81126500	-0.86036000
C	5.57914200	-1.83378800	-1.78130800
C	6.36951800	-0.27241100	-0.11460000
C	6.87984000	-2.30869400	-1.95123400
H	4.76448700	-2.23485700	-2.37584800
C	7.67024600	-0.75076800	-0.28244000
H	6.18184700	0.53371000	0.58974400
C	7.92725200	-1.77022100	-1.20043400
H	7.07756700	-3.09575500	-2.67463800
H	8.48244800	-0.32289200	0.29949400
H	8.94058600	-2.13990800	-1.33463600
C	3.74576200	1.56861300	-0.44771300
C	3.53430700	2.23135100	0.76702600
C	4.13474200	2.31328500	-1.57416000
C	3.72669200	3.61353600	0.86024200
H	3.22045200	1.66640600	1.63774500
C	4.31357100	3.69276400	-1.48319100
H	4.29649700	1.80613100	-2.52100400
C	4.11570000	4.34517400	-0.26217500
H	3.57455200	4.11378300	1.81337300
H	4.61279600	4.25944900	-2.36137300
H	4.26548400	5.41948500	-0.18897800
N	2.89603900	-0.99423900	0.69246600
N	2.84364000	-0.55450500	-2.02211500
Li	0.92592200	-1.34894400	0.36023000
C	1.53653200	-0.48350200	-2.18034200
O	0.63237900	-0.32137100	-1.31229800
O	1.05690400	-0.63772300	-3.45359100
C	2.00433700	-0.79566900	-4.51181600
H	1.40990600	-0.86022300	-5.42622100
H	2.59438100	-1.70768600	-4.38137600
H	2.68701200	0.05734200	-4.56185100
C	3.63521800	-1.45397900	1.87860600
H	4.70562300	-1.57464300	1.65272600
C	3.12147100	-2.84284000	2.30214200
H	2.04936600	-2.81378100	2.52657000
H	3.64739800	-3.19493200	3.19768200
H	3.28070100	-3.56437400	1.49436300
C	3.54932600	-0.48488900	3.06038000
C	4.71416400	-0.02430300	3.68574800
C	2.31031200	-0.04855000	3.55672500
C	4.65447100	0.85510600	4.77082300
H	5.68277800	-0.35619600	3.31608100
C	2.24729400	0.82768200	4.64054100
H	1.38870000	-0.38979600	3.09395800
C	3.41868200	1.28637700	5.25149600
H	5.57368100	1.20279800	5.23642500
H	1.27746800	1.15080700	5.01201900
H	3.36633400	1.97067500	6.09471600
O	-0.76793300	-0.72583000	1.01349300
Li	-1.00315300	0.46589100	-0.53348400
C	-1.63432500	-0.75841600	1.93344700
N	-3.05588300	0.25483600	-0.80173300
N	-2.92721000	-0.52112200	1.86826500
O	-1.11611200	-1.05386400	3.16084700
P	-3.80483700	-0.36842100	0.47931000
C	-3.79480600	1.01067200	-1.83080900
C	-2.01702900	-1.16588300	4.26476400
C	-4.49533400	-2.06508200	0.21682000
C	-5.26436300	0.61371900	1.02055500
H	-4.55928000	1.64959600	-1.36200600
C	-4.53376100	0.11675100	-2.85273500
C	-2.87033200	1.94721600	-2.60379000
H	-1.39326900	-1.43370700	5.12025700
H	-2.76617500	-1.94156700	4.08309500
H	-2.53146600	-0.21875300	4.45249900
C	-4.20796900	-2.77117000	-0.95663700
C	-5.26773500	-2.68541800	1.21227100
C	-6.51248200	0.47591800	0.39541600
C	-5.11209600	1.58599100	2.01976200
H	-3.82410900	-0.53272600	-3.37745000
H	-5.04812300	0.73138900	-3.60144400
H	-5.27835200	-0.51957900	-2.36295400
C	-3.20786400	3.29730300	-2.76455200
C	-1.71674700	1.47008000	-3.24309700
C	-4.68780500	-4.07117500	-1.13963400

H	-3.60531000	-2.29326200	-1.72208000
C	-5.74875500	-3.98098900	1.03004400
H	-5.49161200	-2.15045200	2.13097100
C	-7.58380200	1.29404200	0.75880300
H	-6.65727500	-0.28419500	-0.36718100
C	-6.18252300	2.40283000	2.38397600
H	-4.15493400	1.68073100	2.52289100
C	-2.42441800	4.14946900	-3.54744200
H	-4.10122400	3.68343500	-2.27758600
C	-0.92663900	2.31983100	-4.01914000
H	-1.42572200	0.42874000	-3.13934500
C	-5.45980900	-4.67651900	-0.14793700
H	-4.46192600	-4.60734000	-2.05806300
H	-6.34851100	-4.45001800	1.80593800
C	-7.42020700	2.25993500	1.75274300
H	-8.54603200	1.17296000	0.26814200
H	-6.05276900	3.14685800	3.16584600
C	-1.27961100	3.66184900	-4.18033500
H	-2.70979600	5.19261700	-3.66176300
H	-0.03422300	1.92478000	-4.49662100
H	-5.83622100	-5.68637400	-0.28984000
H	-8.25478400	2.89502900	2.03835500
H	-0.66726800	4.32120500	-4.79040600
O	0.61294600	-3.29241900	-0.13811500
C	1.56785500	-4.00858600	-0.94892500
C	-0.73612700	-3.64134000	-0.54117000
C	0.79765200	-4.42290100	-2.20141000
H	1.92768000	-4.88578300	-0.39221900
H	2.40867800	-3.33839600	-1.13730600
C	-0.59249700	-4.72238200	-1.61980600
H	-1.21311700	-2.73657400	-0.92692700
H	-1.28766100	-3.97915800	0.34089600
H	0.74568200	-3.58454800	-2.90580900
H	1.25002300	-5.27932200	-2.71144300
H	-1.39452600	-4.67325900	-2.36227900
H	-0.60889100	-5.72296200	-1.17130000
O	-0.52180700	2.29339400	0.20939600
C	-0.77118500	2.63131900	1.58312500
C	0.01538700	3.44385800	-0.48969200
C	-1.02318700	4.13725800	1.57222600
H	0.10470800	2.37179000	2.19463800
H	-1.62544000	2.03860200	1.91780300
C	-0.01490800	4.61172500	0.51252000
H	-0.62106000	3.62545100	-1.35839400
H	1.02897600	3.21021400	-0.82786900
H	-2.05069600	4.34264800	1.24977500
H	-0.86977000	4.60063900	2.55219900
H	-0.30417600	5.55404100	0.03732600
H	0.97280000	4.75143200	0.96431900

(*u*,*d*)-**D3a(THF)$_2$**

B3LYP SCF energy: -3386.03984390 a.u.
B3LYP enthalpy: -3384.97500800 a.u.
B3LYP free energy: -3385.05905500 a.u.
M06-2X SCF energy in solution: -3385.67456697 a.u.
M06-2X enthalpy in solution: -3384.60973107 a.u.
M06-2X free energy in solution: -3384.69377807 a.u.

Cartesian coordinates

ATOM	X	Y	Z
P	3.81729000	0.26942000	0.61251900
C	4.44081300	1.96631100	1.00600200
C	4.73173200	2.34925800	2.32508100
C	4.64316100	2.88912900	-0.02787900
C	5.21335000	3.62900900	2.60034600
H	4.57041100	1.64161500	3.13256900
C	5.13317700	4.16914500	0.24569500
H	4.40056800	2.60026900	-1.04624900
C	5.41722400	4.54081300	1.56076700
H	5.43040300	3.91648300	3.62603100
H	5.29216300	4.87409800	-0.56679200
H	5.79546300	5.53683800	1.77655900
C	5.31174000	-0.78347900	0.78064700
C	6.55560700	-0.35536600	0.29333700
C	5.20334800	-2.06711100	1.33355800
C	7.66735800	-1.19800200	0.34958000
H	6.66354800	0.64524200	-0.11656700
C	6.31516200	-2.90689900	1.39326900
H	4.24669100	-2.39467800	1.72733300
C	7.54825300	-2.47564800	0.89889400
H	8.62634300	-0.85300000	-0.02818200
H	6.22011600	-3.89850300	1.82825700
H	8.41431300	-3.13070800	0.94736500
N	3.12639200	0.19843000	-0.83138200
N	2.90229900	-0.13994400	1.92483700
Li	1.20601500	0.86484300	-0.71385200
C	1.59793800	0.01221200	2.00402600
O	0.77172000	0.42353600	1.13700600
O	1.00742100	-0.32136100	3.19271000
C	1.84785200	-0.75178600	4.26392400
H	1.17552900	-0.93050700	5.10608000
H	2.58063500	0.01775900	4.52292300
H	2.38386400	-1.66998200	4.00501800
C	3.79640400	-0.28717800	-2.04759900
H	4.89121200	-0.24694700	-1.94614300
C	3.43028600	0.62009100	-3.23805200
H	2.34602600	0.63753900	-3.39663300
H	3.90322900	0.26387400	-4.16114300
H	3.76295900	1.64786900	-3.05187800
C	3.45749000	-1.74234300	-2.38067900
C	4.47673700	-2.69399700	-2.49922500
C	2.13568800	-2.14774200	-2.62206400
C	4.19479200	-4.01556000	-2.85654700
H	5.50580200	-2.39830100	-2.30635600
C	1.85265600	-3.46330200	-2.99084700
H	1.32376700	-1.43222500	-2.51921800
C	2.88029300	-4.40409300	-3.10986200
H	5.00420500	-4.73708500	-2.93953700
H	0.82488800	-3.75442900	-3.19610400
H	2.65570200	-5.42801000	-3.39852100
O	-0.50473000	0.12326700	-1.32930500
Li	-0.94631200	-0.30431400	0.53943900

C	-1.28335100	0.67280300	-2.16607500
N	-2.87534600	0.39639800	0.62443500
N	-2.57835200	0.88373300	-2.10807200
O	-0.63459000	1.10164900	-3.29626100
P	-3.53529700	0.42772300	-0.83534300
C	-3.44581300	1.04821800	1.80778000
C	-1.41822000	1.68038400	-4.34038000
C	-4.97697000	1.55854900	-0.96612500
C	-4.20986800	-1.21617700	-1.33455700
H	-4.22453200	1.77072300	1.52289300
C	-2.35386200	1.85042900	2.54314100
C	-4.10594900	0.07122300	2.78547500
H	-0.71239600	1.90377800	-5.14379700
H	-1.91267900	2.59737700	-4.00550100
H	-2.18189300	0.98172000	-4.69366800
C	-4.85167100	2.79568900	-1.61241700
C	-6.20223500	1.22220700	-0.36991000
C	-4.62702400	-2.12410200	-0.35078100
C	-4.34500500	-1.56724400	-2.68720400
H	-1.52194000	1.20310000	2.84107000
H	-2.75720600	2.32876500	3.44398100
H	-1.95903400	2.62780300	1.87978100
C	-5.27468900	0.44052300	3.46432600
C	-3.54551000	-1.18365600	3.06441000
C	-5.92963600	3.68096400	-1.65916000
H	-3.90955800	3.04686600	-2.08852500
C	-7.27879000	2.10824900	-0.41676500
H	-6.32024000	0.26403400	0.12881500
C	-5.17597100	-3.35697900	-0.71267200
H	-4.50856300	-1.86804900	0.69751500
C	-4.88509300	-2.80226400	-3.04690600
H	-4.01833300	-0.86988600	-3.45213100
C	-5.86753500	-0.41104500	4.39938900
H	-5.72702700	1.40843600	3.25551500
C	-4.13435300	-2.03729800	3.99908400
H	-2.65731000	-1.49658800	2.52320700
C	-7.14403200	3.33976200	-1.06127300
H	-5.82257300	4.63595500	-2.16749400
H	-8.22318800	1.83482800	0.04646700
C	-5.30406800	-3.69835900	-2.06014500
H	-5.50067900	-4.04996500	0.05952000
H	-4.97963000	-3.06577500	-4.09734900
C	-5.29732000	-1.65496300	4.67218900
H	-6.77740300	-0.10412700	4.90987400
H	-3.68488000	-3.00707600	4.20155500
H	-7.98403600	4.02853300	-1.10078700
H	-5.72709400	-4.65941100	-2.34163700
H	-5.75655000	-2.32209800	5.39732700
O	1.05963900	2.88087100	-0.79842600
C	1.24849800	3.72086100	-1.95085100
C	0.86202100	3.69181800	0.38606200
C	0.63357600	5.06535700	-1.56641000
H	2.32345000	3.82193200	-2.15848500
H	0.76907100	3.22625200	-2.79799500
C	0.99279400	5.15020500	-0.07393200
H	-0.13375100	3.46738700	0.78066100
H	1.60842000	3.40855900	1.13252400
O	-0.84234500	-2.33942100	0.82202400
C	-0.99913300	-3.21228500	-0.31147700
C	-0.06286500	-3.07171800	1.78406800
C	-1.29412600	-4.57952100	0.30929900
H	-0.06710200	-3.22379200	-0.89157800
H	-1.80668400	-2.81360000	-0.92617400
C	-0.47046600	-4.55627900	1.62337700
H	-0.28231500	-2.64858500	2.76510200
H	1.00404400	-2.92637100	1.56892400
H	-2.36389100	-4.66639900	0.52285700
H	-1.01326600	-5.40382900	-0.35325700
H	-1.06540300	-4.90627800	2.47222600
H	0.41589000	-5.19485400	1.55825800
H	1.03134600	5.89679000	-2.15672400
H	-0.45430900	5.03729300	-1.70015100
H	2.02549100	5.49632900	0.04828700
H	0.34066700	5.82273600	0.49139700

Table S8. Vibrational analyses of all calculated species up to ca. 100 cm^{-1} (copy of screen)

M1a

G3:M1:V1 - Display Vibrations

Mode #	Freq	Infrared
1	14.11	0.3750
2	16.21	0.1872
3	33.99	0.1443
4	37.63	0.0540
5	41.94	0.0802
6	45.43	0.0574
7	50.31	0.1228
8	55.02	0.0911
9	64.16	0.1217
10	94.40	0.6351
11	114.33	1.6285

M1b

G5:M3:V1 - Display Vibrations

Mode #	Freq	Infrared
1	11.85	0.1319
2	17.57	0.5332
3	35.32	0.1554
4	36.79	0.4623
5	40.50	0.1015
6	46.37	0.2619
7	49.93	0.7812
8	59.89	2.1743
9	64.98	0.1101
10	96.29	2.7441
11	114.65	0.0843

M2a

G3:M2:V1 - Display Vibrations

Mode #	Freq	Infrared
1	7.20	0.0165
2	24.29	0.4644
3	29.71	0.0815
4	36.61	0.0623
5	40.59	0.0986
6	44.31	0.0341
7	46.64	0.0143
8	66.82	0.0162
9	67.00	0.1002
10	87.97	1.1030
11	103.72	0.6544

M2b

G2:M1:V1 - Display Vibrations

Mode #	Freq	Infrared
1	9.84	0.1314
2	25.32	0.1883
3	28.75	0.6123
4	35.45	0.0020
5	37.49	0.0190
6	42.68	0.1665
7	52.55	0.8405
8	59.97	0.2346
9	70.32	0.1895
10	84.25	3.1885
11	101.91	1.3630

M1a(THF)

G5:M1:V1 - Display Vibrations

Mode #	Freq	Infrared
1	5.91	0.0718
2	14.89	0.4541
3	24.12	0.6601
4	28.00	0.6112
5	31.26	0.1582
6	38.00	0.1412
7	40.68	0.1315
8	42.57	0.1931
9	45.01	0.5598
10	47.90	0.3961
11	52.87	0.4030
12	59.09	0.4180
13	64.55	1.4006
14	66.24	0.9428
15	84.25	1.5207
16	109.49	0.2106

M2a(THF)

G6:M1:V1 - Display Vibrations

Mode #	Freq	Infrared
1	14.03	0.6282
2	19.28	0.0353
3	25.44	0.4499
4	29.57	0.4856
5	36.25	0.2032
6	41.48	0.0393
7	43.83	0.0762
8	46.93	0.0628
9	50.75	0.6108
10	54.89	0.3216
11	59.42	0.1374
12	65.50	0.4991
13	75.25	1.5593
14	84.96	0.1488
15	96.01	1.3543
16	115.83	1.0331

M1a(THF)$_2$

G8:M1:V1 - Display Vibrations

Mode #	Freq	Infrared
1	1.52	0.3571
2	11.67	0.0522
3	20.05	0.0607
4	24.14	0.7888
5	26.65	0.5618
6	32.59	0.1215
7	33.74	0.2114
8	38.54	0.7049
9	40.97	0.3381
10	42.83	0.3496
11	45.04	0.0984
12	53.59	0.1664
13	56.77	0.3298
14	58.56	0.2055
15	67.15	0.0942
16	74.44	0.1413
17	83.35	0.6061
18	86.92	0.9666
19	99.84	2.1638
20	106.55	3.7866

M1b(THF)$_2$

G9:M1:V1 - Display Vibrations

Mode #	Freq	Infrared
1	3.56	0.1939
2	11.15	0.3017
3	19.06	0.0210
4	21.43	0.4176
5	23.72	0.0846
6	31.56	1.0842
7	33.75	0.1302
8	37.05	0.2078
9	38.90	0.3221
10	43.34	0.2306
11	46.81	0.5984
12	47.48	0.4135
13	52.74	0.3868
14	57.25	0.0941
15	65.34	0.2740
16	68.10	0.1416
17	81.57	0.0743
18	83.18	0.6575
19	87.03	0.2691
20	96.55	0.4132
21	105.61	1.3688

M2a(THF)$_2$

G11:M1:V1 - Display Vibrations

Mode #	Freq	Infrared
1	9.97	0.0894
2	16.31	0.0292
3	24.45	0.7023
4	27.51	0.0768
5	30.78	0.5697
6	31.18	0.2170
7	35.53	0.0814
8	39.66	0.1140
9	42.89	0.0596
10	45.50	0.0111
11	47.41	0.2836
12	48.39	0.2923
13	57.02	0.3880
14	59.62	0.8793
15	63.28	0.1563
16	68.13	0.7773
17	74.97	0.4388
18	85.90	1.3902
19	93.56	1.4406
20	100.18	4.3279

M2b(THF)$_2$

G12:M1:V1 - Display Vibrations

Mode #	Freq	Infrared
1	13.42	0.0364
2	19.59	0.3716
3	23.89	0.2599
4	26.53	0.2985
5	29.79	0.2611
6	36.00	1.1233
7	36.60	0.0292
8	41.70	0.0146
9	43.08	0.0492
10	46.46	0.6768
11	48.65	0.3399
12	55.97	0.1382
13	58.01	0.3458
14	65.18	0.5921
15	67.03	0.6950
16	77.29	0.1183
17	79.28	0.8071
18	88.00	0.5368
19	94.96	0.8649
20	101.66	0.6970

M3a(THF)$_2$

G13:M1:V1 - Display Vibrations

Mode #	Freq	Infrared
1	5.73	0.3658
2	12.89	0.2085
3	15.86	0.1786
4	20.23	0.5026
5	26.95	0.6609
6	27.91	0.2256
7	31.58	0.1681
8	35.32	0.6894
9	38.64	0.0362
10	43.25	0.1060
11	45.55	0.1522
12	50.19	0.1882
13	53.01	0.5459
14	56.95	0.4765
15	62.39	0.5004
16	65.33	0.2251
17	74.17	1.4241
18	78.54	0.0908
19	92.08	0.8266
20	96.24	0.6600
21	97.70	1.7918
22	107.20	1.6691

M3b(THF)$_2$

G14:M1:V1 - Display Vibrations

Mode #	Freq	Infrared
1	12.83	0.2750
2	15.93	0.0978
3	20.83	0.5507
4	26.10	0.1933
5	27.92	0.5016
6	32.73	0.1703
7	36.86	0.0103
8	39.10	1.1669
9	44.43	0.4991
10	44.85	0.4467
11	48.84	0.6594
12	50.44	0.3005
13	57.25	0.8228
14	63.01	0.1523
15	65.35	0.2856
16	71.95	0.0762
17	75.37	0.6722
18	80.64	1.3918
19	83.19	0.6075
20	100.62	0.2338

D1a

G16:M1:V1 - Display Vibrations

Mode #	Freq	Infrared
1	9.28	0.1082
2	9.55	0.0022
3	12.24	0.0653
4	15.76	0.0775
5	15.79	0.0121
6	24.04	0.2567
7	25.81	0.0252
8	31.37	0.1886
9	34.48	0.0159
10	34.92	0.0054
11	36.87	0.0005
12	40.15	0.0098
13	40.78	0.1862
14	44.08	0.1352
15	46.41	0.0343
16	49.81	0.2372
17	50.28	0.0128
18	54.50	0.0002
19	56.64	0.2756
20	59.69	0.2960
21	64.86	0.1841
22	72.02	0.0028
23	79.08	0.2623
24	94.48	0.3557
25	96.09	0.1081
26	108.15	0.0989

D1b

G17:M1:V1 - Display Vibrations

Mode #	Freq	Infrared
1	5.67	0.0407
2	6.71	0.0762
3	10.03	0.0843
4	12.33	0.0206
5	16.01	0.1549
6	19.25	0.0349
7	26.62	0.1538
8	28.46	0.1144
9	33.04	0.0026
10	35.96	0.6190
11	38.38	0.1313
12	40.84	0.2924
13	42.73	0.1012
14	43.74	0.2159
15	45.94	0.0777
16	49.80	0.5877
17	51.38	0.0764
18	53.54	0.1499
19	59.00	0.0835
20	62.13	0.2552
21	67.03	0.2308
22	77.32	0.3625
23	80.93	0.5509
24	98.02	0.8087
25	100.41	1.9246

D2a

G1:M1:V1 - Display Vibrations

Mode #	Freq	Infrared
1	11.73	0.0080
2	12.42	0.0103
3	12.97	0.0712
4	16.10	0.1035
5	16.21	0.0237
6	17.46	0.0480
7	27.64	0.0643
8	29.18	0.0526
9	32.00	0.0019
10	35.52	0.0324
11	38.50	0.0268
12	41.08	0.0148
13	41.14	0.0687
14	43.47	0.0567
15	44.09	0.0322
16	50.35	0.6175
17	52.12	0.3584
18	55.38	0.2967
19	60.88	0.0242
20	66.06	0.2622
21	68.01	0.1924
22	73.99	0.0065
23	79.22	0.1565
24	87.80	0.0036
25	88.83	0.0063
26	105.47	0.1640

D1c

G18:M1:V1 - Display Vibrations

Mode #	Freq	Infrared
1	7.61	0.0083
2	9.79	0.0423
3	12.70	0.1464
4	18.54	0.0435
5	19.50	0.0360
6	27.64	0.2758
7	29.27	0.0930
8	32.19	0.0894
9	37.10	0.3622
10	39.24	0.0015
11	40.45	0.2746
12	41.49	0.2164
13	43.73	0.0046
14	44.14	0.9353
15	46.33	0.0013
16	47.08	0.1317
17	50.26	0.7579
18	52.58	0.0322
19	62.08	0.0474
20	69.96	2.0075
21	76.03	0.0213
22	81.12	0.7317
23	82.87	1.1302
24	103.29	1.5207

D2b

G3:M1:V1 - Display Vibrations

Mode #	Freq	Infrared
1	10.08	0.0597
2	13.50	0.0502
3	15.69	0.0422
4	18.78	0.0503
5	19.70	0.0645
6	22.52	0.0745
7	28.74	0.1029
8	31.27	0.0709
9	32.81	0.0016
10	35.26	0.3801
11	38.43	0.2483
12	40.21	0.4096
13	43.13	0.1376
14	44.88	0.2042
15	47.63	0.5749
16	48.67	0.5397
17	54.40	0.3786
18	55.82	0.0507
19	61.13	0.0424
20	63.22	0.2284
21	74.63	0.1583
22	83.59	0.3510
23	89.34	0.2425
24	91.60	0.8404
25	92.41	0.0851
26	103.86	1.1426

D2c

G11:M14:V1 - Display Vibrations

Mode #	Freq	Infrared
1	8.14	0.1105
2	16.67	0.3553
3	17.71	0.0760
4	22.06	0.0539
5	22.98	0.0750
6	24.78	0.2392
7	29.87	0.1128
8	31.14	0.1998
9	36.99	0.1253
10	37.27	0.4008
11	38.65	0.0800
12	40.56	0.6436
13	41.56	0.7224
14	46.53	0.6006
15	49.69	0.6922
16	50.08	0.1909
17	52.84	0.0961
18	53.68	0.5164
19	59.30	1.2748
20	64.72	0.0208
21	70.62	0.2104
22	79.90	0.3154
23	87.86	1.7412
24	90.16	0.0688
25	92.69	0.4204
26	114.34	2.1339
27	117.13	0.7147

D3a

G2:M1:V1 - Display Vibrations

Mode #	Freq	Infrared
1	5.71	0.0014
2	9.40	0.0872
3	11.26	0.0840
4	15.21	0.0139
5	17.95	0.0222
6	21.65	0.0946
7	24.81	0.2109
8	28.88	0.0916
9	32.35	0.0691
10	35.83	0.0254
11	39.31	0.0037
12	41.82	0.0272
13	43.67	0.2565
14	46.90	0.1659
15	48.00	0.0781
16	52.17	0.2747
17	54.59	0.0879
18	56.01	0.3579
19	57.40	0.0667
20	62.89	0.1428
21	66.74	0.0247
22	69.84	0.0111
23	74.18	0.1885
24	86.45	0.0912
25	92.37	0.0067
26	108.68	0.2879

D4a

G10:M1:V1 - Display Vibrations

Mode #	Freq	Infrared
1	14.94	0.0118
2	18.27	0.1721
3	22.96	0.1203
4	28.40	0.3409
5	31.01	0.0832
6	31.71	0.1605
7	33.76	0.0204
8	34.57	0.4247
9	44.88	0.8490
10	45.41	0.1656
11	47.46	0.0363
12	47.67	0.7318
13	51.34	0.0467
14	54.69	0.0150
15	60.49	1.1967
16	60.54	0.4842
17	65.59	0.0410
18	65.68	0.3278
19	69.29	5.8085
20	73.70	0.0966
21	73.97	0.3273
22	78.85	0.9421
23	81.32	0.4578
24	85.66	0.0114
25	102.78	0.1279

D5a

G9:M1:V1 - Display Vibrations

Mode #	Freq	Infrared
1	11.24	0.2360
2	14.26	0.0211
3	16.72	0.0020
4	24.55	0.1801
5	25.76	0.0565
6	28.11	0.1479
7	37.86	0.0294
8	40.07	0.0081
9	42.07	0.3016
10	44.21	0.0061
11	46.23	0.2311
12	49.67	0.6922
13	51.81	0.2344
14	54.98	0.2121
15	58.33	0.0474
16	64.87	0.2501
17	67.79	0.1963
18	70.33	0.5057
19	74.35	1.6344
20	78.78	0.8394
21	79.77	2.9789
22	81.86	0.9626
23	86.17	3.0434
24	90.75	0.8733
25	100.87	0.1581

D5a'

G12:M1:V1 - Display Vibrations

Mode #	Freq	Infrared
1	8.84	0.1296
2	16.17	0.0858
3	19.25	0.0261
4	21.23	0.5088
5	26.87	0.2293
6	29.20	0.1206
7	37.97	0.1090
8	40.21	0.0499
9	42.93	0.4053
10	46.18	0.6604
11	48.31	0.2680
12	51.98	0.0421
13	54.14	0.0176
14	59.51	0.0812
15	60.03	0.1066
16	63.61	0.1982
17	70.60	0.2482
18	73.67	0.2048
19	76.66	6.7326
20	80.73	0.1140
21	81.30	0.8145
22	87.48	0.4232
23	90.99	3.9510
24	97.47	0.6326
25	103.43	0.3499

(*d*,*d*)-**D1a(THF)$_2$**

G5:M1:V1 - Display Vibrations

Mode #	Freq	Infrared
1	7.32	0.9012
2	8.94	0.0831
3	10.41	0.1163
4	13.97	0.5674
5	20.26	0.2801
6	22.56	0.2129
7	24.62	0.5954
8	25.01	0.3445
9	26.30	0.3412
10	28.06	0.1817
11	28.96	0.0693
12	33.66	0.0508
13	35.43	0.1004
14	37.34	0.1245
15	37.86	0.6160
16	41.44	0.1389
17	43.75	0.1988
18	47.03	0.0551
19	49.74	0.0187
20	50.57	0.1286
21	53.89	0.1100
22	55.02	0.2766
23	56.06	0.1830
24	57.95	0.0740
25	59.95	0.0440
26	60.71	0.1376
27	66.54	1.1234
28	70.18	0.4030
29	72.11	0.3311
30	76.50	0.1220
31	78.54	0.1291
32	84.44	0.9149
33	86.79	2.3348
34	93.85	0.9517
35	102.03	2.7929

(*u*,*u*)-**D1a(THF)$_2$**

G6:M1:V1 - Display Vibrations

Mode #	Freq	Infrared
1	14.68	0.0023
2	15.40	0.0070
3	16.07	0.0511
4	16.54	0.7175
5	18.57	0.2195
6	20.12	0.0397
7	20.38	0.0038
8	25.16	0.0008
9	27.97	0.8965
10	29.15	0.1672
11	32.50	0.0668
12	35.13	0.2062
13	37.09	0.0101
14	38.54	0.0441
15	39.32	0.5412
16	41.22	0.1176
17	47.87	0.4941
18	48.52	0.0032
19	51.26	0.4270
20	54.11	0.0728
21	56.71	0.1458
22	58.99	0.0168
23	59.30	0.0180
24	61.09	0.0113
25	61.24	0.4210
26	64.69	0.1066
27	69.15	1.3011
28	69.37	1.1165
29	71.91	0.2754
30	73.78	0.0816
31	81.53	0.0936
32	83.41	0.1096
33	88.59	1.6557
34	92.97	0.0161
35	94.93	4.0039
36	96.37	1.4184
37	97.71	0.8884
38	109.74	0.6079

(*d*,*u*)-**D1a(THF)$_2$**

G7:M1:V1 - Display Vibrations

Mode #	Freq	Infrared
1	9.88	0.1240
2	12.69	0.0918
3	14.26	0.2266
4	15.78	0.5127
5	17.64	0.0561
6	20.95	0.1034
7	21.15	0.0615
8	26.92	0.0719
9	29.57	0.3905
10	32.63	0.1457
11	35.84	0.2808
12	36.26	0.2850
13	37.61	0.2361
14	39.42	0.1885
15	39.92	0.1513
16	43.40	0.2320
17	46.11	0.6136
18	47.18	0.7982
19	49.15	0.3350
20	50.68	0.0672
21	54.60	0.0736
22	57.10	0.8219
23	59.87	0.3385
24	62.22	0.3690
25	63.28	0.4782
26	65.16	0.0405
27	68.72	0.0668
28	71.06	0.1058
29	72.24	0.3857
30	81.07	0.2638
31	84.00	0.4652
32	87.21	0.1423
33	92.05	2.5658
34	99.23	0.4613
35	100.20	0.3696

(*d*,*u*)-**D2a(THF)$_2$**

G8:M1:V1 - Display Vibrations

Mode #	Freq	Infrared
1	10.99	0.0554
2	13.17	0.0782
3	15.13	0.0692
4	19.12	0.0436
5	21.60	0.0097
6	23.15	0.0063
7	24.61	0.1972
8	27.00	0.1379
9	28.48	0.0990
10	30.63	0.0589
11	33.92	0.9968
12	36.51	0.0372
13	39.91	0.1129
14	40.93	0.8842
15	41.85	0.7925
16	47.42	0.3625
17	48.30	0.2500
18	50.22	0.1764
19	53.02	0.0467
20	54.48	0.6357
21	56.31	0.1830
22	59.44	0.3880
23	61.73	0.0286
24	64.72	0.2409
25	66.08	0.2273
26	67.37	0.1561
27	73.99	0.0211
28	78.42	0.3556
29	79.07	0.0635
30	82.31	0.5174
31	82.91	0.5937
32	89.46	0.6781
33	90.41	0.0949
34	97.43	0.4520
35	100.30	0.3493

(*d*,*d*)-**D2a(THF)$_2$**

G10:M60:V1 - Display Vibrations

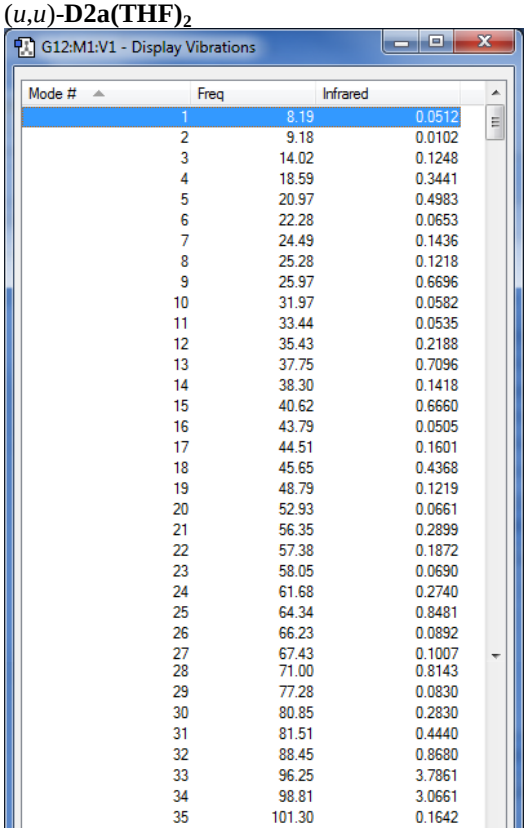
Mode #	Freq	Infrared
1	6.99	0.1619
2	8.97	0.1236
3	11.28	0.0284
4	13.57	0.1034
5	18.84	1.2561
6	20.97	0.2501
7	21.56	0.0656
8	22.70	0.2671
9	26.34	0.1259
10	28.98	0.0615
11	30.31	0.2095
12	32.92	0.0500
13	35.96	0.8869
14	36.88	0.0628
15	42.95	0.1834
16	43.87	0.2546
17	46.98	0.2157
18	48.27	0.2624
19	49.91	0.0521
20	50.95	0.1791
21	53.62	0.0917
22	55.99	0.1399
23	58.46	0.0234
24	60.86	0.0077
25	66.18	0.1849
26	66.75	0.5014
27	69.94	0.2874
28	71.43	0.0405
29	74.42	0.6829
30	79.39	0.7260
31	81.77	0.1997
32	86.17	0.9957
33	93.71	0.4356
34	94.91	0.8818
35	95.79	0.8166
36	105.28	0.1461

(*d*,*u*)-**D3a(THF)$_2$**

G9:M1:V1 - Display Vibrations

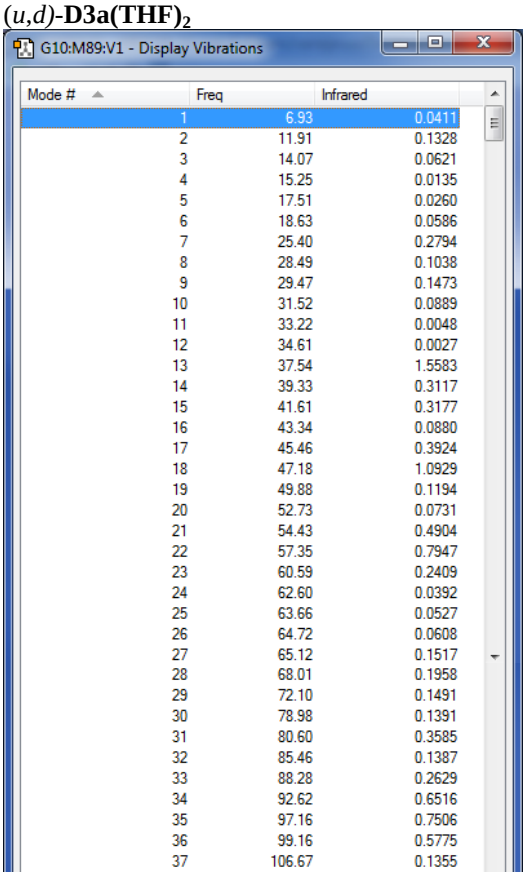
Mode #	Freq	Infrared
1	8.17	0.1014
2	11.29	0.0267
3	13.07	0.0442
4	18.18	0.1065
5	21.34	0.1928
6	22.54	0.0599
7	25.58	0.0866
8	29.66	0.0672
9	31.98	0.4369
10	32.29	0.8215
11	34.08	0.1774
12	37.35	0.2328
13	39.54	0.3144
14	42.18	0.0908
15	43.00	0.5788
16	44.95	0.3544
17	48.93	0.0809
18	51.96	0.2747
19	53.20	0.2772
20	54.60	0.4200
21	56.37	0.2949
22	57.53	0.1687
23	59.67	0.1773
24	61.48	0.4950
25	62.38	0.0750
26	66.45	0.0754
27	69.99	0.0210
28	73.40	0.1135
29	78.60	0.0561
30	81.00	0.3846
31	86.50	1.1612
32	91.98	0.6821
33	92.66	0.6172
34	94.51	0.3094
35	101.76	1.9652

(*u*,*u*)-**D2a(THF)$_2$**


G12:M1:V1 - Display Vibrations

Mode #	Freq	Infrared
1	8.19	0.0512
2	9.18	0.0102
3	14.02	0.1248
4	18.59	0.3441
5	20.97	0.4983
6	22.28	0.0653
7	24.49	0.1436
8	25.28	0.1218
9	25.97	0.6696
10	31.97	0.0582
11	33.44	0.0535
12	35.43	0.2188
13	37.75	0.7096
14	38.30	0.1418
15	40.62	0.6660
16	43.79	0.0505
17	44.51	0.1601
18	45.65	0.4368
19	48.79	0.1219
20	52.93	0.0661
21	56.35	0.2899
22	57.38	0.1872
23	58.05	0.0690
24	61.68	0.2740
25	64.34	0.8481
26	66.23	0.0892
27	67.43	0.1007
28	71.00	0.8143
29	77.28	0.0830
30	80.85	0.2830
31	81.51	0.4440
32	88.45	0.8680
33	96.25	3.7861
34	98.81	3.0661
35	101.30	0.1642

(*u*,*d*)-**D3a(THF)$_2$**


G10:M89:V1 - Display Vibrations

Mode #	Freq	Infrared
1	6.93	0.0411
2	11.91	0.1328
3	14.07	0.0621
4	15.25	0.0135
5	17.51	0.0260
6	18.63	0.0586
7	25.40	0.2794
8	28.49	0.1038
9	29.47	0.1473
10	31.52	0.0889
11	33.22	0.0048
12	34.61	0.0027
13	37.54	1.5583
14	39.33	0.3117
15	41.61	0.3177
16	43.34	0.0880
17	45.46	0.3924
18	47.18	1.0929
19	49.88	0.1194
20	52.73	0.0731
21	54.43	0.4904
22	57.35	0.7947
23	60.59	0.2409
24	62.60	0.0392
25	63.66	0.0527
26	64.72	0.0608
27	65.12	0.1517
28	68.01	0.1958
29	72.10	0.1491
30	78.98	0.1391
31	80.60	0.3585
32	85.46	0.1387
33	88.28	0.2629
34	92.62	0.6516
35	97.16	0.7506
36	99.16	0.5775
37	106.67	0.1355