

Supporting Information

Design of selective divalent chain transfer agent for coordinative chain transfer polymerization of ethylene and its copolymerization with butadiene

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NMR Spectra

Figure S1. ^1H NMR in TCE/ C_6D_6 at 363K of the polyethylene obtained with $\{(\text{Me}_2\text{Si}(\text{C}_{13}\text{H}_8)_2)\text{Nd}(\mu\text{-BH}_4)[(\mu\text{-BH}_4)\text{Li}(\text{THF})]\}_2/\text{MgPh}_2$ (run 2). *: solvent impurity.

Figure S2. ^1H NMR in C_6D_6 at 298K of an aliquot of $\text{PhMg}(\text{CH}_2)_5\text{MgPh}$ (**2b**) in solution in toluene. The solvent was evaporated before addition of C_6D_6 . Δ : MeTHF, * toluene, ψ : dibutylether.

Figure S3. ^1H NMR in TCE/ C_6D_6 at 363K of the polyethylene obtained with $\{(\text{Me}_2\text{Si}(\text{C}_{13}\text{H}_8)_2)\text{Nd}(\mu\text{-BH}_4)[(\mu\text{-BH}_4)\text{Li}(\text{THF})]\}_2/\mathbf{2b}$ (run 2).

Figure S4. ^1H NMR in TCE/ C_6D_6 at 363K of the poly(ethylene-*co*-butadiene) obtained with $\{(\text{Me}_2\text{Si}(\text{C}_{13}\text{H}_8)_2)\text{Nd}(\mu\text{-BH}_4)[(\mu\text{-BH}_4)\text{Li}(\text{THF})]\}_2/\mathbf{2b}$ (run 3).

Figure S5. ^{13}C NMR in C_6D_6 at 340K of $\text{MesMg}(\text{CH}_2)_5\text{MgMes}$ (**2c**). Δ : MeTHF. Ω : dioxane.

Figure S6. Two-dimensional NMR correlations $^1\text{H}/^{13}\text{C}$ HMBC in C_6D_6 at 340K of $\text{MesMg}(\text{CH}_2)_5\text{MgMes}$ (**2c**).

Figure S7. Two-dimensional NMR correlations $^1\text{H}/^1\text{H}$ NOESY at 298K of $\text{MesMg}(\text{CH}_2)_5\text{MgMes}$ (**2c**).

Figure S8. Two-dimensional NMR correlations $^1\text{H}/^1\text{H}$ COSY at 298K of $\text{MesMg}(\text{CH}_2)_5\text{MgMes}$ (**2c**).

Figure S9. Two-dimensional NMR correlations $^1\text{H}/^{13}\text{C}$ HMQC in C_6D_6 at 298K of $\text{MesMg}(\text{CH}_2)_5\text{MgMes}$ (**2c**).

Figure S10. ^1H NMR in TCE/ C_6D_6 at 363K of the polyethylene obtained with $\{(\text{Me}_2\text{Si}(\text{C}_{13}\text{H}_8)_2)\text{Nd}(\mu\text{-BH}_4)[(\mu\text{-BH}_4)\text{Li}(\text{THF})]\}_2/\mathbf{2c}$ after deactivation with MeOH (run 4).

Figure S11. ^{13}C NMR in TCE/ C_6D_6 at 363K of the polyethylene with deuterated chain-ends obtained with $\{(\text{Me}_2\text{Si}(\text{C}_{13}\text{H}_8)_2)\text{Nd}(\mu\text{-BH}_4)[(\mu\text{-BH}_4)\text{Li}(\text{THF})]\}_2/\mathbf{2c}$ (run 5).

Figure S12. ^1H NMR in TCE/ C_6D_6 at 363K of a typical poly(ethylene-*co*-butadiene) (run 7)

Molecular Modeling

➤ Speciation

Figure S13. Speciation of **A** : polymetallic neodymium species for phenyl and mesityl groups, **B** : phenyl organomagnesium co-catalyst and **C** : mesityl organomagnesium co-catalyst. ΔG in purple in kcal.mol $^{-1}$. [Nd] correspond to $[(\text{Me}_2\text{Si}(\text{C}_{13}\text{H}_8)_2)\text{Nd}]$.

➤ Dependence on DFT functionals

Figure S14. Isodesmic equilibria considered to assess initiation selectivity depending on the CTA.

Table S1. Gibbs activation energy differences for ethylene insertion between alkyl and aryl groups as illustrated in Figure S14.

➤ Cartesian coordinates and associated energies of optimized structures

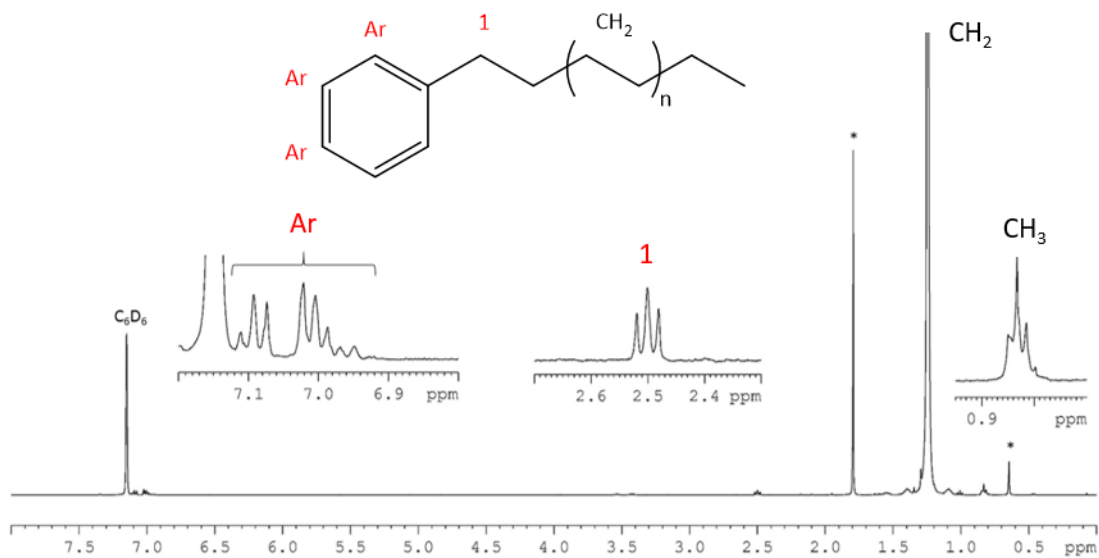


Figure S1. ^1H NMR in TCE/ C_6D_6 at 363K of the polyethylene obtained with $\{(\text{Me}_2\text{Si}(\text{C}_{13}\text{H}_8)_2)\text{Nd}(\mu\text{-BH}_4)[(\mu\text{-BH}_4)\text{Li}(\text{THF})]\}_2/\text{MgPh}_2$ (run 1). *: solvent impurity

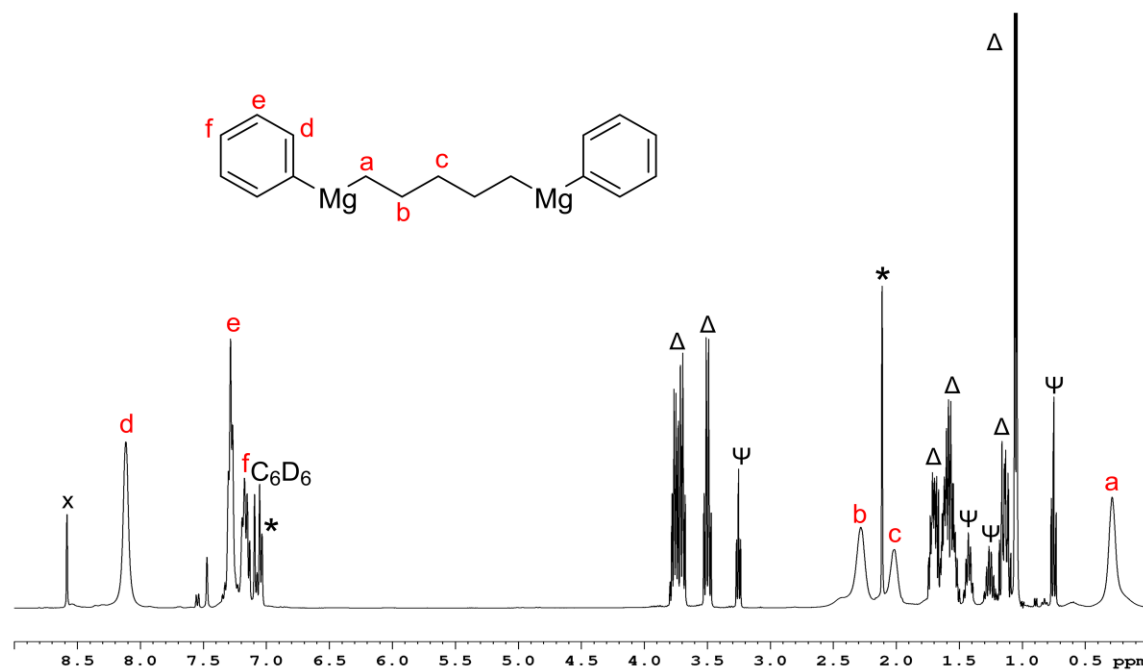


Figure S2. ^1H NMR in C_6D_6 at 298K of an aliquot of $\text{PhMg}(\text{CH}_2)_5\text{MgPh}$ (**2b**) in solution in toluene. The solvent was evaporated before addition of C_6D_6 . Δ : MeTHF, * toluene, ψ : dibutylether

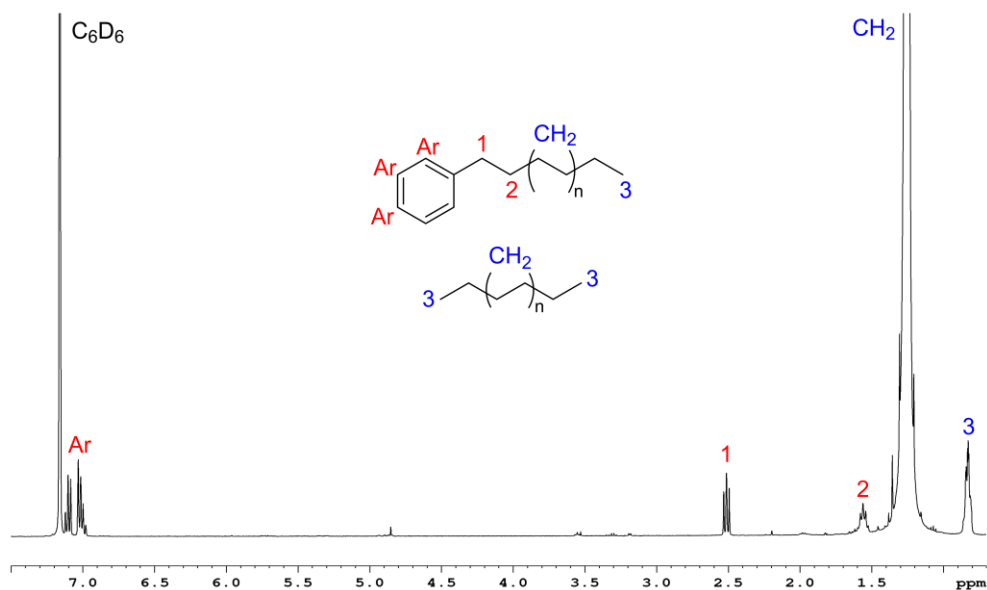


Figure S3. ^1H NMR in TCE/ C_6D_6 at 363K of the polyethylene obtained with $\{(\text{Me}_2\text{Si}(\text{C}_{13}\text{H}_8)_2)\text{Nd}(\mu\text{-BH}_4)[(\mu\text{-BH}_4)\text{Li}(\text{THF})]\}_2/\mathbf{2b}$ (run 2)

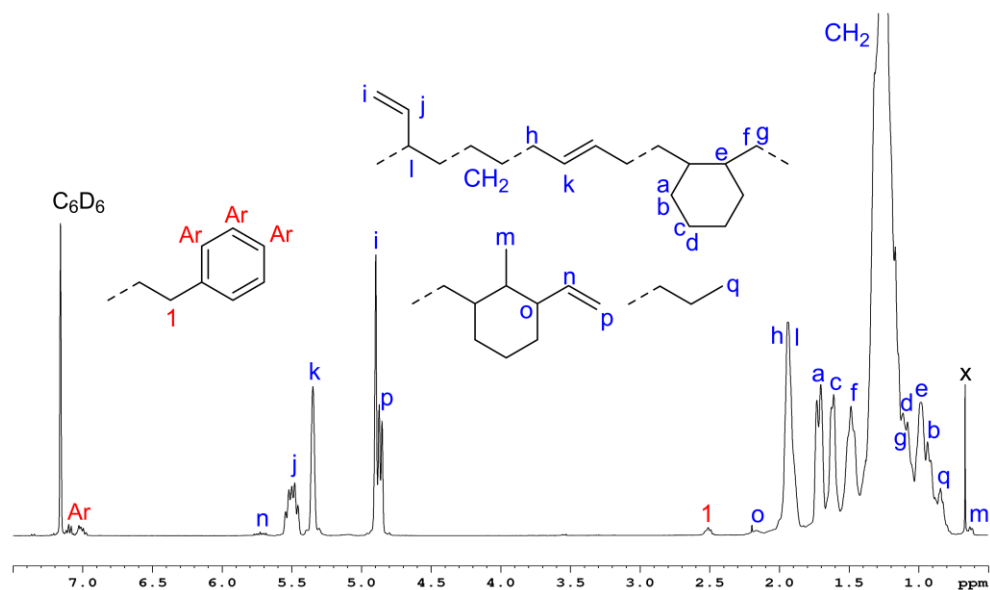


Figure S4. ¹H NMR in TCE/C₆D₆ at 363K of the poly(ethylene-*co*-butadiene) obtained with $\{(\text{Me}_2\text{Si}(\text{C}_{13}\text{H}_8)_2\text{Nd}(\mu\text{-BH}_4)[(\mu\text{-BH}_4)\text{Li}(\text{THF})]\}_2/\mathbf{2b}$ (run 3)

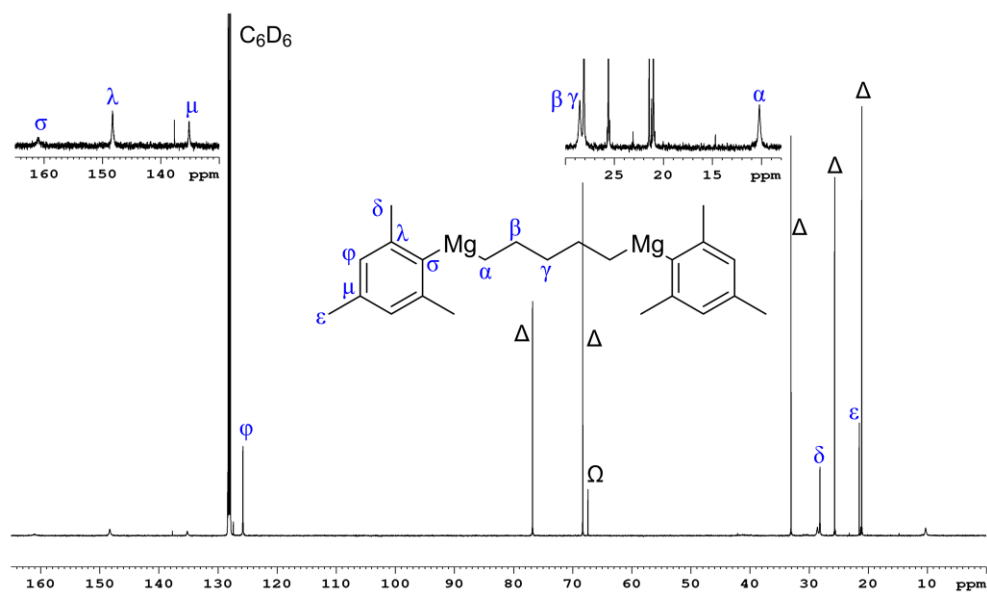


Figure S5. ^{13}C NMR in C_6D_6 at 340K of $\text{MesMg}(\text{CH}_2)_5\text{MgMes}$ (**2c**). Δ : MeTHF. Ω : dioxane

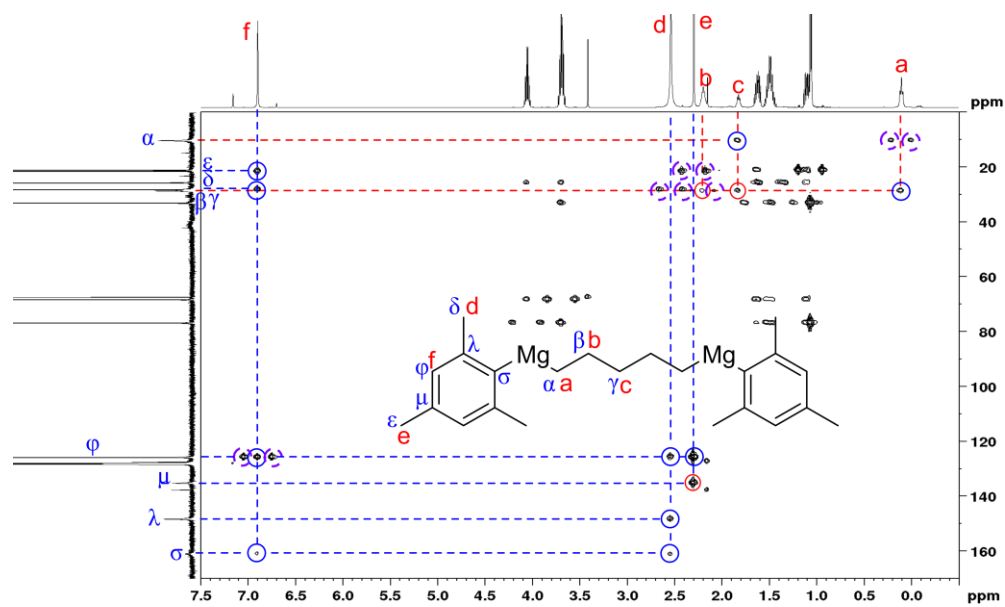


Figure S6. Two-dimensional NMR correlations $^1\text{H}/^{13}\text{C}$ HMBC in C_6D_6 at 340K of $\text{MesMg}(\text{CH}_2)_5\text{MgMes}$ (**2c**)

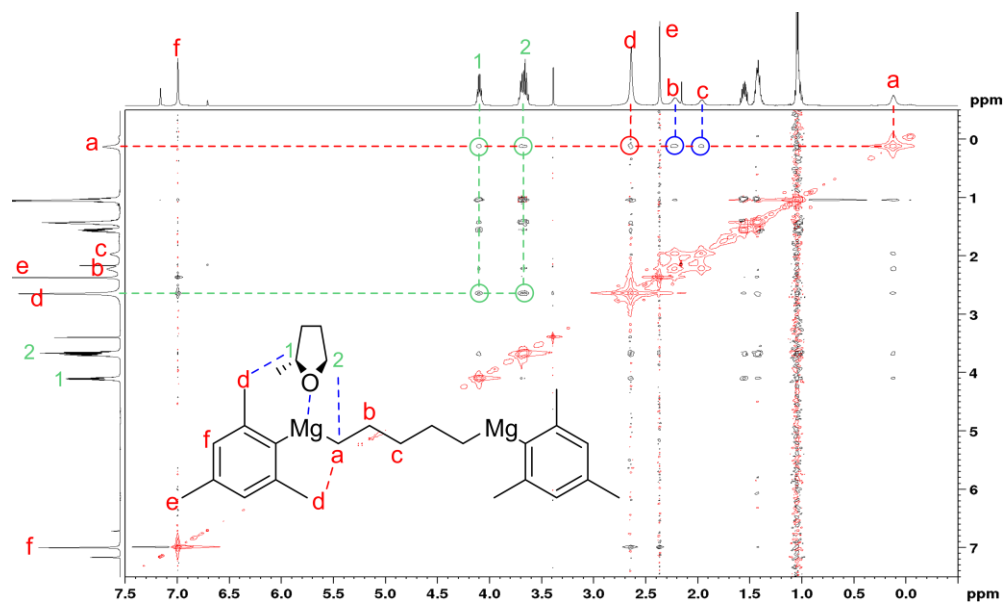


Figure S7. Two-dimensional NMR correlations $^1\text{H}/^1\text{H}$ NOESY at 298K of $\text{MesMg}(\text{CH}_2)_5\text{MgMes}$ (**2c**)

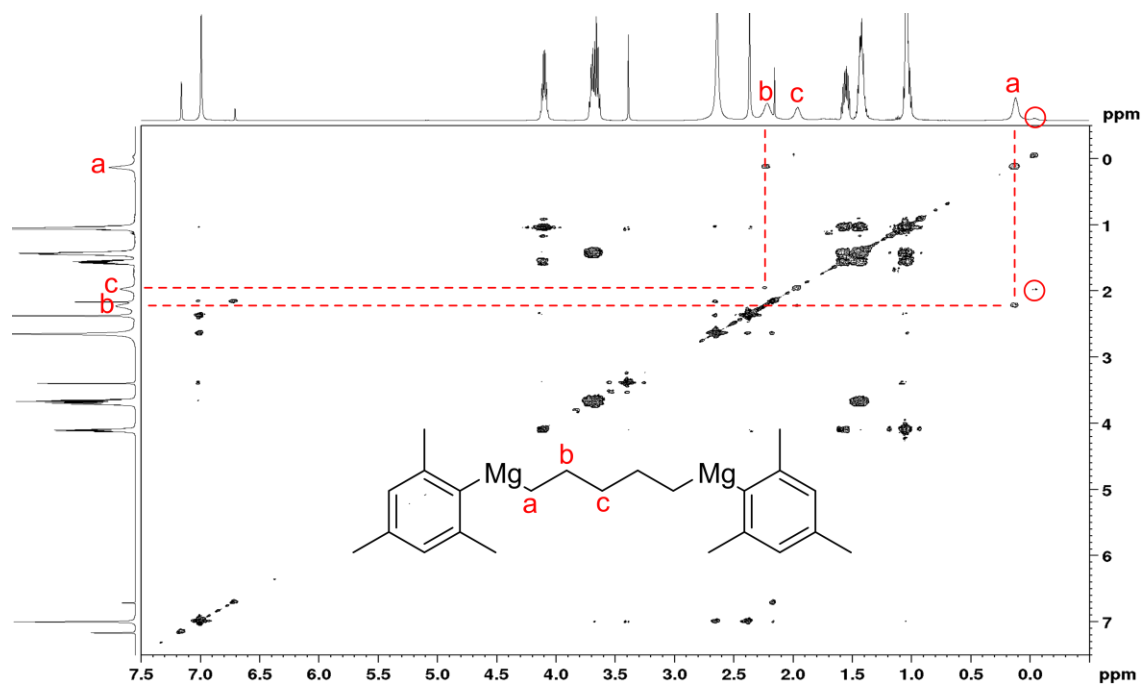


Figure S8. Two-dimensional NMR correlations ¹H/¹H COSY at 298K of MesMg(CH₂)₅MgMes (2c)

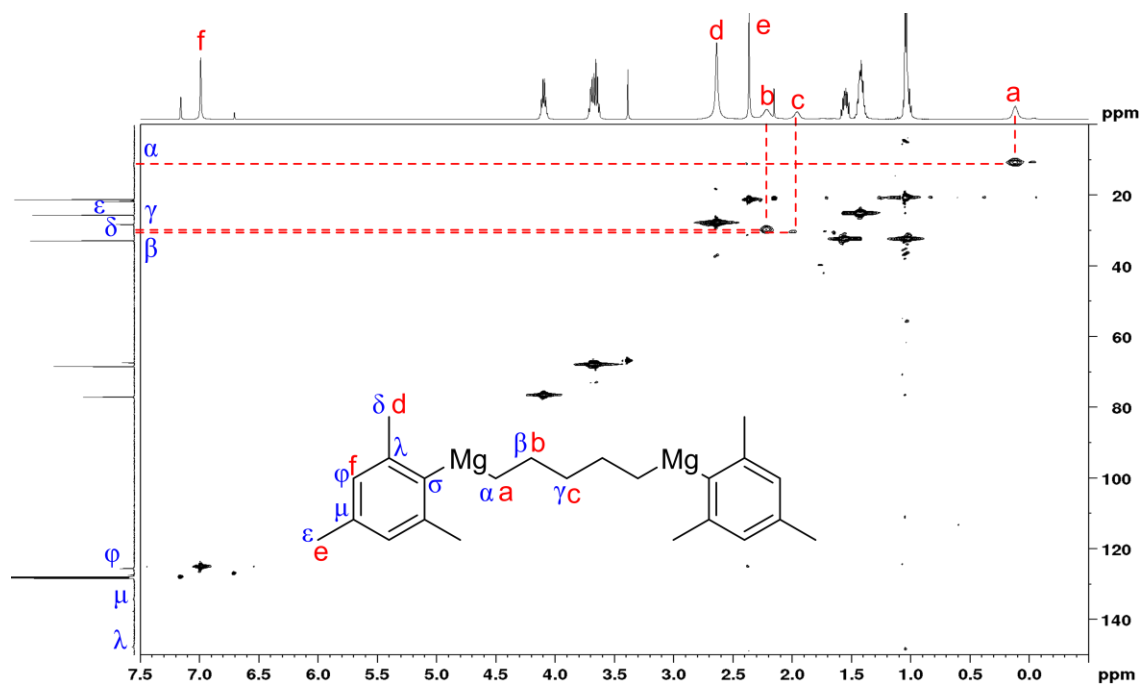


Figure S9. Two-dimensional NMR correlations $^1\text{H}/^{13}\text{C}$ HMQC in C_6D_6 at 298K of MesMg(CH₂)₅MgMes (**2c**)

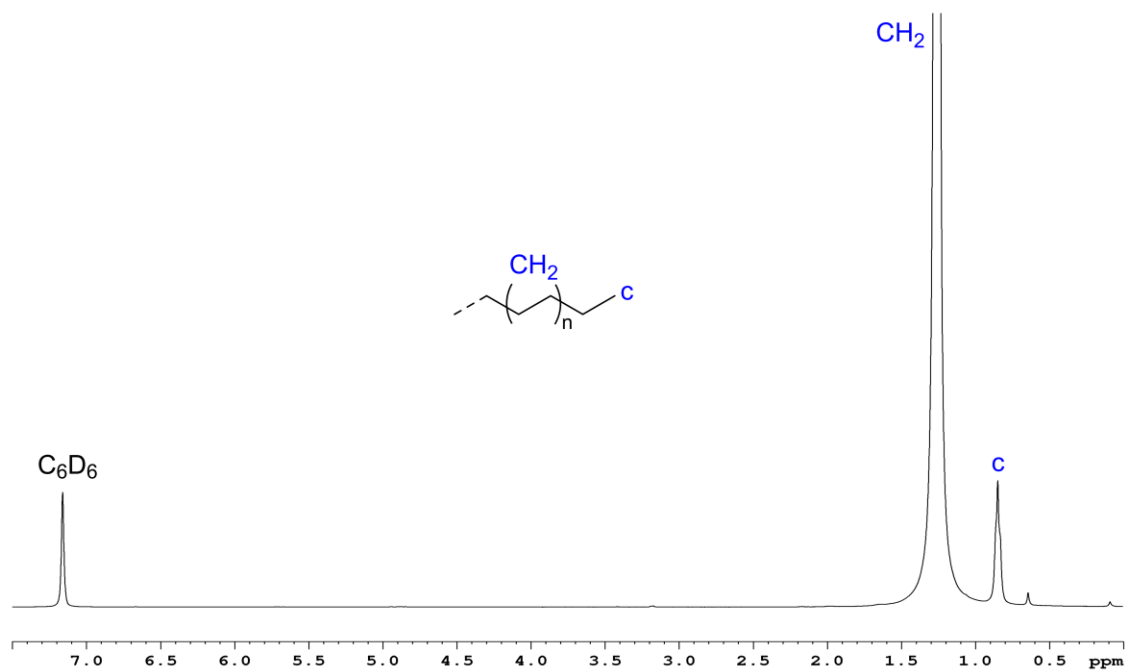


Figure S10. ^1H NMR in TCE/ C_6D_6 at 363K of the polyethylene obtained with $\{(\text{Me}_2\text{Si}(\text{C}_{13}\text{H}_8)_2)\text{Nd}(\mu\text{-BH}_4)[(\mu\text{-BH}_4)\text{Li}(\text{THF})]\}_2/\mathbf{2c}$ after deactivation with MeOH (run 4)

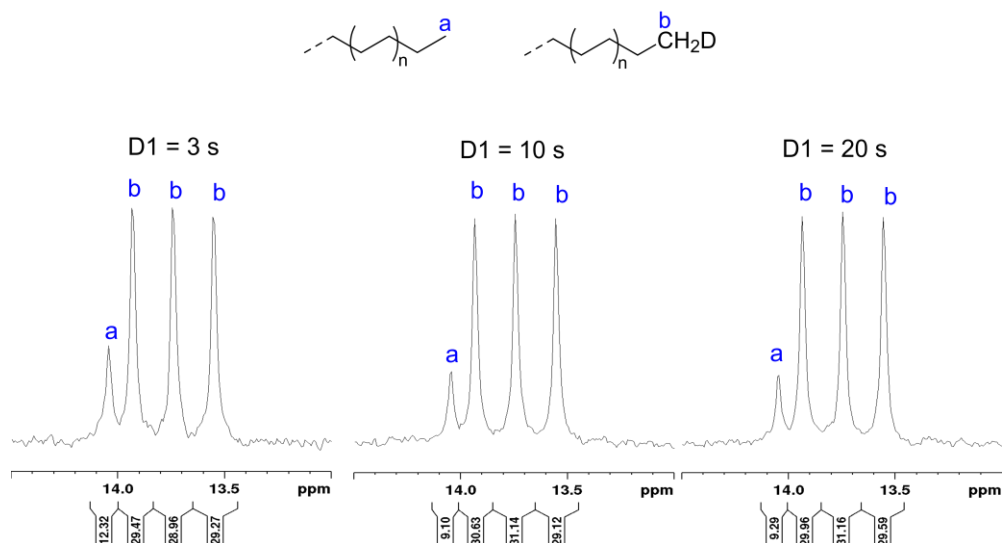


Figure S11. ^{13}C NMR in TCE/ C_6D_6 at 363K of the polyethylene with deuterated chain-ends obtained with $\{(\text{Me}_2\text{Si}(\text{C}_{13}\text{H}_8)_2)\text{Nd}(\mu\text{-BH}_4)[(\mu\text{-BH}_4)\text{Li}(\text{THF})]\}_2/2\mathbf{c}$ (run 5)

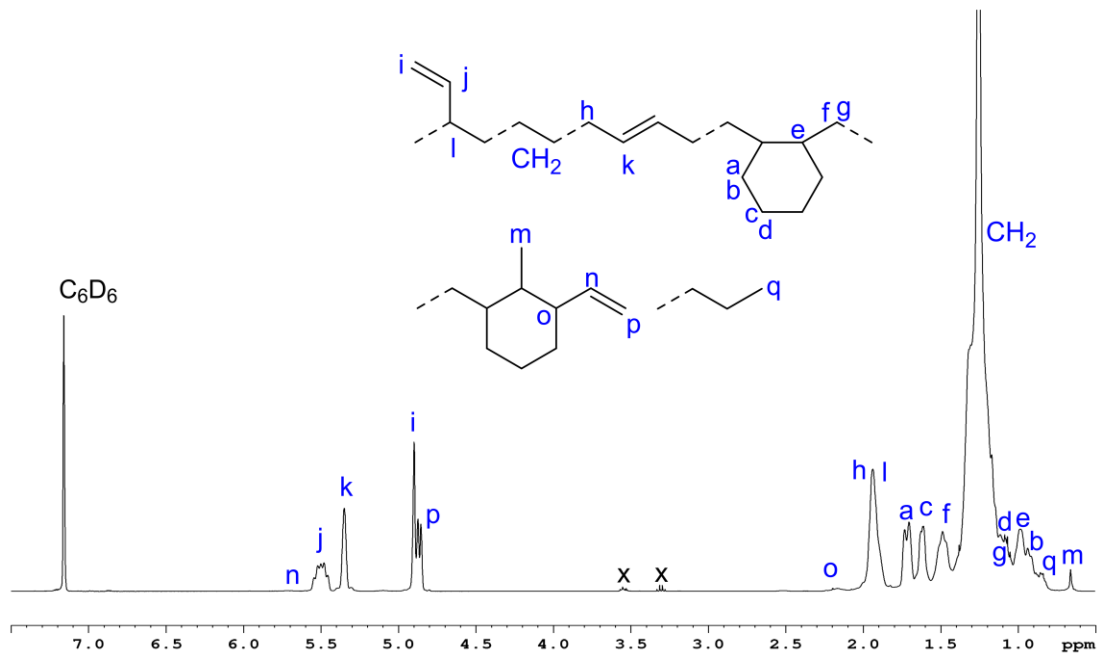


Figure S12. ^1H NMR in TCE/ C_6D_6 at 363K of a typical poly(ethylene-co-butadiene) (run 7)

DFT Calculations

- **Speciation**

Structure of polymetallic species are based on our previous papers:

> H. Nsiri, I. Belaid, P. Larini, J. Thuilliez, C. Boisson, L. Perrin, Ethylene-Butadiene Copolymerization by Neodymocene Complexes: A Ligand Structure/Activity/Polymer Microstructure Relationship based on DFT Calculations, *ACS Catal.*, **2016**, 6, 1028-1036.

> I. Belaid, B. Macqueron, M.-N. Poradowski, S. Bouaouli, J. Thuilliez, F. Da Cruz-Boisson, V. Monteil, F. D'Agosto, L. Perrin, C. Boisson, Identification of a Transient but Key Motif in the Living Coordinative Chain Transfer Cyclocopolymerization of Ethylene with Butadiene, *ACS Catal.* **2019**, 9, 9298-9309.

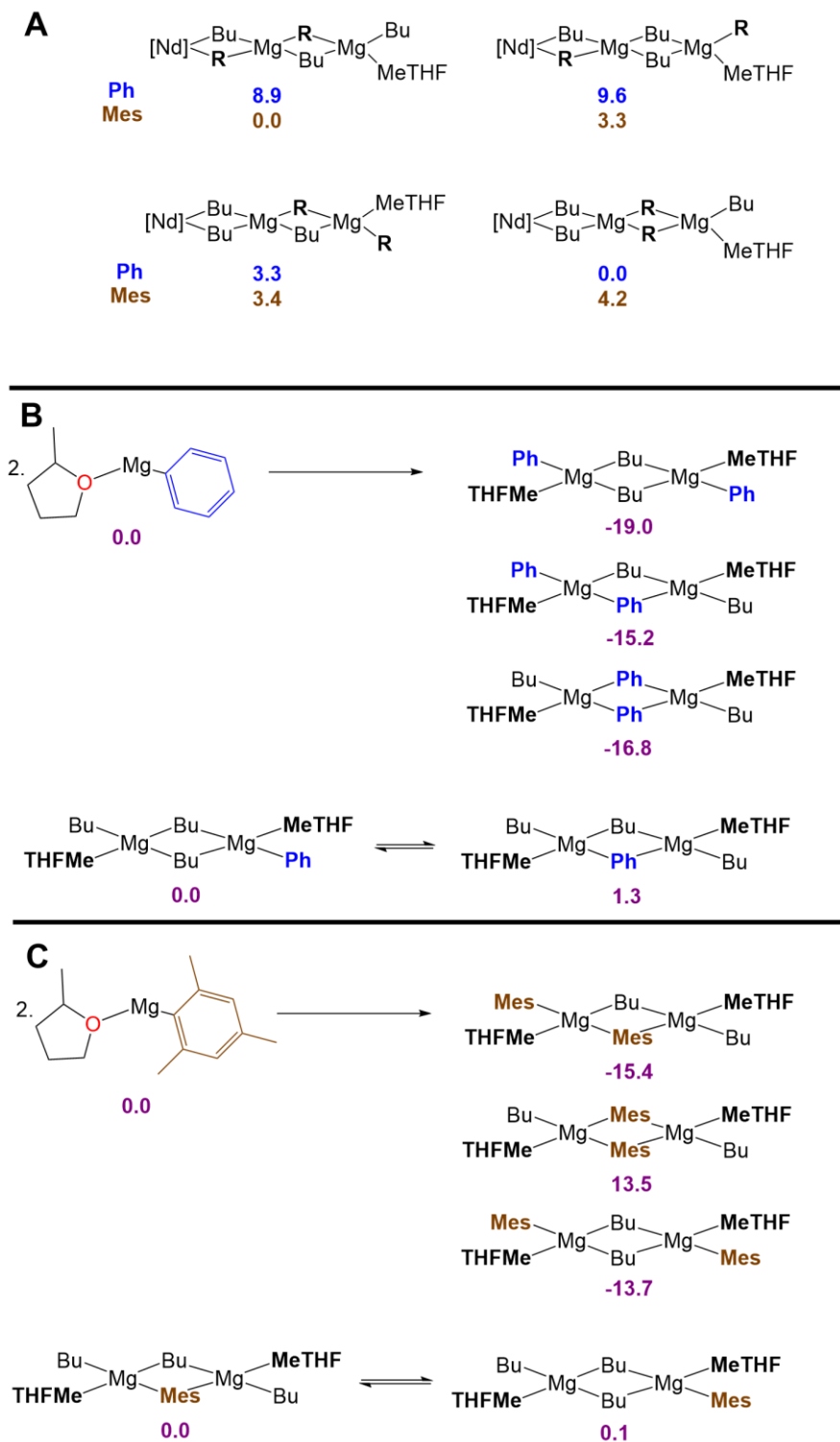


Figure S13. Speciation of **A** : polymetallic neodymium species for phenyl and mesityl groups, **B** : phenyl organomagnesium co-catalyst and **C** : mesityl organomagnesium co-catalyst. ΔG in purple in kcal mol⁻¹. [Nd] correspond to [(Me₂Si(C₁₃H₈)₂)Nd].

- **Dependence on DFT functionals**

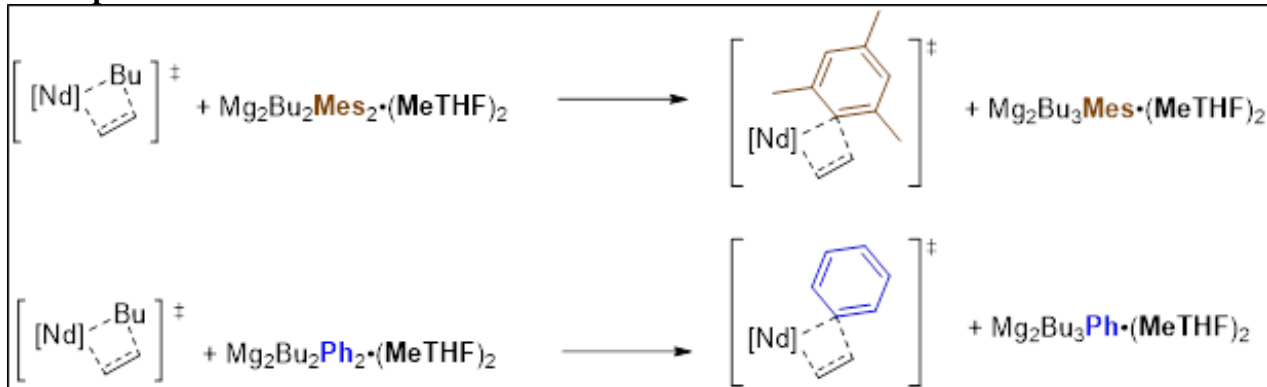


Figure S14. Isodesmic equilibria considered to assess initiation selectivity depending on the CTA.

ΔG (kcal mol ⁻¹)			
Ar	B3PW91	M06	WB97xd
Ph	3.9	2.6	2.6
Mes	11.1	4.0	7.2

Table S1. Gibbs activation energy differences for ethylene insertion between alkyl and aryl groups as illustrated in **Figure S14**.

- **Cartesian coordinates and associated energies of optimized structures**

SiFlu2_Bu_MeTHF	H	0.13531144	3.47113885	0.54926997
81	H	1.82622554	1.67086650	0.68923595
E: -1547.25420209 ; H: -1546.539785 ; G: -	H	2.42786738	0.36225964	-1.32783418
1546.655840 ; D: -0.2308113	H	1.38447174	0.81601634	-3.49390222
C	C	-2.63636761	6.08666762	-1.88147929
C	C	-2.88408249	5.93919328	-3.25981440
C	H	-1.60294073	5.31954909	-0.16604152
C	H	-3.11710482	6.88903664	-1.33193284
C	H	-3.56103922	6.62900167	-3.75420072
C	H	-2.49409206	4.86205708	-5.05845067
C	C	-3.15280831	-2.81793113	-4.07692639
C	C	-1.87944157	-2.28629675	-3.82399302
C	H	-5.09076550	-2.46797363	-4.93622644
C	H	-3.39068442	-3.82645954	-3.75482038
Nd	H	-1.13999818	-2.89224379	-3.30857669
C	H	-0.53072409	-0.64252386	-4.04847238
C	Si	-0.80903432	2.15485165	-5.60631986
C	C	0.67322322	1.07801920	-6.09324361
C	H	0.55720148	0.80863125	-7.14913775
C	H	1.60665891	1.64225642	-5.99586601
C	H	0.77470065	0.14328813	-5.54007273
C	C	-0.86956496	3.46886744	-6.96938712
C	H	0.12430164	3.92452172	-7.04506876
C	H	-1.09148877	2.99443567	-7.93093320
C	H	-1.58356712	4.27965184	-6.82110121

C	-5.52583702	2.43336046	-7.25277440	C	-5.59097926	-0.38023706	-6.84977620
C	-6.34587797	1.30846899	-7.05611225	C	-3.91580323	-2.30167827	-4.76572330
H	-3.62032954	3.35352579	-6.95165647	C	-1.64090304	-0.89349904	-3.88254320
H	-5.91847588	3.28776375	-7.79626403	C	1.44520883	2.11226706	-0.30997448
H	-7.35889542	1.30547273	-7.44508724	C	1.66785758	1.22842767	-1.38535718
H	-6.48885884	-0.66591403	-6.22516786	H	0.42133931	3.87419631	0.36289797
C	-4.85997346	2.86082325	-2.05012973	H	1.97392689	1.96465634	0.62614151
H	-4.95391586	2.51803002	-1.00146452	H	2.37458332	0.41294553	-1.26387223
H	-4.63395131	3.93633080	-1.97324826	H	1.25825582	0.72050536	-3.41775363
C	-6.20190125	2.67193826	-2.76228287	C	-2.26546715	6.43424761	-2.21003225
H	-6.41924142	1.60210467	-2.91016410	C	-2.63300017	6.14186255	-3.53568233
H	-6.14443861	3.09097616	-3.77607869	H	-1.15678758	5.80030643	-0.48805957
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H	-7.22920360	4.37212971	-1.92914704	H	-2.44263188	4.83935440	-5.21487930
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H	-8.95922109	2.01457040	-2.89447026	C	-1.88792287	-2.19461358	-3.45259748
H	-9.57131494	3.54655511	-2.26228876	H	-4.78636471	-2.85444584	-5.10800050
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C	-1.65312393	-0.49462614	-0.31093417	Si	-0.90170035	2.03672376	-5.59700332
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H	-4.27796290	0.86121047	0.49623948	H	0.40043220	0.56222300	-7.07907820
C	-5.12054754	-0.77020316	-0.62488900	H	1.49315820	1.42362704	-5.98628146
C	-1.88113566	-0.62630103	1.18050682	H	0.61105014	-0.01624850	-5.43587676
H	-1.54731992	-1.47098094	-0.79507914	C	-0.95869091	3.26690033	-7.03534380
H	-0.80077853	0.13336096	-0.57613514	H	0.00797110	3.78059614	-7.08397962
H	-3.52235142	-2.02883266	1.02047589	H	-1.09203978	2.71991125	-7.97441401
H	-3.83127832	-0.74160774	2.19438895	H	-1.73150653	4.03452088	-6.98450009
H	-5.93980772	-0.96771059	0.07343770	C	-5.38064737	1.82659193	-7.80704664
H	-5.51425282	-0.12475805	-1.41371824	C	-6.07398108	0.61198624	-7.68717605
H	-4.80813779	-1.71975374	-1.06756160	H	-3.70573296	3.01528318	-7.21584589
H	-1.24734138	-1.39452500	1.62792444	H	-5.76666758	2.59585821	-8.46958169
H	-1.67650001	0.32529373	1.67992838	H	-6.98543673	0.45160494	-8.25408427

SiFlu2_Mes_MeTHF

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E: -1738.96414132 ; H: -1738.193398 ; G: -

1738.316082 ; D: -0.26545047

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C	-2.52517276	-0.26983583	-4.79074355	C	-2.19479723	-0.86214166	1.13957936
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C	-4.41039891	-0.15871225	-6.13327976	H	-1.02438051	0.61642348	0.00846260
C	0.13048064	2.47263468	-2.78793622	H	-3.47141726	-2.31895562	0.16227796
C	-0.63240234	2.90631759	-3.93690720	H	-4.23350815	-1.56380464	1.57438170
C	-1.27886788	4.13159350	-3.51472574	H	-5.97874490	-1.14137189	-0.71257662
C	-0.95548410	4.41772583	-2.14128989	H	-5.46519176	0.13980693	-1.79448048
C	-0.08425290	3.36769222	-1.68042580	H	-4.68603217	-1.46859334	-1.88301381
Nd	-2.79094607	1.86048599	-2.77665785	H	-1.51846541	-1.64430176	1.48975305
C	1.02738693	1.39176878	-2.59870672	H	-2.28730725	-0.11215218	1.93059376
C	0.57532194	3.17612163	-0.45483030	C	-4.84237460	3.01853461	-1.75535579
C	-1.43739405	5.57625881	-1.51283497	C	-4.85593091	3.47809663	-0.42173691
C	-2.16185165	5.01512896	-4.18361064	C	-6.06043534	3.15198931	-2.47126501
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H -8.27179599 5.00347294 1.10475555

SiFlu2_Ph_MeTHF

79

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H -2.96808114 6.91388818 -1.28885449
H -3.50810228 6.63299918 -3.68677565
H -2.49314480 4.85695985 -5.01855199
C -3.05615861 -2.82490467 -4.03690712
C -1.77972922 -2.28366380 -3.82171756
H -5.02195237 -2.48910506 -4.83586407
H -3.27829153 -3.83326767 -3.70335862

H -1.02284051 -2.88158606 -3.32270315
H -0.44966042 -0.63220113 -4.09033626
Si -0.79144026 2.16449013 -5.62726873
C 0.69010729 1.10437828 -6.15145453
H 0.56111421 0.85343491 -7.21036333
H 1.62233012 1.67067458 -6.05565840
H 0.80173235 0.16059331 -5.61607967
C -0.89851030 3.48921221 -6.97594748
H 0.08418387 3.96630874 -7.06341895
H -1.12602320 3.01805522 -7.93786428
H -1.62695502 4.28308658 -6.80909679
C -5.57535138 2.42653846 -7.09744969
C -6.38074911 1.29500733 -6.87685556
H -3.66171636 3.35151095 -6.87400971
H -5.99735335 3.28688135 -7.60828781
H -7.41078258 1.29215922 -7.21833637
H -6.47864097 -0.68877217 -6.06131065
O -2.85055184 0.14771489 -0.85118780
C -4.00664490 -0.14740255 0.01804375
C -1.65685240 -0.46437905 -0.30122200
C -3.42213147 -0.95492491 1.17813694
H -4.36772924 0.82479106 0.36288850
C -5.08861021 -0.85435379 -0.76392856
C -1.94172304 -0.58247454 1.18145308
H -1.51562619 -1.44429149 -0.76909664
H -0.80423332 0.17434859 -0.54025639
H -3.54277576 -2.02636732 0.98685882
H -3.92845627 -0.72149897 2.11667628
H -5.92778847 -1.07730343 -0.09731012
H -5.47552419 -0.22797320 -1.57127357
H -4.72022675 -1.79464338 -1.18294370
H -1.30928296 -1.33023039 1.66422174
H -1.77808557 0.37985969 1.67571087
C -4.89731129 2.76462495 -2.09757336
C -5.02135046 3.35895594 -0.82611164
C -6.07770121 2.73407960 -2.86644343
C -6.22553981 3.87488908 -0.34628799
H -4.14924451 3.43765125 -0.17546384
C -7.29185123 3.24349477 -2.40455906
H -6.06603483 2.30470274 -3.86854860
C -7.36893678 3.81659054 -1.13843378
H -6.27234595 4.32776398 0.64115100
H -8.17655822 3.19755228 -3.03451492
H -8.31034605 4.21678240 -0.77330324

MeTHF

16

E: -271.749069419 ; H: -271.597593 ; G: -271.634729 ; D: -0.02082247

C -2.10158663 -0.33652445 0.44516239
O -0.66768798 -0.35740157 0.40637013
C -0.16727008 0.92179022 0.01153099
C -1.38154567 1.77826555 -0.34536950
C -2.47479462 1.14248160 0.51053827
H -2.48242930 -0.76253045 -0.49722593
H 0.39382186 1.35636909 0.84942309

H 0.52454032 0.79582916 -0.82863294
H -1.22337662 2.83860623 -0.13554947
H -1.62634029 1.67649984 -1.40759194
H -2.40983121 1.49658449 1.54600019
H -3.48562572 1.33773452 0.14468272
C -2.57858712 -1.18652299 1.60314651
H -3.67238213 -1.22103399 1.63100061
H -2.20987698 -2.21147524 1.50827632
H -2.21742778 -0.78066457 2.55301905

BuMgMes_MeTHF

50

E: -979.204956167 ; H: -978.740988 ; G: -978.827358
; D: -0.09457181

C 0.24387856 1.29373077 0.36464307
C -0.57701932 2.32563586 -0.42235525
H 0.90116331 0.75297267 -0.33782021
H 0.93966032 1.83461156 1.02933737
H -1.26502443 1.81221409 -1.11111178
H -1.22845340 2.88891700 0.26242166
Mg -0.89952224 -0.12761424 1.49757283
C 0.24288044 3.33361037 -1.23684538
H 0.88514463 2.78398078 -1.93804462
H 0.92348593 3.86642539 -0.55936154
C -0.60584468 4.34250322 -2.00570479
H -1.27882082 3.84092964 -2.71039178
H -1.22793743 4.93855039 -1.32848561
C -2.84064864 -0.52504586 2.34470875
C -3.10856085 -0.34243970 3.71734198
C -3.92350338 -0.94998477 1.54344161
C -4.37656247 -0.59029223 4.25464688
C -5.18555239 -1.19575783 2.09163399
C -5.43208849 -1.02214976 3.45381133
H -4.54887491 -0.44177805 5.31949962
H -5.99861614 -1.52428546 1.44564481
H 0.01224021 5.03924798 -2.58196282
O 0.41851385 -1.71243730 1.95293904
C 0.09272351 -3.03825750 2.49957340
C 1.85502644 -1.52493420 1.92305929
C 1.44962281 -3.67643975 2.79614380
H -0.45828755 -2.85323992 3.42628739
C -0.77361423 -3.80458457 1.52653439
C 2.38338441 -2.48182481 2.97291083
H 2.22527884 -1.77377336 0.92275583
H 1.77035985 -4.28568337 1.94409728
H 1.40291763 -4.32373407 3.67400830
H -0.98057626 -4.80184718 1.92767583
H -1.73347544 -3.30633444 1.37315455
H -0.26903649 -3.92060859 0.56269734
H 3.43522466 -2.72862440 2.81513275
H 2.27677953 -2.04754245 3.97162559
H 2.06202421 -0.47315499 2.12408713
C -3.74880843 -1.11165906 0.05020398
H -3.86598059 -0.15246019 -0.46940881
H -2.75236611 -1.49190398 -0.20394174
H -4.48027404 -1.80295541 -0.37970352

C -6.80056537 -1.27038053 4.02910421
H -7.50906394 -0.49175022 3.72311178
H -7.21114484 -2.22760794 3.69174774
H -6.77848442 -1.28233200 5.12207002
C -2.00978051 0.11250986 4.65130592
H -1.34627568 -0.71583913 4.93072922
H -1.38655531 0.88512401 4.18600219
H -2.40626138 0.53258154 5.58049323

BuMgPh_MeTHF

41

E: -861.267066606 ; H: -860.890316 ; G: -860.965159
; D: -0.07382036

C 0.19224060 1.21555946 0.21024459
C -0.63277799 2.21823853 -0.60932436
H 0.83735240 0.64023291 -0.47554736
H 0.90004152 1.78006806 0.84197775
H -1.32253305 1.68077750 -1.27771015
H -1.28209983 2.80520548 0.05732738
Mg -0.91454858 -0.13987994 1.44932454
C 0.18343860 3.19779483 -1.46093341
H 0.82210449 2.62490583 -2.14662049
H 0.86742258 3.75242533 -0.80466684
C -0.66902024 4.18104140 -2.25824139
H -1.34686831 3.65651022 -2.94129213
H -1.28637971 4.80023813 -1.59764282
C -2.84125363 -0.54601259 2.30815403
C -3.04723108 -0.76110223 3.68591126
C -4.00986961 -0.58108046 1.52025000
C -4.30622555 -0.99752323 4.23888282
H -2.19817693 -0.74206549 4.37042410
C -5.27790082 -0.81938984 2.05114556
H -3.94244178 -0.41547714 0.44448626
C -5.43022154 -1.02943663 3.41851488
H -4.41247712 -1.15450935 5.30960618
H -6.14806283 -0.83807494 1.39957797
H -6.41399975 -1.21340186 3.84051624
H -0.05383332 4.85700859 -2.86168151
O 0.44740490 -1.58599604 2.13966153
C 0.14410528 -2.92825828 2.65853067
C 1.87546377 -1.34707967 2.17529698
C 1.50760571 -3.51847564 3.01816768
H -0.45992919 -2.77189938 3.55701412
C -0.64292318 -3.71427494 1.63426930
C 2.38894444 -2.29216653 3.24301232
H 2.29975638 -1.57508776 1.19177756
H 1.89058194 -4.11238549 2.18134007
H 1.44260405 -4.17045100 3.89130930
H -0.84242135 -4.71998582 2.01749342
H -1.60756776 -3.24385305 1.42800893
H -0.08215009 -3.80853305 0.69922304
H 3.45489369 -2.50063053 3.13164546
H 2.22274685 -1.86850484 4.23815762
H 2.03627804 -0.29024457 2.39225690

MeTHFMes_Mg_Bu2_Mg_MesMeTHF

100
 E: -1958.41878363 ; H: -1957.487837 ; G: -
 1957.631296 ; D: -0.23440921
 C 0.68273982 0.55008600 -0.14615603
 C -0.37839733 1.18466681 -1.06364167
 H 0.68060832 -0.53985044 -0.33362780
 H 1.66971767 0.81884656 -0.56429103
 H -1.38562372 0.90145658 -0.72965577
 H -0.34211140 2.27725376 -0.96400139
 C 0.75189721 1.17345097 3.51054854
 C 1.86237004 0.58584441 4.40008222
 H -0.21021483 0.84347742 3.94397928
 H 0.69904214 2.25822844 3.71734134
 H 1.89862938 -0.50388623 4.27104094
 H 2.84496595 0.94484124 4.06588701
 Mg -0.30272751 -0.08598873 1.84488215
 Mg 1.70020892 1.84257424 1.50730835
 C 1.71725464 0.88962771 5.89516151
 H 1.68493815 1.97811600 6.03375872
 H 0.74573593 0.51474629 6.24483451
 C -0.23892756 0.83148189 -2.54822849
 H -0.25506410 -0.26094191 -2.65708152
 H 0.75079919 1.15177636 -2.90062826
 C -1.32119310 1.44563693 -3.43111595
 H -2.31920052 1.11347071 -3.12506530
 H -1.30983490 2.54010711 -3.37524748
 C 2.83248212 0.30136401 6.75438297
 H 2.86253107 -0.79150084 6.67770657
 H 3.81341588 0.67782091 6.44460637
 C 3.84987648 2.27363689 1.60799321
 C 4.84902922 1.63807392 0.82496084
 C 4.32148827 3.24642713 2.51773934
 C 6.20198567 1.95933918 0.95051248
 C 5.68353263 3.56332765 2.62906761
 C 6.64491309 2.92842228 1.85294208
 H 6.93335902 1.44456541 0.32859640
 H 5.99877407 4.32146376 3.34507833
 C -2.47115687 -0.38943288 1.74746214
 C -3.43011780 0.26742180 2.55360029
 C -2.99531647 -1.29378734 0.79083641
 C -4.80303189 0.03320263 2.40866478
 C -4.36913802 -1.51830927 0.65703798
 C -5.29736205 -0.85871278 1.46038013
 H -5.50587982 0.55828060 3.05383061
 H -4.72537245 -2.22484847 -0.09187018
 H -1.19028473 1.17082197 -4.48292014
 H 2.70259532 0.55065018 7.81263098
 O 0.73335106 3.70200941 1.06928364
 C 1.32633991 4.87998428 0.42115234
 C -0.61061909 3.99959714 1.52244272
 C 0.16881074 5.86443167 0.30002259
 H 2.08009258 5.26374107 1.11599746
 C 1.98336552 4.49443956 -0.88326280
 C -0.71539777 5.51358267 1.49259338
 H -1.32266301 3.52699009 0.83884370
 H -0.36959138 5.69568579 -0.63907766

H 0.52048167 6.89809821 0.30981381
 H 2.41375725 5.38827023 -1.34619264
 H 2.79804563 3.78510401 -0.72162164
 H 1.25912066 4.06332829 -1.57953721
 H -1.74809656 5.84957768 1.38175713
 H -0.31066528 5.94386917 2.41381131
 O 0.63945984 -1.97359361 2.31014526
 C 0.30193156 -2.89358587 3.40616139
 C 1.97441041 -2.25141430 1.81673160
 C 1.41853747 -3.93102832 3.38633486
 H 0.35443823 -2.30340400 4.32848600
 C -1.09009684 -3.45109270 3.22790706
 C 2.61767858 -3.15253216 2.85570479
 H 1.88658640 -2.74903061 0.84538410
 H 1.15491384 -4.74619304 2.70346658
 H 1.58440446 -4.35889070 4.37711046
 H -1.32089635 -4.10982072 4.07146072
 H -1.84160333 -2.65983186 3.19891319
 H -1.16493660 -4.03582857 2.30716458
 H 3.38902618 -3.78984511 2.41896003
 H 3.07694965 -2.55657239 3.64905030
 H -0.73573861 3.57170548 2.51806101
 H 2.49653645 -1.30185547 1.68416364
 C -3.00583968 1.23824220 3.63190246
 H -2.55608597 0.72067887 4.48782436
 H -2.26400116 1.95284304 3.26403976
 H -3.85463659 1.81295445 4.01513332
 C -2.07905150 -2.04098969 -0.15128918
 H -1.85656016 -1.44665767 -1.04530961
 H -1.12483152 -2.29106990 0.32109118
 H -2.52861570 -2.97787601 -0.49591285
 C -6.77463432 -1.09693902 1.29868218
 H -7.13694063 -0.72301622 0.33400350
 H -7.01680444 -2.16438288 1.33858643
 H -7.34795913 -0.59527485 2.08279207
 C 3.38487069 3.97775306 3.45402189
 H 3.65259986 5.03605394 3.54814728
 H 2.34464550 3.93084792 3.12189894
 H 3.42082241 3.55511005 4.46527398
 C 4.48076620 0.59696630 -0.20706855
 H 3.74263087 -0.11379790 0.17511830
 H 4.04875106 1.05351541 -1.10596794
 H 5.35387890 0.02167751 -0.53026389
 C 8.10737659 3.26138081 1.97571330
 H 8.52310180 3.60175273 1.02085987
 H 8.27631013 4.05174458 2.71186882
 H 8.69237828 2.38807347 2.28547654

MeTHFBu_Mg_Mes2_Mg_BuMeTHF
 100
 E: -1958.40969197 ; H: -1957.478556 ; G: -
 1957.619619 ; D: -0.20269607
 C -1.98131488 -0.59095937 2.96457516
 C -3.05103777 0.21379570 3.70870109
 H -1.70706230 -1.44016160 3.61517027
 H -2.46443159 -1.06790043 2.09150845

H 1.07547961 1.84248247 -1.73480138
 Mg -0.28188269 0.05620849 1.65016871
 Mg 1.77519432 2.01225216 1.29584199
 C -4.92034251 0.26182568 1.31206296
 H -5.02226999 -0.79207034 1.02014848
 H -4.99312699 0.83836683 0.38017134
 C 1.01039668 -0.05482709 -2.73504496
 H 0.58459766 -1.05276883 -2.56480608
 H 2.09828950 -0.19424428 -2.78111690
 C 0.50722342 0.48924262 -4.06876411
 H -0.58229772 0.60672026 -4.06462158
 H 0.94248563 1.47078220 -4.28754499
 C -6.06703182 0.64834895 2.24211210
 H -6.01793451 1.70897902 2.51442098
 H -6.03777013 0.07159693 3.17366529
 H -7.04446036 0.47452565 1.77938138
 H 0.76258245 -0.17501487 -4.90091639
 C 3.80073444 2.85604641 1.44564827
 C 4.80537433 2.64416952 0.46382748
 C 4.18930573 3.65077534 2.54690213
 C 6.08666088 3.18483796 0.58528741
 C 5.48245968 4.18543136 2.65671894
 C 6.45106929 3.96246875 1.68663974
 H 6.82185698 2.99943009 -0.19679709
 H 5.73448376 4.79565891 3.52372870
 C 0.90274079 1.10404615 3.32059672
 C 0.09304840 1.82423533 4.23259606
 C 1.94624779 0.32658639 3.89948862
 C 0.29744812 1.75270164 5.61548451
 C 2.14075837 0.27534467 5.28001421
 C 1.32048207 0.98314798 6.16051551
 H -0.35484939 2.31313920 6.28278958
 H 2.95206912 -0.32829096 5.68299867
 O 0.65193270 3.68141045 0.51555162
 C 1.15850337 5.05281411 0.40857756
 C -0.71827300 3.67606159 0.07272976
 C -0.09882422 5.94528791 0.38686314
 H 1.75610863 5.20878667 1.30779887
 C 2.03167019 5.20491319 -0.81906746
 C -1.27644665 4.98533710 0.59365698
 H -0.74823171 3.63302907 -1.02197026
 H -1.19802308 2.78005645 0.46788170
 H -0.17932339 6.44708443 -0.58168809
 H -0.05385163 6.71925319 1.15546820
 H 2.39137938 6.23697763 -0.88464864
 H 2.90322020 4.55064884 -0.76082281
 H 1.47287848 4.98457929 -1.73409306
 H -2.17596884 5.29380146 0.05677556
 H -1.52608184 4.89188332 1.65306071
 O -0.00998000 -2.03715067 2.15751341
 C -0.06766576 -2.62621119 3.50051282
 C -0.01609251 -3.08128221 1.15457032
 C -0.27913685 -4.11731435 3.25808435
 H 0.91375797 -2.45026335 3.95233542
 C -1.14217848 -1.95590224 4.32416530
 C 0.36981096 -4.34708557 1.89722914

H -1.02119642 -3.15163874 0.72471160
 H 0.68749773 -2.80579936 0.36705398
 H -1.35082740 -4.34081455 3.21440926
 H 0.16127749 -4.71871216 4.05598851
 H -1.16417193 -2.40398596 5.32265051
 H -0.94415899 -0.88865504 4.45056383
 H -2.12593487 -2.08868065 3.86583990
 H 0.01149618 -5.24528436 1.39038095
 H 1.45759839 -4.41664540 1.99317077
 C 3.23084625 3.98859764 3.66610999
 H 3.60572665 3.64163646 4.63577064
 H 3.08201380 5.07190072 3.75612456
 H 2.25258405 3.52463443 3.52629833
 C 4.52034663 1.80801283 -0.76266158
 H 4.46930163 0.74009264 -0.51904652
 H 3.56673439 2.07725820 -1.22772861
 H 5.29947886 1.92514359 -1.52237229
 C 7.84468567 4.51462361 1.81956505
 H 8.55720983 3.73215168 2.10726214
 H 8.20124602 4.94081626 0.87625743
 H 7.89360139 5.29743791 2.58133123
 C -1.00304299 2.73790154 3.74470265
 H -1.86451726 2.73657201 4.41942244
 H -0.64416646 3.77268899 3.68831021
 H -1.35459550 2.45153478 2.75124160
 C 2.91307346 -0.43939518 3.02766619
 H 3.64709430 0.24155971 2.57789932
 H 3.47738794 -1.17977529 3.60190232
 H 2.40779534 -0.96136606 2.21051510
 C 1.55204427 0.92521012 7.64494309
 H 2.47706605 1.44523212 7.91866685
 H 0.73335806 1.39408203 8.19633925
 H 1.64940710 -0.10690194 7.99642165

MeTHFPh_Mg_Bu2_Mg_PhMeTHF

82

E: -1722.55705177 ; H: -1721.800616 ; G: -1721.926800 ; D: -0.18140678

C 0.83942619 0.38565898 -0.14717270
 C 0.06906389 1.06994709 -1.28993119
 H 0.60017875 -0.69457402 -0.19436907
 H 1.91070363 0.36348595 -0.42037267
 H -1.00519072 1.08340393 -1.06034254
 H 0.36169556 2.12668765 -1.35694385
 C 0.47466219 1.43512395 3.40214271
 C 1.22996676 0.76849573 4.56506003
 H -0.59933547 1.45492990 3.66262471
 H 0.71216645 2.51628246 3.44003783
 H 0.93991104 -0.28882534 4.64092464
 H 2.30773796 0.75616478 4.35296375
 Mg -0.26177516 -0.09246681 1.83319499
 Mg 1.59360074 1.89034227 1.42242998
 C 1.01519823 1.42094201 5.93454520
 H 1.32858665 2.47192930 5.87968938
 H -0.05992503 1.43764208 6.15716022
 C 0.26059314 0.43194239 -2.66952759

H	-0.05171195	-0.61970301	-2.62109165
H	1.33191850	0.41791067	-2.91018783
C	-0.50427701	1.13956465	-3.78378830
H	-1.58192479	1.14384144	-3.58613383
H	-0.18479314	2.18285240	-3.88550862
C	1.76151484	0.72616169	7.06928111
H	1.43869898	-0.31528767	7.17945430
H	2.84210656	0.71810748	6.88868853
C	3.72589247	2.21530191	1.58767489
C	4.62272891	1.81070018	0.57714182
C	4.33533329	2.82667435	2.70339726
C	6.00340716	1.99793839	0.66004425
H	4.24006009	1.32687925	-0.32239485
C	5.71290951	3.02393732	2.80930727
H	3.71990742	3.16795567	3.53643170
C	6.55575785	2.60820801	1.78231918
H	6.64957250	1.66727883	-0.14979551
H	6.13068040	3.49994726	3.69339373
H	7.62924774	2.75684211	1.85627454
C	-2.39999570	-0.40434543	1.78036641
C	-3.23591285	-0.04367534	2.85691293
C	-3.07528508	-0.95066110	0.66872183
C	-4.62167247	-0.21211801	2.83887330
H	-2.79939944	0.39036820	3.75734177
C	-4.45890713	-1.12606018	0.62623902
H	-2.50817265	-1.25979298	-0.20965878
C	-5.24047867	-0.75663502	1.71756126
H	-5.21942976	0.08099303	3.69883021
H	-4.92880646	-1.55152353	-0.25744891
H	-6.31824049	-0.89019514	1.69356989
H	-0.35011702	0.65375186	-4.75288601
H	1.59291585	1.22419026	8.02967581
O	0.66080323	3.71814772	0.91787904
C	1.34140711	5.01950616	0.83813930
C	-0.76921728	3.91719876	1.00611360
C	0.22095186	6.05442836	0.97140674
H	2.01041118	5.05904846	1.70268481
C	2.14394026	5.11087326	-0.43977194
C	-0.91868709	5.28602163	1.63832420
H	-1.19754064	3.88762882	-0.00135706
H	-0.08681663	6.40066595	-0.02084085
H	0.54799922	6.92437650	1.54400119
H	2.64697782	6.08199929	-0.48745472
H	2.91273423	4.33595858	-0.47761625
H	1.49674992	5.01732353	-1.31681453
H	-1.90108145	5.72404848	1.45091022
H	-0.77009016	5.22257882	2.72039491
O	0.78894777	-1.87774380	2.30448855
C	0.27194147	-3.08785890	2.95839991
C	2.23173717	-1.94478703	2.20783694
C	1.51785280	-3.90267467	3.31414049
H	-0.23792129	-2.74239787	3.86328501
C	-0.70376579	-3.80503126	2.05287506
C	2.64739740	-2.87607403	3.32921193
H	2.50429404	-2.34458535	1.22498914
H	1.69952433	-4.65640402	2.54060000

H	1.39555308	-4.42309021	4.26606755
H	-1.06057216	-4.71258589	2.55076779
H	-1.57141896	-3.18263753	1.82576210
H	-0.21978731	-4.09735804	1.11608695
H	3.63099527	-3.31661977	3.15464906
H	2.67666150	-2.33636629	4.27964132
H	-1.19011818	3.09907283	1.59274310
H	2.62731057	-0.93194757	2.29882531

MeTHFBu_Mg_Ph2_Mg_BuMeTHF

82

E: -1722.55289545 ; H: -1721.796997 ; G: -1721.924349 ; D: -0.18042961

C	-1.97507390	-0.71862923	2.92445849
C	-3.04856684	0.33879052	3.20759215
H	-1.80037347	-1.28436314	3.85662771
H	-2.39971007	-1.45934160	2.22488302
H	-2.66880775	1.07248144	3.93399189
H	-3.26134790	0.91470926	2.29369545
C	3.81339219	1.63052468	0.53509107
C	4.29085336	2.26651227	-0.77738823
H	4.06583844	0.55627884	0.50531473
H	4.42865468	2.03299973	1.35890638
H	3.68817152	1.89377480	-1.61977988
H	4.11153022	3.35224538	-0.75300106
Mg	-0.05551335	-0.10796296	2.14103734
Mg	1.73173054	1.89050957	1.07801415
C	-4.38175169	-0.20324250	3.73947710
H	-4.18987117	-0.77287778	4.65863962
H	-4.78463733	-0.92438451	3.01578942
C	5.77012601	2.04477921	-1.11889193
H	6.38484504	2.42688842	-0.29287416
H	5.96419363	0.96465680	-1.16295157
C	6.21168849	2.69506727	-2.42738016
H	6.06388263	3.78097678	-2.40261199
H	5.63968919	2.30703312	-3.27793743
C	-5.42285541	0.87764351	4.01710996
H	-5.66029663	1.44405431	3.10918584
H	-5.06319093	1.59432641	4.76454993
C	0.10055233	0.67481470	-0.04275543
C	0.64316179	-0.14429845	-1.05605370
C	-1.13248169	1.28255985	-0.36903321
C	0.02085347	-0.34453976	-2.28806367
H	1.59526760	-0.64430402	-0.88587961
C	-1.77549101	1.09312828	-1.59216400
H	-1.62255512	1.92826676	0.35908346
C	-1.19577468	0.27567046	-2.55835744
H	0.48217620	-0.98313812	-3.03675366
H	-2.72704034	1.57898566	-1.79158143
H	-1.68957537	0.12191170	-3.51340526
C	1.16735508	1.51905887	3.29644593
C	0.18652121	2.33450918	3.90401207
C	2.28604453	1.23745069	4.11103885
C	0.29853343	2.82566448	5.20492328
H	-0.71453100	2.59466153	3.34929286
C	2.41998430	1.71695535	5.41329211

H	3.09983659	0.63085706	3.71721504
C	1.42137750	2.51479573	5.96533953
H	-0.48908882	3.44475235	5.62610883
H	3.30292683	1.47201022	5.99778404
H	1.51750276	2.88971249	6.98007311
H	7.27173154	2.51382251	-2.63539736
H	-6.36051674	0.45466886	4.39354555
O	1.12157150	3.88210592	0.64944865
C	1.07540733	5.04222114	1.54615395
C	0.84195237	4.29420857	-0.70893215
C	0.68671808	6.21676700	0.64531334
H	0.27963766	4.82958488	2.26585791
C	2.39423753	5.20300358	2.26856108
C	0.01304254	5.55272847	-0.55432153
H	1.78734773	4.49270998	-1.22592604
H	0.32817208	3.47140086	-1.20745197
H	1.58526197	6.75493331	0.32512010
H	0.03936893	6.92389066	1.16772108
H	2.33882015	6.06329654	2.94345213
H	2.62979290	4.32413066	2.87358969
H	3.21135981	5.37175985	1.56157636
H	0.02766060	6.17152116	-1.45381843
H	-1.02667703	5.29658535	-0.32891040
O	1.13133026	-1.87595784	2.15114112
C	0.61119827	-3.17672272	2.59001531
C	2.56174384	-1.96554476	2.00617299
C	1.85283871	-3.98199996	3.00397451
H	-0.02605398	-2.95754731	3.44950124
C	-0.20167937	-3.81465615	1.48424454
C	2.97580206	-2.94605802	3.08454324
H	2.80522427	-2.34004570	1.00488346
H	2.97356620	-0.96244921	2.11449083
H	2.08147685	-4.72955078	2.23785981
H	1.69191424	-4.50887859	3.94633740
H	-0.59117034	-4.77986223	1.82386548
H	-1.05086481	-3.18823102	1.20355247
H	0.41420174	-3.98840560	0.59672070
H	3.96506268	-3.37241571	2.90559713
H	2.98345931	-2.45004332	4.05926330

MeTHFBu_Mg_PhBu_Mg_PhMeTHF

82

E: -1722.55496096 ; H: -1721.798066 ; G: -1721.921197 ; D: -0.18099071

C	-2.42104870	-0.63621366	1.60271943
C	-3.46939875	0.46819777	1.41850191
H	-2.67679892	-1.19839371	2.51766840
H	-2.54393087	-1.36757400	0.78429398
H	-3.40309068	1.19042108	2.24642888
H	-3.25493770	1.04940396	0.50863431
C	0.73673716	0.52889588	-0.25381486
C	-0.25917249	1.06825423	-1.29535534
H	0.74931016	-0.57335269	-0.34993306
H	1.75636741	0.77108939	-0.60854736
H	-1.28369393	0.79158201	-1.00981414
H	-0.24328536	2.16651893	-1.29227579

Mg	-0.31985474	-0.14697200	1.69246027
Mg	1.48954958	1.97221299	1.37675255
C	-4.92386063	-0.01267371	1.33462343
H	-5.16482936	-0.57105380	2.24899592
H	-5.01137391	-0.73242955	0.51000036
C	-0.01555152	0.59096617	-2.73029784
H	-0.03872419	-0.50666680	-2.74798718
H	1.00049849	0.87684270	-3.03357655
C	-1.02263422	1.13825678	-3.73724824
H	-2.04416677	0.83354391	-3.48409299
H	-1.00459706	2.23378857	-3.76301639
C	-5.93738615	1.11135608	1.13953327
H	-5.74692085	1.66323249	0.21178425
H	-5.89660700	1.83340575	1.96326903
H	-6.96331069	0.73129472	1.08875214
H	-0.81519898	0.78307514	-4.75194935
C	3.64173197	2.21818690	1.47192518
C	4.49720347	1.83884174	0.41702790
C	4.29718969	2.77685421	2.58901841
C	5.88334221	2.00015540	0.46060762
H	4.07585929	1.39541287	-0.48631639
C	5.68036437	2.95093737	2.65459831
H	3.71214284	3.08880390	3.45480213
C	6.48196298	2.56120518	1.58484202
H	6.49712040	1.68879384	-0.38157080
H	6.13494695	3.38850762	3.54053011
H	7.55967552	2.69080060	1.62791352
C	0.46903410	1.31616305	3.34688138
C	-0.65321672	1.90837608	3.96645573
C	1.49670309	0.92953447	4.23534505
C	-0.75126226	2.10085441	5.34419751
H	-1.50080795	2.22435801	3.36029765
C	1.42190763	1.11479442	5.61563147
H	2.40614644	0.48111229	3.83929506
C	0.29164901	1.70263330	6.17530251
H	-1.64060016	2.55796336	5.76979525
H	2.24523126	0.80439143	6.25355266
H	0.22430659	1.84983560	7.24921724
O	0.68895380	3.84537147	0.83123454
C	1.50302861	5.06784389	0.73407937
C	-0.70613134	4.20674999	0.89717713
C	0.51892601	6.21756902	0.98818564
H	2.24047057	4.99040689	1.53639829
C	2.20106782	5.12389722	-0.60634858
C	-0.70710368	5.54468095	1.60703097
H	-1.10856865	4.28638285	-0.11887460
H	-1.23471597	3.41165620	1.42264390
H	0.24982377	6.69276073	0.03946280
H	0.95726796	6.98211195	1.63217121
H	2.79072684	6.04390940	-0.67379355
H	2.88362524	4.28043687	-0.73070539
H	1.47631927	5.12181598	-1.42605805
H	-1.63114447	6.10294411	1.44222025
H	-0.57575439	5.39892812	2.68300859
O	0.81702403	-1.90792144	2.08730665
C	0.39057392	-2.99011574	2.98361422

C 2.23067546 -2.02835941 1.81069019
 C 1.67662996 -3.74797516 3.32793828
 H -0.01866203 -2.49583247 3.87014326
 C -0.67062037 -3.83635311 2.31605448
 C 2.79405792 -2.75498268 3.01514489
 H 2.36558195 -2.60662481 0.88940914
 H 2.63554383 -1.02678854 1.65836338
 H 1.76562817 -4.63334605 2.68968442
 H 1.67728611 -4.08243035 4.36710839
 H -0.97789899 -4.63986688 2.99350104
 H -1.55499994 -3.24683538 2.06777949
 H -0.28345984 -4.29181936 1.39972878
 H 3.74920454 -3.23693232 2.79700379
 H 2.94154200 -2.05787789 3.84440383

MeTHFBu_Mg_BuMes_Mg_BuMeTHF
 93

E: -1766.70206691 ; H: -1765.826789 ; G: -
 1765.964773 ; D: -0.19943155

C -2.26047582 -0.31997977 1.96065664
 C -3.22702377 0.85552449 2.15963062
 H -2.39185636 -1.01269484 2.81074340
 H -2.60314969 -0.89805626 1.08516229
 H -2.93863356 1.43438337 3.05017412
 H -3.14349796 1.56123551 1.31828033
 C 0.95124158 0.56242102 -0.25510308
 C -0.18245805 0.00101186 -1.13921228
 H 1.80248365 -0.13499092 -0.32166882
 H 1.32277632 1.45120031 -0.80017505
 H -0.55267953 -0.95175855 -0.73232734
 H -1.05452459 0.67051018 -1.11592973
 Mg -0.14703056 0.09911093 1.73906760
 Mg 1.79684167 2.03264868 1.33409615
 C -4.70513185 0.47136326 2.30443630
 H -4.80598565 -0.22644078 3.14634257
 H -5.01293150 -0.08930665 1.41174292
 C 0.20437964 -0.23783855 -2.60282586
 H 1.06621345 -0.91680929 -2.63434642
 H 0.55122712 0.70887556 -3.03765971
 C -0.92939378 -0.80626691 -3.45064585
 H -1.27234192 -1.77179555 -3.06244588
 H -1.79424086 -0.13365905 -3.46315877
 C -5.64327626 1.65718232 2.51071709
 H -5.59331863 2.35839282 1.66954161
 H -5.38605003 2.21704660 3.41732527
 H -6.68679884 1.33872089 2.60800041
 H -0.61864031 -0.96143022 -4.48902042
 C 3.96726316 2.24334265 1.26717830
 C 4.60898192 2.72567530 0.09709238
 C 4.82113789 1.93148127 2.34685307
 C 5.99388982 2.88398780 0.02675450
 C 6.21219561 2.09011977 2.26103760
 C 6.82104420 2.56924958 1.10723837
 H 6.44436622 3.25821122 -0.89172321
 H 6.83278769 1.83573132 3.11945414
 C 0.55770410 1.72125512 3.25837224

H 1.26223743 2.54679455 3.48085854
 H -0.40938601 2.24711771 3.16975436
 C 0.50591149 0.86014060 4.53337773
 H 1.45422545 0.32249188 4.66852451
 H -0.25976184 0.07601870 4.42957871
 C 0.20598308 1.63108832 5.82372693
 H -0.74963650 2.15842141 5.70844896
 H 0.96946757 2.40914248 5.95558120
 C 0.15671626 0.74841770 7.06709276
 H 1.10808549 0.22765023 7.22383881
 H -0.04923122 1.33286663 7.96972894
 H -0.62601947 -0.01393412 6.98469754
 O 0.81590854 3.86695828 0.82563660
 C 0.80507022 5.08819691 1.64318539
 C -0.25045175 3.91165083 -0.15530900
 C -0.21606589 5.99173103 0.96077495
 H 0.43980170 4.78933349 2.63200493
 C 2.19886132 5.66126219 1.75209820
 C -1.18834222 5.00373722 0.32400548
 H 0.18528406 4.15156391 -1.13126386
 H -0.70879011 2.92332495 -0.20610695
 H 0.27745711 6.59607939 0.19169800
 H -0.69052794 6.66940182 1.67322555
 H 2.17350586 6.55328446 2.38626125
 H 2.89766218 4.95046732 2.19851184
 H 2.58255634 5.94922760 0.76967926
 H -1.76900229 5.43324780 -0.49473587
 H -1.88520946 4.61003561 1.06966880
 O 0.89928194 -1.72466414 2.14799842
 C 0.32737221 -2.93090397 2.75601633
 C 2.33538413 -1.85382401 2.06787928
 C 1.53640570 -3.77371165 3.17827841
 H -0.23132862 -2.58549986 3.63056396
 C -0.60210791 -3.62395017 1.78394747
 C 2.69633811 -2.78036340 3.21139949
 H 2.60584764 -2.28446461 1.09711277
 H 2.77137799 -0.85683625 2.14000542
 H 1.72500679 -4.55068081 2.43001808
 H 1.36476379 -4.26769276 4.13666697
 H -1.00451437 -4.53116381 2.24665656
 H -1.44400708 -2.98531841 1.51015361
 H -0.06661074 -3.91427731 0.87500197
 H 3.67029995 -3.25295196 3.06885787
 H 2.71639803 -2.22873833 4.15560727
 C 4.27241717 1.43413647 3.66445447
 H 4.25763337 2.23013573 4.42013308
 H 3.24809760 1.06968623 3.56230298
 H 4.87978503 0.62065154 4.07656071
 C 3.80234702 3.06191671 -1.13600214
 H 2.87710017 3.58669773 -0.87884747
 H 4.36252693 3.69985666 -1.82684009
 H 3.52251733 2.15651892 -1.68784939
 C 8.31142005 2.76072834 1.02325529
 H 8.57793827 3.82439223 1.02449225
 H 8.82281935 2.29330089 1.86905392
 H 8.72186621 2.32962359 0.10420741

MeTHFMes_Mg_Bu2_Mg_BuMeTHF

93

E: -1766.69971370 ; H: -1765.824706 ; G: -1765.961623 ; D: -0.20269607

C	-2.34833901	-0.62948557	1.72297096
C	-3.21476966	0.15825921	0.73261969
H	-2.86618554	-0.65752643	2.69725862
H	-2.33583329	-1.68536907	1.39635691
H	-3.24046952	1.22361877	1.01000817
H	-2.75560969	0.13310953	-0.26723616
C	0.88607409	0.42305428	0.03846148
C	0.57814388	1.20092022	-1.25407579
H	0.35632262	-0.54283905	-0.07806532
H	1.94612304	0.11741863	-0.00188234
H	-0.48309947	1.48287969	-1.27672359
H	1.13544383	2.15010580	-1.27049483
Mg	-0.26721441	-0.08982706	2.00248426
Mg	1.50653849	2.08406193	1.53477762
C	-4.66624526	-0.32078670	0.59667773
H	-5.14453388	-0.28229741	1.58469357
H	-4.66425523	-1.37959631	0.30487320
C	0.90360195	0.44990669	-2.54976650
H	0.33976817	-0.49222020	-2.56229228
H	1.96469498	0.16927998	-2.54023345
C	0.59629095	1.24493214	-3.81501130
H	-0.46511371	1.51187050	-3.86963709
H	1.17242732	2.17638608	-3.85009249
C	-5.49379423	0.48269897	-0.40293794
H	-5.06377142	0.42923977	-1.40967556
H	-5.53858472	1.54147911	-0.12252082
H	-6.52444212	0.11745870	-0.46718408
H	0.83815404	0.67594432	-4.71868773
C	0.62452197	1.35092206	3.60574994
C	-0.44140994	2.02051719	4.26765823
C	1.71611043	0.96989963	4.42944477
C	-0.40781850	2.28306834	5.63838080
C	1.73175786	1.24163423	5.80246504
C	0.67595394	1.89864609	6.42838151
H	-1.24911276	2.79244594	6.10573623
H	2.58984285	0.93518765	6.39792525
C	3.56491069	2.65581248	1.13890937
H	3.51766473	3.53385007	0.47053118
H	4.02174129	3.04725058	2.06440307
C	4.52783418	1.63810659	0.51664875
H	4.13507218	1.29507076	-0.45212446
H	4.58170830	0.73146895	1.13943203
C	5.96160376	2.13732300	0.29362489
H	5.92973288	3.03217983	-0.34215635
H	6.37396558	2.46810753	1.25641246
C	6.89085106	1.10003079	-0.33101515
H	6.52478196	0.77744707	-1.31253926
H	7.90426385	1.49140677	-0.47156118
H	6.96958182	0.20568801	0.29796357
O	0.71314700	-1.95772336	2.47541441
C	0.68926899	-2.64697395	3.76997034

C	1.29024743	-2.81708477	1.46089365
C	1.07506011	-4.08444083	3.44184123
H	1.46951243	-2.17923336	4.37977259
C	-0.65486017	-2.48332703	4.44095748
C	1.98276666	-3.93061381	2.22617564
H	0.48185808	-3.20344029	0.83062443
H	1.96351750	-2.21812667	0.84660062
H	0.18022276	-4.66124934	3.18352476
H	1.56187043	-4.57167454	4.28915276
H	-0.63623167	-2.99912104	5.40645111
H	-0.88480295	-1.43343100	4.63662535
H	-1.45580171	-2.91377774	3.83479550
H	2.07145546	-4.84186520	1.63127129
H	2.98698411	-3.61969064	2.52999375
O	0.41075133	3.95774403	1.33002154
C	0.43799794	5.07114287	2.28476974
C	-0.40764668	4.30209117	0.18445258
C	-0.14723366	6.24361150	1.50886642
H	-0.23436676	4.79168416	3.10306015
C	1.83306144	5.28725063	2.82119803
C	-1.14750501	5.57053561	0.57501904
H	0.25198429	4.46899955	-0.67285454
H	-1.06671569	3.46075891	-0.03506823
H	0.64158182	6.74279890	0.93535060
H	-0.60272093	6.97863684	2.17571163
H	1.81617768	6.12432929	3.52662681
H	2.19940324	4.41216440	3.36197755
H	2.53573475	5.52240982	2.01829980
H	-1.40468369	6.17626400	-0.29634809
H	-2.07196669	5.33013228	1.10845869
C	-1.68305456	2.42514815	3.51070501
H	-2.40233806	1.59996699	3.46816461
H	-2.19120303	3.27029247	3.98535326
H	-1.44828438	2.70010931	2.48023388
C	0.69487397	2.18995447	7.90360052
H	0.66111062	3.26782976	8.09629915
H	-0.17112403	1.74772530	8.40767262
H	1.59641845	1.79546704	8.37845685
C	2.93271714	0.29410765	3.84229540
H	3.64032413	1.03562965	3.45495424
H	3.46700082	-0.29803741	4.59156171
H	2.66906357	-0.36550767	3.01184120

MeTHFBu_Mg_Bu2_Mg_PhMeTHF

84

E: -1648.77158812 ; H: -1647.983666 ; G: -1648.111688 ; D: -0.1741955

C	-2.38103051	-0.51677275	2.16931258
C	-3.35630123	0.64108174	2.42262663
H	-2.48622519	-1.23880714	2.99849028
H	-2.72690455	-1.07052433	1.27926972
H	-3.05623258	1.19745600	3.32394317
H	-3.29784621	1.37292378	1.60221305
C	0.57875533	0.50811630	-0.15385582
C	-0.45974316	1.09786795	-1.12295306
H	0.47360477	-0.59266436	-0.19079396

H 1.57598617 0.62969406 -0.61777410
 H -1.47175330 0.97227172 -0.71259077
 H -0.31477668 2.18372644 -1.20926629
 Mg -0.28590108 -0.05131755 1.93783272
 Mg 1.57668021 1.90725406 1.38134225
 C -4.82679169 0.23641256 2.58604324
 H -4.90628187 -0.47609515 3.41781715
 H -5.14282867 -0.31277002 1.68915089
 C -0.44020773 0.49945210 -2.53332884
 H -0.60382137 -0.58362815 -2.45894694
 H 0.56399618 0.62434564 -2.95990644
 C -1.47596692 1.10799155 -3.47362437
 H -2.49230480 0.97051519 -3.08812928
 H -1.31602053 2.18485541 -3.59983332
 C -5.77355621 1.40893295 2.82617030
 H -5.74415996 2.12257763 1.99464438
 H -5.50644583 1.95803791 3.73644105
 H -6.81194630 1.07820970 2.93624425
 H -1.43742123 0.65286113 -4.46863340
 C 3.74056454 2.02666245 1.34243947
 C 4.53691957 1.37018767 0.38170888
 C 4.46502069 2.78200258 2.28874615
 C 5.93005208 1.45685066 0.35412958
 H 4.06092286 0.75950398 -0.38671328
 C 5.85676765 2.88296100 2.28249555
 H 3.93106999 3.31984063 3.07309299
 C 6.59774190 2.21785138 1.30917806
 H 6.49578715 0.93052948 -0.41131084
 H 6.36532890 3.47845774 3.03720116
 H 7.68152499 2.29047050 1.29652963
 C 0.63033456 1.47318501 3.43411387
 H 0.91165406 2.54306443 3.48221326
 H -0.42478884 1.51912198 3.75988053
 C 1.43646196 0.75664353 4.53158410
 H 2.49874077 0.72753607 4.25318752
 H 1.12552721 -0.29550329 4.60048915
 C 1.31949380 1.37863439 5.92693158
 H 0.26070728 1.40650939 6.21645707
 H 1.64683682 2.42555831 5.87629489
 C 2.12336595 0.64505677 6.99617842
 H 3.19127398 0.63094144 6.75158365
 H 2.01737856 1.11816193 7.97795927
 H 1.79523105 -0.39571242 7.09710206
 O 0.93519893 3.86481652 0.85564872
 C -0.41166658 4.44838370 0.85835333
 C 1.82930297 4.72176654 0.10475824
 C -0.33787275 5.62480968 -0.12500964
 H -1.07199565 3.66458720 0.47788579
 C -0.82359099 4.84087184 2.26076215
 C 0.93489851 5.36965467 -0.93102365
 H 2.27159355 5.45964092 0.78361969
 H 2.62750075 4.09824265 -0.29751159
 H -0.25052205 6.56534049 0.42868712
 H -1.23499108 5.68439732 -0.74411799
 H -1.81460573 5.30530647 2.23098081
 H -0.88152229 3.97554017 2.92362787

H -0.12164137 5.56352536 2.68739506
 H 1.37097861 6.28245081 -1.34249381
 H 0.74872741 4.67570899 -1.75581432
 O 0.86266167 -1.83505108 2.20372198
 C 0.41138476 -3.14759913 2.67703023
 C 2.29804159 -1.84064254 2.02571426
 C 1.69424889 -3.96755436 2.84059961
 H -0.06008657 -2.97061939 3.64888922
 C -0.59128256 -3.73967836 1.71138973
 C 2.79402973 -2.91592830 2.97085726
 H 2.52842839 -2.08176267 0.98191797
 H 2.67269200 -0.84020934 2.24742037
 H 1.85980962 -4.57774927 1.94646119
 H 1.63350695 -4.63918973 3.69921252
 H -0.90746073 -4.72499217 2.06917560
 H -1.48060257 -3.11234767 1.62444609
 H -0.14744222 -3.86272060 0.71883262
 H 3.78148545 -3.28735628 2.68989558
 H 2.84928925 -2.52830414 3.99196931

MeTHFBu_Mg_PhBu_Mg_BuMeTHF

84

E: -1648.76908148 ; H: -1647.981224 ; G: -1648.109085 ; D: -0.17465063

C -2.34920755 -0.56261182 1.62272377
 C -3.30702161 0.24270194 0.73621794
 H -2.75660030 -0.58330214 2.64823920
 H -2.38755788 -1.61771117 1.29605500
 H -3.32228988 1.29709592 1.05373647
 H -2.93612988 0.26079764 -0.29953738
 C 0.86970780 0.56198969 -0.19611011
 C 0.42437498 1.46605865 -1.36099604
 H 0.37969272 -0.41517661 -0.37417505
 H 1.93585289 0.31578830 -0.34737842
 H -0.64306171 1.70346428 -1.26168702
 H 0.94232560 2.43568850 -1.31102427
 Mg -0.24297355 -0.07908471 1.75150778
 Mg 1.56917937 2.05134895 1.41862011
 C -4.75768615 -0.25633805 0.70980274
 H -5.14745503 -0.26322600 1.73643861
 H -4.76465030 -1.30353768 0.37901202
 C 0.65887058 0.88022150 -2.75734422
 H 0.12602209 -0.07685670 -2.83351745
 H 1.72501886 0.64408580 -2.86923294
 C 0.21704411 1.80021809 -3.89124104
 H -0.85298476 2.02764321 -3.82605680
 H 0.75812300 2.75272456 -3.86542293
 C -5.68307350 0.56670157 -0.18235117
 H -5.34313230 0.55895395 -1.22433573
 H -5.72104247 1.61341046 0.14104000
 H -6.70910719 0.18370540 -0.16987187
 H 0.39620671 1.34831064 -4.87233208
 C 0.58895972 1.29373442 3.41332402
 C -0.49137664 1.89682806 4.09336713
 C 1.70826152 1.00403350 4.22371113
 C -0.46821763 2.18582433 5.45730294

H -1.40129703 2.13987589 3.54626281
 C 1.75807129 1.29238312 5.58800948
 H 2.58778653 0.54160865 3.77735925
 C 0.66381032 1.88533209 6.21016162
 H -1.33135287 2.64306525 5.93409276
 H 2.64863276 1.05595455 6.16441920
 H 0.69204257 2.11110792 7.27214222
 C 3.67721960 2.51828694 1.32133409
 H 3.86255743 2.98750341 0.33878356
 H 3.92057534 3.30523988 2.05594790
 C 4.68633023 1.37540384 1.49187361
 H 4.48299259 0.57806862 0.76008855
 H 4.55959683 0.90169273 2.47737987
 C 6.16066081 1.77575489 1.35299169
 H 6.31116362 2.23400916 0.36644822
 H 6.38189736 2.56204161 2.08686104
 C 7.13844672 0.61820766 1.53380035
 H 6.96970359 -0.16670027 0.78737687
 H 8.17961905 0.94401967 1.43623370
 H 7.03079285 0.15712848 2.52248698
 O 0.84135059 -1.88376137 2.15023654
 C 0.95968330 -2.54336933 3.45493218
 C 1.40508392 -2.72065964 1.11007393
 C 1.40742396 -3.96113769 3.12121600
 H 1.75274947 -2.01518397 3.99519269
 C -0.34020982 -2.43997719 4.21825750
 C 2.21686479 -3.77445172 1.84183834
 H 0.58323439 -3.16726286 0.53961372
 H 1.99812182 -2.08915316 0.44770205
 H 0.53290658 -4.59419340 2.93475694
 H 1.98143494 -4.40361662 3.93790184
 H -0.22937366 -2.93666085 5.18749510
 H -0.61195042 -1.39986003 4.41437451
 H -1.15630892 -2.92231312 3.67382128
 H 2.32183739 -4.68981576 1.25591959
 H 3.21776901 -3.39572417 2.06986190
 O 0.46248523 3.85461398 1.14500358
 C 0.92959392 5.17748702 1.58267567
 C -0.96452863 3.88623802 0.92895005
 C -0.33805156 6.03113696 1.67487904
 H 1.36524138 5.02552045 2.57513020
 C 1.97183565 5.71005888 0.62541056
 C -1.46420943 5.00986749 1.81509381
 H -1.16078094 4.08986386 -0.12928390
 H -1.36694911 2.90284857 1.17763458
 H -0.46375676 6.60958181 0.75340958
 H -0.28652979 6.73374410 2.50893378
 H 2.29994333 6.70062123 0.95706993
 H 2.84799408 5.06069192 0.58595756
 H 1.55828207 5.80669486 -0.38298825
 H -2.43485252 5.39084138 1.49088235
 H -1.55277472 4.66853263 2.85003345

SiFlu2_EE_adduct
 71

E: -1354.07472335 ; H: -1353.45976 ; G: -
 1353.566357 ; D: -0.20824444
 C -1.31890119 0.93319698 -2.05598351
 C -0.56707655 0.06260996 -2.92116143
 C 0.81941207 0.42210924 -2.78771400
 C 0.88943724 1.52472291 -1.85776929
 C -0.42617150 1.82156454 -1.34077864
 Nd 0.13123741 -0.46521656 -0.01904222
 C -1.54329667 0.57792184 2.06575438
 C -0.88988094 -0.37935984 2.92024543
 C 0.48295320 0.03098896 3.04924703
 C 0.64830774 1.23219581 2.26813455
 C -0.59189699 1.56936757 1.60420013
 C -1.34542940 -2.48569040 -0.23955772
 C -0.75462126 -3.89929027 -0.33607727
 C 2.91771354 -2.65596791 0.46592788
 C 3.42839160 -1.43246788 0.33392161
 H -1.97252604 -2.42385466 0.66565221
 H -2.04089499 -2.32926286 -1.07959228
 H -0.02848879 -4.07568229 0.47437726
 H -1.53085109 -4.66808440 -0.18332136
 C -0.07398241 -4.19910066 -1.67271054
 H 3.55481899 -0.77439862 1.19007492
 H 3.77616848 -1.06253718 -0.62712182
 H 2.83082110 -3.33289089 -0.37907181
 H 2.60666648 -3.04054318 1.43365248
 C 0.47236501 -5.61912761 -1.78339520
 H -0.79549905 -4.02250153 -2.47971923
 H 0.73993452 -3.47937974 -1.84530888
 H 0.96741722 -5.78985476 -2.74514064
 H 1.20125044 -5.83516588 -0.99396113
 H -0.33111711 -6.35801714 -1.69300043
 Si -0.83902248 2.83367989 0.21131128
 C 0.25901001 4.36731733 0.39680525
 H 1.33464831 4.19260058 0.42081053
 H 0.05621142 5.04493706 -0.43998805
 H -0.00983782 4.88793634 1.32228373
 C -2.58771960 3.56020054 0.17480280
 H -2.74171444 4.15188137 1.08377014
 H -2.67603647 4.23497716 -0.68369748
 H -3.40470322 2.84163932 0.11186612
 C 1.92327381 1.85237258 2.27496199
 C 2.94525995 1.32727952 3.04049076
 H 2.08999177 2.76643687 1.71909026
 H 3.90711477 1.83098980 3.05929043
 C 1.54244003 -0.48421243 3.81795183
 C 2.76299637 0.16144896 3.81410313
 H 1.39307597 -1.37043188 4.42809239
 H 3.58188276 -0.21678524 4.41722887
 C -2.92536925 0.39625477 1.81195151
 C -3.60331447 -0.65292713 2.39746210
 H -3.46572917 1.09238136 1.18332756
 H -4.66532546 -0.77013446 2.20538078
 C -1.60339930 -1.43998536 3.50330206
 C -2.95165751 -1.57347148 3.24248750
 H -1.09981091 -2.14116218 4.16239979

H -3.51598865 -2.38448964 3.69040079
C -1.21423614 -0.87470695 -3.74610479
C -2.58913236 -0.97029304 -3.71192660
H -0.63664807 -1.50714214 -4.41358576
H -3.10147159 -1.68387215 -4.34855168
C -2.72882581 0.79378990 -2.04039410
C -3.33803664 -0.13507051 -2.85685215
H -3.33538679 1.44247498 -1.42126459
H -4.42042114 -0.21921988 -2.84973589
C 2.16882575 2.07886619 -1.59236691
C 3.28440102 1.59024821 -2.24160418
H 2.27208029 2.91817118 -0.91621515
H 4.25092178 2.04624103 -2.04952099
C 1.97484877 -0.05614858 -3.43601452
C 3.19619014 0.52573784 -3.16507396
H 1.89944667 -0.86256634 -4.15973205
H 4.09063196 0.17678109 -3.67058291

SiFlu2_EE_product

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E: -1354.11171496 ; H: -1353.4930000 ; G: -1353.59701 ; D: -0.20317239

C -1.43604701 1.51382851 -1.93209781
C -0.76509998 0.67903504 -2.90034066
C 0.63470908 1.00301790 -2.84683211
C 0.80400638 2.00501579 -1.82756986
C -0.47108625 2.31430409 -1.21079874
Nd -0.14645556 -0.08287766 -0.02668911
C -1.65540542 0.97068285 2.09308477
C -1.07257370 -0.16526998 2.76727867
C 0.33598198 0.09559708 2.90353409
C 0.59568405 1.37079746 2.28234740
C -0.62533445 1.91414213 1.72390329
C 0.47031831 -3.53369668 -0.82011688
C 0.09033383 -5.01135915 -0.68551955
C 1.57599230 -3.03507409 0.11637838
C 1.90676945 -1.54847594 -0.08520103
H -0.44450428 -2.93919101 -0.64496652
H 0.76005616 -3.32822304 -1.86008944
H -0.15617629 -5.22896533 0.36284362
H -0.82886771 -5.19657688 -1.25683951
C 1.16160279 -5.99186310 -1.16473731
H 2.63497141 -1.22149586 0.67145941
H 2.41054767 -1.41427563 -1.05683052
H 2.46251801 -3.67299840 -0.02037817
H 1.25361253 -3.21273506 1.15376046
C 0.71004096 -7.44636653 -1.08432691
H 1.43014489 -5.75018183 -2.20127733
H 2.07600542 -5.86365728 -0.57538740
H 1.49111120 -8.12876926 -1.43374709
H 0.46110094 -7.73020185 -0.05597721
H -0.18007456 -7.62190999 -1.69854385
Si -0.76610575 3.27361924 0.40219340
C 0.47371488 4.67926786 0.66142425
H 1.52312224 4.39066027 0.71300308
H 0.37192860 5.40127863 -0.15609585

H 0.23065923 5.19652267 1.59605259
C -2.43893319 4.16188498 0.42553644
H -2.57297131 4.65274863 1.39565718
H -2.42817859 4.94056234 -0.34510660
H -3.31732541 3.54174878 0.24600078
C 1.92955344 1.85167123 2.30096942
C 2.91592779 1.12383080 2.93215808
H 2.17302128 2.81098040 1.86240741
H 3.92819955 1.51519833 2.95771560
C 1.36194276 -0.62451201 3.54205595
C 2.64067515 -0.11059055 3.55672037
H 1.14403301 -1.56939447 4.03094838
H 3.43976740 -0.65117737 4.05259131
C -3.05839812 0.96092067 1.87947952
C -3.81776269 -0.10526908 2.31425207
H -3.54384387 1.80692868 1.40887680
H -4.89255103 -0.08894793 2.16109345
C -1.87380648 -1.23993289 3.20336770
C -3.23300522 -1.21023925 2.97199860
H -1.42428660 -2.07596624 3.73114558
H -3.86158456 -2.02726095 3.31043515
C -1.48674390 -0.21784086 -3.70993296
C -2.85491156 -0.32252340 -3.55814371
H -0.97042619 -0.81543664 -4.45560065
H -3.42188176 -1.00583245 -4.18160630
C -2.84040127 1.36397194 -1.79957642
C -3.52296881 0.46854823 -2.60008744
H -3.39153606 1.97259052 -1.09388779
H -4.60058671 0.38250013 -2.49930418
C 2.11428634 2.48841562 -1.58972987
C 3.16986297 2.01942589 -2.34432471
H 2.29036209 3.25301838 -0.84379492
H 4.16637700 2.41020508 -2.16230149
C 1.72666976 0.54480092 -3.60354179
C 2.98453814 1.05223536 -3.35284052
H 1.57925207 -0.19578261 -4.38409695
H 3.83555612 0.71151509 -3.93303272

SiFlu2_EE_TS

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E: -1354.06555719 ; H: -1353.448510 ; G: -1353.551091 ; D:

C -0.85717569 0.48915675 -1.99598365
C -0.07882312 -0.35009453 -2.87398560
C 1.29869164 0.03174594 -2.71890825
C 1.33892693 1.10592906 -1.75677696
C 0.01068033 1.37438479 -1.25134858
Nd 0.53205667 -0.97657634 0.01124311
C -1.10978054 0.03581631 2.12595982
C -0.42723351 -0.98647234 2.88220922
C 0.95157457 -0.59407764 2.98378765
C 1.09381139 0.65762093 2.28019226
C -0.17078940 1.04848509 1.69560916
C -0.39109980 -3.32535992 -0.39486900
C -0.59840634 -4.82379503 -0.49123428
C 1.90180329 -3.49660418 -0.18930206

H	2.30644359	-3.86066984	0.00000000
H	0.98275205	-4.33494022	0.00000000
C	1.18030050	-1.20309775	0.00000000
H	2.18172494	-1.52091537	0.00000000
H	0.45885682	-1.64868912	0.00000000
H	1.13796340	-0.12059445	0.00000000
C	-1.84069236	2.64869739	0.00000000
C	-1.98666285	4.04070743	0.00000000
H	-2.93028773	4.47896035	0.00000000
C	-0.94827773	4.87814491	0.00000000
C	0.22041426	4.28217057	0.00000000
C	0.38346899	2.89769989	0.00000000
H	1.02260819	4.91723810	0.00000000
C	1.61689364	2.35208507	0.00000000
H	2.47526372	3.01770361	0.00000000
H	1.44243592	2.25123456	0.00000000
H	1.91434340	1.36622637	0.00000000
C	-3.05956936	1.82206664	0.00000000
H	-3.82161886	1.92962030	0.00000000
H	-3.52499575	2.11634650	0.00000000
H	-2.83597072	0.75167373	0.00000000
C	-1.07543078	6.37413890	0.00000000
H	-0.90940855	6.84012489	0.00000000
H	-0.33586986	6.79951175	0.00000000
H	-2.06584453	6.67552404	0.00000000

SiFlu2_MesE_product

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E: -1545.82582223 ; H: -1545.150592 ; G: -1545.260801 ; D: -0.24122375

C	1.97579299	-1.00740090	0.00000000
C	2.36686292	0.38724420	0.00000000
C	3.26103715	0.66482579	0.00000000
C	3.44003613	-0.56190975	0.00000000
C	-1.86462946	-0.59612755	0.00000000
C	-0.88965960	-1.54936414	0.00000000
C	-1.60866400	-2.35372099	0.00000000
C	-2.96639908	-1.89147535	0.00000000
C	-3.12990459	-0.80291954	0.00000000
Si	0.87752360	-1.86341869	0.00000000
C	4.19354831	-0.86168182	0.00000000
H	4.77781313	-0.08777851	0.00000000
C	2.70298467	-2.88667196	0.00000000
H	2.16306467	-3.69006205	0.00000000
C	4.19514527	-2.15378112	0.00000000
H	4.77719570	-2.39799537	0.00000000
C	3.45222837	-3.15863382	0.00000000
H	3.47366823	-4.17091808	0.00000000
C	1.97870436	1.47070260	0.00000000
H	1.29323762	1.32170387	0.00000000
C	3.80564104	1.94292950	0.00000000
H	4.51618767	2.12639899	0.00000000
C	3.43724044	2.96936494	0.00000000
H	3.85733609	3.96157458	0.00000000
C	2.51258251	2.73111984	0.00000000
H	2.22123699	3.54765095	0.00000000

C	-4.24613199	-0.02435786	0.00000000
H	-5.20267730	-0.20560422	0.00000000
C	-1.77165821	0.44062476	0.00000000
H	-0.84050742	0.62278017	0.00000000
C	-4.12441480	0.97276513	0.00000000
H	-4.98498597	1.57570611	0.00000000
C	-2.88604730	1.20198972	0.00000000
H	-2.80622116	1.98356843	0.00000000
C	-3.85990964	-2.50715356	0.00000000
H	-4.88863320	-2.16430704	0.00000000
C	-3.42795510	-3.56669397	0.00000000
H	-4.11673484	-4.05489794	0.00000000
C	-1.19557641	-3.42111147	0.00000000
H	-0.18073233	-3.79942808	0.00000000
C	-2.09959029	-4.01449100	0.00000000
H	-1.77438899	-4.84239815	0.00000000
C	-0.93996509	0.43683692	0.00000000
C	-0.64570837	-0.94688695	0.00000000
H	-0.30907639	0.83525871	0.00000000
H	-1.98830470	0.63496996	0.00000000
H	-1.50089824	-1.62080062	0.00000000
H	0.22746423	-1.40757244	0.00000000
C	1.24954406	-3.71380361	0.00000000
H	0.68034819	-4.09623443	0.00000000
H	2.31350333	-3.86018823	0.00000000
H	0.98792663	-4.33303637	0.00000000
C	1.18579596	-1.19948716	0.00000000
H	2.18828920	-1.51491423	0.00000000
H	0.46609069	-1.64547394	0.00000000
H	1.14164625	-0.11689339	0.00000000
C	-1.87445034	2.55995111	0.00000000
C	-1.96019460	3.95284910	0.00000000
H	-2.87891790	4.37839737	0.00000000
C	-0.92501791	4.79998147	0.00000000
C	0.23912434	4.20175316	0.00000000
C	0.35926848	2.81943750	0.00000000
H	1.07413355	4.83222961	0.00000000
C	1.60464445	2.30296030	0.00000000
H	2.45694805	2.95423402	0.00000000
H	1.47025222	2.27239133	0.00000000
H	1.87888318	1.29251427	0.00000000
C	-3.09659972	1.75640921	0.00000000
H	-3.86647012	1.86073344	0.00000000
H	-3.53824627	2.08498227	0.00000000
H	-2.88820184	0.68557982	0.00000000
C	-1.04595280	6.29708400	0.00000000
H	-0.91136840	6.76611168	0.00000000
H	-0.28126293	6.71432663	0.00000000
H	-2.02368893	6.59666837	0.00000000

SiFlu2_MesE_TS

78

E: -1545.769300 ; H: -1545.096535 ; G: -1545.205782 ; D: -0.24064059

Nd	-0.601925	-0.182476	-0.384755
C	0.769007	-0.747979	1.763962

C -0.912578 2.583358 -1.809154
 C -2.050850 1.887908 -1.239098
 C -2.069393 2.278944 0.156038
 C -0.976883 3.173820 0.432217
 C -0.244562 3.350732 -0.794508
 C -3.221441 -1.953375 -0.826584
 C -2.732933 -0.977706 -1.778796
 C -1.762261 -1.694774 -2.582289
 C -1.646662 -3.054622 -2.121645
 C -2.574914 -3.218754 -1.034393
 Si -3.332007 0.789980 -2.094427
 C 0.898882 4.103940 -1.096449
 H 1.389566 4.688456 -0.323417
 C -0.384201 2.612071 -3.120148
 H -0.874955 2.075149 -3.923758
 C 1.392900 4.104865 -2.389082
 H 2.275011 4.687273 -2.634486
 C 0.746200 3.361572 -3.393416
 H 1.136140 3.384759 -4.406633
 C -2.895318 1.890433 1.239693
 H -3.721867 1.204853 1.091963
 C -0.798728 3.719233 1.709532
 H 0.003192 4.428370 1.892891
 C -1.650760 3.350914 2.736113
 H -1.520753 3.768985 3.728728
 C -2.680895 2.425084 2.499422
 H -3.331789 2.132048 3.317442
 C -2.907206 -4.335131 -0.256641
 H -2.425196 -5.291806 -0.437202
 C -4.178077 -1.859169 0.209839
 H -4.700253 -0.927236 0.393323
 C -3.859439 -4.212505 0.740262
 H -4.130570 -5.072291 1.344289
 C -4.484254 -2.973424 0.970568
 H -5.232389 -2.892756 1.753657
 C -0.764703 -3.948310 -2.740651
 H -0.700531 -4.977731 -2.399819
 C 0.016048 -3.516774 -3.801955
 H 0.693835 -4.207045 -4.293396
 C -0.932316 -1.282118 -3.652165
 H -0.984491 -0.269368 -4.035888
 C -0.069896 -2.187973 -4.249031
 H 0.547545 -1.864784 -5.081453
 C 2.234321 -1.054006 -0.022891
 C 1.825693 -0.783812 -1.308779
 H 2.852836 -0.348440 0.516250
 H 2.300036 -2.077897 0.325428
 H 1.532660 -1.590510 -1.976952
 H 2.068088 0.169811 -1.775336
 C -3.498979 1.162607 -3.944502
 H -4.356281 0.595846 -4.324606
 H -3.711555 2.227133 -4.088811
 H -2.643827 0.900254 -4.567403
 C -5.077490 1.100150 -1.428161
 H -5.386391 2.103338 -1.742705
 H -5.774432 0.381916 -1.872619

H -5.195137 1.056371 -0.345341
 C 0.350277 -1.950779 2.370655
 C 0.283130 -2.068509 3.763717
 H -0.068511 -3.000136 4.202752
 C 0.664855 -1.024657 4.599857
 C 1.158744 0.139213 4.005139
 C 1.236301 0.280274 2.620514
 H 1.500897 0.953505 4.641292
 C 1.920075 1.511512 2.081750
 H 1.760193 2.375847 2.729767
 H 3.004958 1.350702 2.028721
 H 1.593335 1.787873 1.076504
 C 0.021754 -3.171890 1.549579
 H 0.810534 -3.927613 1.647909
 H -0.914218 -3.641701 1.862042
 H -0.056814 -2.951538 0.480392
 C 0.574758 -1.143578 6.095575
 H 1.554256 -1.008266 6.566875
 H -0.090214 -0.379984 6.513346
 H 0.191634 -2.121387 6.396901

SiFlu2_BuMes_Mg_BuBu_Mg_MesMeTHF
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E: -2962.15131480 ; H: -2960.809940 ; G: -2961.008607 ; D: -0.42656169

C 3.42352101 -1.74908092 0.71939447
 C 2.22612305 -1.28131741 1.41280648
 C 1.32724289 -2.42045706 1.38929035
 C 1.93017917 -3.52111187 0.68769730
 C 3.24866164 -3.09862434 0.28297067
 C -0.62322300 1.28869784 2.80373617
 C 0.74197602 1.19395670 2.31084984
 C 0.91262162 2.35266544 1.45724457
 C -0.31465612 3.10196110 1.39076661
 C -1.27313464 2.43423423 2.23431720
 Si 2.12836032 0.00452189 2.80568311
 C 4.64136862 -1.10831000 0.43199843
 C 5.63516062 -1.78988382 -0.25350258
 H 4.81557381 -0.08509070 0.74488181
 H 6.57503185 -1.28825869 -0.46455070
 C 4.25925279 -3.76972358 -0.41343717
 C 5.45197126 -3.11500454 -0.67820145
 H 6.24788457 -3.62595762 -1.21048065
 C 0.00950027 -2.57534613 1.87319433
 C -0.66687577 -3.77861770 1.67143297
 H -0.46325462 -1.80068843 2.47323515
 H -1.67133865 -3.89562151 2.06606302
 C 1.23643777 -4.71431796 0.50708776
 C -0.06161959 -4.84152810 0.99667781
 H 1.70420679 -5.54821172 -0.00885780
 H -0.60258722 -5.77259604 0.86293680
 C 1.77545731 -0.85206561 4.45885892
 H 2.68513619 -1.38188915 4.76314632
 H 1.53664843 -0.12155695 5.23838498
 H 0.97558791 -1.59360687 4.41773719
 C 3.76322175 0.91764843 3.08611040

H	4.53928623	0.20150945	3.37439558	C	-5.23582215	-3.42361768	-0.74930297
H	4.13697814	1.49970773	2.24331539	H	-5.70134835	-3.11801967	-1.69292670
H	3.62142194	1.61187271	3.92180431	H	-4.65191960	-4.32850754	-0.94962026
C	-1.35640150	0.48997399	3.70836279	C	0.54142698	0.35459221	-2.60872032
C	-2.66454213	0.82055805	4.01745925	C	1.29721140	-0.82485579	-2.85086727
H	-0.89579765	-0.36458134	4.19062711	C	1.09161738	1.56112510	-3.12362923
H	-3.21471717	0.20710724	4.72484609	C	2.53836325	-0.78679060	-3.49427750
C	-2.59605422	2.75225124	2.56552711	C	2.32693386	1.57396738	-3.77341148
C	-3.28968239	1.94447838	3.44994476	C	3.07325755	0.40985015	-3.96050326
H	-3.07008663	3.63391679	2.14457936	H	3.09237517	-1.71150968	-3.63922427
H	-4.31289595	2.18532345	3.71931153	H	2.71925043	2.51742036	-4.14705565
C	-0.38444814	4.30200351	0.67389721	H	-2.64913448	-5.17086100	-6.95096656
C	0.73277045	4.75886381	-0.00674615	H	-6.49590936	4.29205966	-0.37600134
H	-1.30351106	4.88060531	0.66329501	H	-6.04149365	-3.69706001	-0.06057627
H	0.69018280	5.69454417	-0.55413151	C	-2.46064754	2.40758805	-6.44626479
C	2.01819036	2.81860988	0.70289958	C	-3.02254753	3.70269514	-6.49971442
C	1.91967626	4.00938474	-0.00048070	C	-1.45829051	2.13915895	-7.41664655
H	2.96288838	2.28647026	0.71278874	C	-2.61490850	4.65095677	-7.45103198
H	2.78301676	4.37248806	-0.54926347	C	-1.06100283	3.09271758	-8.35457587
H	4.11598121	-4.79696060	-0.73713486	C	-1.63099203	4.36758775	-8.38912030
Mg	-1.75534385	0.09766309	-2.59431584	H	-3.08010253	5.63614050	-7.45536154
C	-3.08947409	1.94327489	-2.73126598	H	-0.28980573	2.83992913	-9.08093918
C	-4.53873556	2.03240618	-2.22357686	C	-4.08323197	4.15819200	-5.52140015
H	-2.87645788	2.84206398	-3.33112250	H	-4.51579573	3.32831666	-4.95737273
H	-2.44308751	2.13476118	-1.85208245	H	-3.67311223	4.86548021	-4.79023076
H	-5.23905655	1.96260764	-3.06757418	H	-4.90436972	4.67722628	-6.02906829
H	-4.77187293	1.16952876	-1.58419419	C	-0.76634694	0.79644095	-7.45555843
C	-2.30393763	-0.78246032	-0.53506477	H	-0.17533035	0.67222340	-8.36817174
C	-3.21594852	-1.89202903	-1.09961727	H	-0.08282956	0.67488957	-6.60791383
H	-2.94156097	0.05824886	-0.20916895	H	-1.48235860	-0.03050476	-7.41409367
H	-1.94811266	-1.19849920	0.43110965	C	-1.19768326	5.38297129	-9.41173446
H	-3.65910306	-1.58533809	-2.06126796	H	-0.11725171	5.55899964	-9.37006282
H	-2.61327540	-2.77875844	-1.33732013	H	-1.42799731	5.05040814	-10.43038684
Nd	0.26866705	-0.05823727	0.01394370	H	-1.69699300	6.34306631	-9.25696259
Mg	-3.04828305	0.96182373	-4.90270067	C	0.33347749	2.85982868	-3.04692299
C	-2.00845898	-1.10202922	-4.56288134	H	1.00667165	3.72002844	-3.04152458
C	-2.92121760	-2.04578264	-5.37013942	H	-0.31932803	2.97182361	-3.92094680
H	-1.63066740	-1.74044867	-3.73866046	H	-0.29963680	2.92555305	-2.16008883
H	-1.09546006	-0.92752825	-5.15117648	C	0.78203179	-2.19393529	-2.45994016
H	-3.81199203	-2.30360317	-4.78169479	H	0.55205350	-2.77863026	-3.35651767
H	-3.30546572	-1.53748840	-6.26550600	H	1.52006404	-2.76767606	-1.89243331
C	-4.36165974	-2.31384092	-0.17372142	H	-0.15301941	-2.16368437	-1.88446300
H	-3.93792010	-2.63888871	0.78437145	C	4.39795280	0.44227504	-4.66869993
H	-4.97898749	-1.43574522	0.05311335	H	5.07529428	-0.32369601	-4.28251094
C	-2.25181730	-3.34910399	-5.81948458	H	4.27007142	0.25620290	-5.74147999
H	-1.90661872	-3.89569137	-4.93209973	H	4.88500992	1.41504590	-4.56329976
H	-1.34999393	-3.10443770	-6.39487847	O	-5.07364262	0.46424911	-5.39951282
C	-4.86802430	3.30827134	-1.44166826	C	-5.78569319	0.96033195	-6.58997899
H	-4.65707436	4.17839209	-2.07597613	C	-5.98828391	-0.31063289	-4.59843029
H	-4.18203972	3.38316764	-0.58909693	C	-7.27084732	0.68828614	-6.30535913
C	-6.30811668	3.37445501	-0.94279448	H	-5.57570555	2.03049964	-6.62521644
H	-6.54217814	2.52980993	-0.28519664	C	-5.26583281	0.29501122	-7.84483090
H	-7.02259307	3.35326932	-1.77336503	C	-7.32799083	0.36308543	-4.81255759
C	-3.15992283	-4.25060595	-6.65005287	H	-5.99869967	-1.34653221	-4.95536592
H	-4.05569299	-4.54130847	-6.08964779	H	-5.63023545	-0.29275703	-3.56878709
H	-3.49221654	-3.74717196	-7.56468849	H	-7.61024266	-0.17130054	-6.89185715

H -7.89204203 1.54322656 -6.57879393
H -5.82152376 0.67366015 -8.70909145
H -4.21063062 0.52465428 -8.00499971
H -5.40086602 -0.78989588 -7.80476534
H -8.16716384 -0.28340929 -4.54726842
H -7.39226967 1.27461294 -4.21212536

SiFlu2_BuBu_Mg_MesBu_Mg_MesMeTHF
149

E: -2962.14838743 ; H: -2960.807635 ; G: -
2961.006030 ; D: -0.43439297

C 2.83438696 -1.60910064 0.88128547
C 1.73212503 -1.67992517 1.83091902
C 1.25827194 -3.05695897 1.73608179
C 2.00778975 -3.77082483 0.74778695
C 2.99969246 -2.86915181 0.21444111
C -0.66543068 1.25946752 2.64883632
C 0.77390063 1.08070836 2.65145340
C 1.31035620 2.43025694 2.52753327
C 0.24444903 3.38038094 2.42308267
C -0.99663295 2.65111746 2.48837095
Si 1.63286442 -0.48176537 3.30301752
C 3.69176183 -0.54408607 0.52569388
C 4.68270429 -0.74161221 -0.42914666
H 3.61810093 0.42121556 1.02027363
H 5.34351739 0.07979357 -0.68722874
C 4.00873031 -3.04600350 -0.73328592
C 4.84896230 -1.98495952 -1.05116041
H 5.63911459 -2.11865207 -1.78273712
C 0.23642924 -3.74222810 2.41946632
C -0.02447213 -5.07077049 2.12158474
H -0.34517250 -3.24551595 3.18840757
H -0.80999868 -5.59228141 2.66062162
C 1.72419335 -5.10863246 0.45455969
C 0.70901066 -5.75665541 1.14068848
H 2.30020280 -5.63965766 -0.29822704
H 0.48383362 -6.79652283 0.92678267
C 0.68617831 -1.21603685 4.77139893
H 1.17185339 -2.13900428 5.10369217
H 0.73279594 -0.49586688 5.59586804
H -0.36807528 -1.43037382 4.59227562
C 3.36294937 -0.11915345 3.98501424
H 3.72228316 -1.02839892 4.47977089
H 4.10312338 0.14576801 3.22865199
H 3.32631535 0.67808969 4.73404885
C -1.72561851 0.32859071 2.74194838
C -3.04430546 0.77193535 2.71000509
H -1.52823230 -0.72652243 2.90735237
H -3.84917145 0.05000218 2.80930759
C -2.32705753 3.06887102 2.45869109
C -3.34768870 2.13172019 2.57585235
H -2.56740130 4.12323660 2.35678868
H -4.38369834 2.45372211 2.56692769
C 0.50632761 4.74687391 2.27905602
C 1.81930666 5.18812250 2.23943938
H -0.31148898 5.45797858 2.20324132

H 2.03604235 6.24625527 2.13410406
C 2.63405100 2.90879958 2.48403496
C 2.87395103 4.26671927 2.34320688
H 3.47105476 2.22559252 2.57343088
H 3.89872410 4.62561354 2.31887772
H 4.14467194 -4.00961985 -1.21650716
Mg -1.47711680 0.29258108 -2.56474363
C -1.79620044 -1.19797130 -0.78063068
C -3.09830572 -1.93216523 -1.14282160
H -1.91301348 -0.98974275 0.30487381
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H -3.94813156 -1.24981820 -1.02779673
H -3.08138626 -2.21666135 -2.20179495
Nd 0.35158501 -0.04665644 0.23787185
Mg -3.25307503 0.74153099 -4.77717219
C -1.86463417 -1.05798318 -4.43773676
C -2.77561153 -2.10294838 -5.11582328
H -1.27580297 -1.63482149 -3.70289439
H -1.10653135 -0.75600100 -5.18057365
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H -3.34969655 -1.63892317 -5.93312900
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H -3.38758692 -2.90033272 0.75944725
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H -1.28294959 -2.95109808 -6.41459220
C -2.95377748 -4.31552497 -6.39192841
H -3.69721288 -4.72128210 -5.69653256
H -3.49736939 -3.85318124 -7.22327947
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H -5.52239492 -3.27735875 -0.53954552
H -4.62774118 -4.26251269 -1.70483472
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C 2.25702980 2.67280842 -2.98543380
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C -1.28364313 0.96038024 -10.20491518
H -1.06365531 -0.11324639 -10.18625476
H -1.48124165 1.23656685 -11.24626902
H -0.37367302 1.48517982 -9.89238910

C -2.65844462 2.21815218 -3.00664550
 C -2.05894436 3.26394496 -3.75111438
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 C -2.42678898 4.60457783 -3.56469393
 C -3.98437802 3.95522084 -1.87713758
 C -3.38130626 4.97190402 -2.62538732
 H -1.95034325 5.37625250 -4.16657133
 H -4.73917494 4.21995726 -1.13893385
 C -4.36339660 1.58298559 -1.22974231
 H -3.69209610 1.10999825 -0.50514378
 H -5.18800144 2.02202376 -0.66157005
 H -4.77270655 0.79074953 -1.86282183
 C -0.99724716 2.98907494 -4.78837566
 H -1.30703104 3.33947359 -5.77812954
 H -0.06325976 3.50294449 -4.54221199
 H -0.76146665 1.92427570 -4.87005289
 C -3.75896614 6.41054399 -2.40760684
 H -3.30728863 7.06235897 -3.15910332
 H -4.84416219 6.54910800 -2.44807347
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 H 0.41728837 4.14245787 -1.75404006
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 H 1.19266170 -1.85634480 -4.18284783
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 H 4.60975813 3.21513340 -4.21848241
 O -5.38568366 0.59675810 -4.33311341
 C -6.27115127 -0.45859966 -4.83922868
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 C -7.53170290 0.26628079 -5.31975776
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 H -8.29918662 0.23553928 -4.53886805
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 H -5.58797353 -1.95201916 -3.42725411
 H -7.02295316 -1.04837380 -2.90116758
 H -7.87689843 2.43114911 -5.49191122
 H -6.57393497 1.80417782 -6.51994163

SiFlu2_BuMes_Mg_BuMes_Mg_BuMeTHF
 149

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 2961.005660 ; D: -0.42929196

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C 0.93992845 -3.51413596 0.59079736
 C 2.12723805 -2.89581128 0.06573094
 C -0.72210626 0.66463636 3.27238553
 C 0.72019547 0.58649631 3.23840127
 C 1.13903509 1.72248339 2.44880911
 C -0.01131267 2.43021158 1.94524339
 C -1.17860434 1.76733388 2.46196992
 Si 1.79944935 -0.88236946 3.75284231
 C 3.80649462 -1.26962864 0.78327338
 C 4.49230667 -1.51072181 -0.39147107
 H 4.21462817 -0.56868674 1.50075333
 H 5.42005613 -0.97985277 -0.58201875
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 C -0.94636978 -4.98846294 0.83069469
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 C 3.55951343 -0.37312980 4.23463840
 H 4.09277010 -1.26010558 4.59377722
 H 4.16714330 0.07257242 3.44763149
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 C -1.70413952 -0.11963166 3.93291671
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 H -1.40806121 -0.94126949 4.57304844
 H -3.77776955 -0.39355729 4.34168058
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 Nd 0.15155106 -0.34531490 0.75771162

Mg -2.66236766 1.16845727 -4.58198398
C -1.32617521 -0.65614716 -3.99393431
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C -1.52888113 3.05677786 -8.56180317
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C -4.66617440 2.02278536 -1.55523490
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C -0.31337061 3.31701309 -3.87558019
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H -3.20767007 7.38293815 -2.48315695
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H -2.24627737 7.17209213 -1.02360209
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H -4.19762157 3.49449363 -4.56080158
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H -0.98402013 0.13699977 -7.22620022
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C -2.36760599 5.01432597 -9.92038268
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H -1.40682328 5.53812306 -9.97815509
O -4.50628947 0.11403711 -5.07878741
C -5.04954015 0.13544370 -6.44715762
C -5.43753305 -0.59820956 -4.24431773
C -6.54444961 -0.19819658 -6.29322659
H -4.88879254 1.15412134 -6.79829504
C -4.29793680 -0.83259675 -7.33498130
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H -5.25927847 -0.30820012 -3.21066064
H -6.74894646 -1.18858179 -6.71119150
H -7.17078071 0.52066450 -6.82470855
H -4.71103855 -0.78906523 -8.34803205
H -3.24021442 -0.57023257 -7.39982916
H -4.39122100 -1.86221392 -6.97632502
H -7.58596337 -0.88643739 -4.48032014
H -7.05805986 0.80413066 -4.42857898

SiFlu2_BuBu_Mg_MesMes_Mg_BuMeTHF
149

E: -2962.13971834 ; H: -2960.798543 ; G: -2960.996648 ; D: -0.43710425

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C 0.83498065 -2.93512339 1.62958728
C 0.83901603 -3.35944570 0.24971126
C 2.02218700 -2.81380624 -0.36115057
C -0.28583690 0.77270056 3.39110581
C 1.09314583 0.55481684 2.98576840
C 1.48530720 1.79128617 2.33259235
C 0.37153837 2.70111290 2.28721406
C -0.73485079 2.06401868 2.94930068
Si 2.19135110 -0.93872466 3.38735041
C 3.98113344 -1.50998921 0.32009770
C 4.50652240 -1.70586926 -0.93909187
H 4.55782184 -0.97545715 1.06492865
H 5.48517708 -1.29933440 -1.17515925
C 2.57761186 -2.98744543 -1.64275339
C 3.80967717 -2.43673949 -1.92549661

H	4.25583914	-2.57667712	-2.90450031	H	-2.58609817	4.97507031	-2.10276075
C	-0.22326904	-3.39329270	2.45671978	H	-6.03073478	2.53919761	-1.44970924
C	-1.17315516	-4.25579197	1.94944985	C	0.49297768	1.24421306	-1.51194276
H	-0.26631510	-3.11024640	3.50082495	H	0.35695214	2.10034208	-0.82300011
H	-1.95975850	-4.62132322	2.60240411	H	0.06130862	1.64831649	-2.44093198
C	-0.14181035	-4.24261648	-0.23954000	C	1.99595894	1.08147573	-1.79478502
C	-1.13686564	-4.68730186	0.60632502	H	2.54965771	0.81606965	-0.87808672
H	-0.10022905	-4.58564983	-1.26851298	H	2.15831363	0.23195965	-2.46774662
H	-1.89026647	-5.37890658	0.24416378	C	2.68308637	2.31991860	-2.38097435
C	1.72078986	-1.78086717	5.01993643	H	2.49983821	3.17121520	-1.71547133
H	2.42655792	-2.59804529	5.20630879	H	2.20065756	2.56818419	-3.33487872
H	1.82051309	-1.05722173	5.83626697	C	4.18292644	2.14827736	-2.59732495
H	0.71691015	-2.20095840	5.07790334	H	4.39986691	1.31281769	-3.27154883
C	4.00010103	-0.45223094	3.67743879	H	4.63016647	3.04781603	-3.03305210
H	4.59272995	-1.35766216	3.84818606	H	4.70086006	1.94801533	-1.65352926
H	4.48504468	0.11648849	2.88421575	C	-4.18904041	-1.01212905	-5.96854284
H	4.05185937	0.15644022	4.58701909	H	-3.55526748	-1.70575712	-6.54787438
C	-1.19702078	-0.03106109	4.11329560	H	-4.70376239	-1.66137110	-5.24209051
C	-2.46980304	0.43653392	4.38440331	C	-5.24209150	-0.42052248	-6.91312979
H	-0.89992101	-1.00506421	4.48174051	H	-4.75891566	0.22365194	-7.66447280
H	-3.15306539	-0.18505478	4.95534824	H	-5.91963928	0.24729467	-6.35865154
C	-2.03421478	2.51171309	3.22338827	C	-6.10342123	-1.44426077	-7.66455444
C	-2.89662633	1.70169201	3.94062251	H	-5.44217204	-2.11389945	-8.23050942
H	-2.35623558	3.49378874	2.88889833	H	-6.61736656	-2.07986366	-6.93141087
H	-3.90118508	2.04187948	4.17043763	C	-7.12864916	-0.82049474	-8.60759135
C	0.49811095	3.97192397	1.71277845	H	-6.64293226	-0.20777355	-9.37606864
C	1.71498564	4.36308908	1.18200385	H	-7.72398193	-1.58095692	-9.12431788
H	-0.34853092	4.65248126	1.69949671	H	-7.82593658	-0.17175894	-8.06516175
H	1.82859712	5.35167820	0.74912802	C	-1.05133097	-1.22177309	-4.01206212
C	2.70732501	2.21759123	1.76154363	C	-1.60932121	-2.53385735	-3.95645942
C	2.81171954	3.48349921	1.21182186	C	0.09966064	-1.09699959	-4.83227443
H	3.57870656	1.57423159	1.77736516	C	-1.07293772	-3.60091719	-4.67387903
H	3.76397681	3.80669252	0.80262104	C	0.62503207	-2.18345822	-5.54687373
H	2.04984703	-3.56711567	-2.39321361	C	0.04930953	-3.44539253	-5.48962862
Mg	-1.51975927	0.13280031	-2.20465043	H	-1.54691274	-4.57832176	-4.60676265
C	-2.22346049	-0.61581657	-0.09671789	H	1.50506068	-2.03107615	-6.16952744
C	-3.74756268	-0.81853523	-0.13063765	C	-2.79891145	-2.83035258	-3.08214431
H	-2.08674668	0.14793264	0.70149011	H	-3.36100734	-3.69561556	-3.44336213
H	-1.82686777	-1.56919423	0.32367657	H	-2.48931910	-3.04852749	-2.05353002
H	-4.22367607	0.13319084	-0.38827906	H	-3.49114467	-1.98716641	-3.04405044
H	-4.02002733	-1.51991850	-0.92599442	C	0.83325600	0.20955640	-5.00770467
Nd	0.31921682	-0.35701365	0.54025064	H	0.87447108	0.50652579	-6.06080176
Mg	-2.79415905	0.28882298	-4.93345479	H	0.37117310	1.02087889	-4.44664951
C	-4.35055139	-1.32994783	1.18168724	H	1.87104870	0.12553763	-4.67228280
H	-3.89666535	-2.29779841	1.42781525	C	0.58746030	-4.59523807	-6.29401742
H	-4.07360117	-0.64702064	1.99310782	H	-0.08662826	-4.84075138	-7.12267496
C	-5.86824963	-1.47653429	1.13172517	H	1.56638136	-4.36312529	-6.72064221
H	-6.35706486	-0.51276558	0.95218015	H	0.68863835	-5.49894406	-5.68502097
H	-6.17953118	-2.15913259	0.33314889	C	-1.25463257	3.40051685	-3.70973304
H	-6.26298289	-1.87173922	2.07338803	H	-1.42804326	4.27438855	-4.34822193
C	-3.15363599	1.75151173	-3.17590486	H	-0.45962617	3.68271543	-3.01334506
C	-2.53311580	3.01948628	-3.00058777	H	-0.88926246	2.60333553	-4.35742208
C	-4.46155114	1.64413027	-2.61073671	C	-5.34470597	0.45316032	-2.89166660
C	-3.11359107	4.03044004	-2.22278174	H	-6.04046573	0.25503679	-2.07231322
C	-5.03031364	2.67167303	-1.85755958	H	-5.94840633	0.63356336	-3.78884773
C	-4.35562348	3.86957245	-1.62122241	H	-4.77981190	-0.45894591	-3.08419486

C -4.95880487 4.94291257 -0.75943721
H -4.44001013 5.89677212 -0.88367991
H -6.01630707 5.09810696 -0.99393508
H -4.90224485 4.67088443 0.30087880
O -2.25208026 1.70493176 -6.49828648
C -1.37487815 1.58663083 -7.66607081
C -3.15134696 2.83155600 -6.66475081
C -1.89679022 2.62808604 -8.65139960
H -0.37429825 1.87263127 -7.32312173
C -1.36019348 0.16782260 -8.18573177
C -2.51638998 3.68666332 -7.74481860
H -4.13125921 2.45463506 -6.97572372
H -3.25518150 3.32587054 -5.69878825
H -2.66003884 2.18181070 -9.29774994
H -1.09686232 3.01340586 -9.28703876
H -0.67158145 0.10220947 -9.03459442
H -1.01995539 -0.54342584 -7.42949808
H -2.35334743 -0.13668103 -8.52417729
H -3.24967602 4.31682489 -8.25205558
H -1.74307719 4.33350017 -7.31934636

SiFlu2_BuPh_Mg_BuBu_Mg_PhMeTHF

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E: -2726.29245412 ; H: -2725.125634 ; G: -2725.307166 ; D: -0.37219244

C 3.13303784 -1.76014479 0.52746529
C 2.08346273 -1.47811513 1.49233859
C 1.14267982 -2.56746898 1.34377327
C 1.57164437 -3.45627142 0.29342491
C 2.82845050 -2.95576324 -0.20164386
C -0.69578344 1.04657205 2.81576620
C 0.69988801 1.00400153 2.42930058
C 0.87875471 2.13979508 1.54871792
C -0.37019169 2.83560762 1.37681473
C -1.35791415 2.14414619 2.16499194
Si 2.04567399 -0.23374874 2.91826132
C 4.32745273 -1.07964139 0.21723204
C 5.16739670 -1.57263730 -0.76636476
H 4.60419685 -0.17812993 0.75126057
H 6.08827959 -1.04307690 -0.99217904
C 3.69035039 -3.43732915 -1.19392182
C 4.85717620 -2.74626960 -1.47430172
H 5.53818001 -3.11222639 -2.23590250
C -0.08937803 -2.83804589 1.98361724
C -0.82606438 -3.96030384 1.62383440
H -0.44782812 -2.21043626 2.79318574
H -1.75855109 -4.16908824 2.13881218
C 0.80859720 -4.57458718 -0.05089563
C -0.38436683 -4.82763571 0.61556947
H 1.15055423 -5.25100016 -0.82933158
H -0.97425368 -5.70166231 0.35975456
C 1.67787635 -1.09769504 4.56438998
H 2.57848373 -1.64815782 4.85920341
H 1.46375603 -0.36506157 5.34933011
H 0.86193936 -1.82124238 4.53311819
C 3.70855026 0.62097664 3.21717624

H 4.46849554 -0.12828671 3.46202803
H 4.08958582 1.23463121 2.40068076
H 3.59478055 1.27678658 4.08768524
C -1.45780995 0.23783951 3.69172470
C -2.79748146 0.51111132 3.89477184
H -0.99081920 -0.57473952 4.23601025
H -3.36776182 -0.10745468 4.58139379
C -2.71849231 2.40269144 2.38963162
C -3.43378246 1.58707808 3.24667559
H -3.20215709 3.24657523 1.90689201
H -4.48427622 1.78310831 3.43503257
C -0.44086275 4.00469945 0.60531154
C 0.69645212 4.47398916 -0.02776039
H -1.37777248 4.54601307 0.51526221
H 0.65374841 5.38477406 -0.61577005
C 2.00691057 2.61463424 0.83499298
C 1.90799468 3.76830048 0.07750042
H 2.96220806 2.10860798 0.90800818
H 2.78589658 4.13661227 -0.44361762
H 3.45212225 -4.34986064 -1.73353413
Mg -1.74915982 0.03110658 -2.57707303
C -2.96255212 2.01294231 -2.64234741
C -4.43654552 2.40250893 -2.41721537
H -2.44488888 2.87877093 -3.08829393
H -2.50360340 1.96460303 -1.63546744
H -4.96055680 2.50533652 -3.38020553
H -4.96125607 1.59232858 -1.89313607
C -2.26576197 -1.16946044 -0.70067775
C -3.73211266 -1.41685427 -1.11011506
H -2.34765118 -0.83057052 0.35589166
H -1.78743800 -2.16392693 -0.63215758
H -4.28121116 -0.46626525 -1.08718310
H -3.78222055 -1.76993047 -2.15041774
Nd 0.11039466 -0.21689454 0.13187275
Mg -3.03005220 1.09840010 -4.76055585
C -1.84714270 -0.91787050 -4.66036288
C -2.18215306 -2.40209463 -4.42313854
H -0.75414645 -0.82486754 -4.76740172
H -2.18516730 -0.70261050 -5.69318444
H -1.80697847 -2.73148912 -3.44174176
H -3.27111837 -2.53865051 -4.37000460
C -4.47574052 -2.42738300 -0.22998617
H -3.94878717 -3.38836888 -0.27191356
H -4.41994327 -2.09278913 0.81339759
C -1.62685057 -3.35990514 -5.48250809
H -0.53643395 -3.24476058 -5.52633331
H -2.00120047 -3.05215464 -6.46775487
C -4.65254783 3.70036708 -1.63316538
H -4.13602421 4.51807419 -2.15125896
H -4.16579660 3.60475031 -0.65453713
C -6.12195241 4.06122873 -1.43899658
H -6.65738602 3.27524323 -0.89436704
H -6.62919243 4.19984483 -2.40033654
C -1.97825614 -4.82346257 -5.23471422
H -1.59275287 -5.16896164 -4.26897436
H -3.06306505 -4.97897754 -5.22883057

C -5.93520789 -2.62405188 -0.62697756
H -6.49710338 -1.68592010 -0.55898864
H -6.02449932 -2.99238324 -1.65500010
C 0.51800169 0.51527233 -2.36471894
C 1.38472269 -0.45346043 -2.91969340
C 0.74426479 1.84131048 -2.78924066
C 2.40148495 -0.13311602 -3.81728629
C 1.74280842 2.17793385 -3.70146662
C 2.57669581 1.18893056 -4.21401710
H 3.04915826 -0.91188190 -4.20781985
H 1.87048655 3.21102208 -4.01099751
H -1.55822879 -5.47549731 -6.00729348
H -6.23768770 4.99028546 -0.87178681
H -6.43216731 -3.35050850 0.02359917
C -2.44198878 2.49833655 -6.29532574
C -3.02961962 3.76908901 -6.46623441
C -1.37098371 2.22362967 -7.17046615
C -2.59966249 4.68754985 -7.42538053
C -0.92275438 3.12599490 -8.13628633
C -1.53977512 4.36636294 -8.26892393
H -3.08828946 5.65525536 -7.51345506
H -0.08873400 2.86346197 -8.78295408
O -4.96812962 0.42187552 -5.26458731
C -5.65692460 0.75828969 -6.52312660
C -5.86088958 -0.32436740 -4.41112597
C -7.10806140 0.31457911 -6.30608420
H -5.58429744 1.84488201 -6.61262144
C -4.96899568 0.09544881 -7.69497411
C -7.24129306 0.17145913 -4.79063984
H -5.74718458 -1.39492845 -4.61603969
H -5.58012059 -0.12729675 -3.37660088
H -7.27803861 -0.65139517 -6.79272470
H -7.81170158 1.03216211 -6.73223728
H -5.50560975 0.34193785 -8.61691479
H -3.94246549 0.45145118 -7.80407220
H -4.96486513 -0.99313708 -7.58385849
H -8.02926129 -0.52340000 -4.49299956
H -7.43783934 1.13846378 -4.31892940
H -1.19667055 5.07541787 -9.01698090
H 3.36018931 1.44762966 -4.91977312
H 1.27200760 -1.50666995 -2.65690056
H 0.12277467 2.64697032 -2.40422120
H -3.85750240 4.07428922 -5.82483216
H -0.85048265 1.26825335 -7.10067649

SiFlu2_BuPh_Mg_BuPh_Mg_BuMeTHF

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E: -2726.29267553 ; H: -2725.126162 ; G: -2725.306820 ; D: -0.37364756

C 2.77716544 -1.57496631 0.50613712
C 1.90878193 -1.60263888 1.67120289
C 1.17123599 -2.85370607 1.55103788
C 1.55683432 -3.54303261 0.35526292
C 2.56482857 -2.74753462 -0.29801612
C -0.54845648 0.91417390 2.95747114
C 0.89249373 0.94589519 2.83443826

C 1.17815849 2.16981692 2.12351862
C -0.04918413 2.83326462 1.75789906
C -1.13302471 2.04307019 2.27721364
Si 2.06751155 -0.49446278 3.20319987
C 3.71422903 -0.61996217 0.04943323
C 4.43107639 -0.85412619 -1.11482389
H 3.90571996 0.28753128 0.61177933
H 5.15750086 -0.11917427 -1.44696857
C 3.30147739 -2.96191615 -1.46655705
C 4.23862282 -2.02185696 -1.86703947
H 4.82124360 -2.18478518 -2.76781666
C 0.19767730 -3.45154197 2.37703062
C -0.35447681 -4.67151124 2.02514198
H -0.11792965 -2.97016363 3.29496587
H -1.09615597 -5.12618213 2.67512183
C 0.98174101 -4.77288793 0.01359944
C 0.02855886 -5.33462310 0.84710588
H 1.28717058 -5.28850747 -0.89256295
H -0.41850150 -6.29132546 0.59727002
C 1.63427330 -1.39760815 4.81047216
H 2.31590621 -2.24556340 4.93700721
H 1.79567714 -0.70984602 5.64808924
H 0.61778830 -1.78094899 4.89442979
C 3.85025900 0.07424567 3.49828419
H 4.44050119 -0.79705073 3.80292449
H 4.36027450 0.51895926 2.64395498
H 3.87191546 0.79735377 4.32075003
C -1.42628821 0.00496510 3.60052528
C -2.78674738 0.23399342 3.59026983
H -1.03442026 -0.84847997 4.13897635
H -3.44463045 -0.45671401 4.10868522
C -2.52381736 2.25126216 2.28024616
C -3.34188741 1.35232707 2.93368091
H -2.94613185 3.12076717 1.78636093
H -4.41531418 1.50895191 2.95465551
C -0.03248922 4.08129206 1.10874204
C 1.17742807 4.66829836 0.80095487
H -0.96424710 4.58473329 0.86891288
H 1.20376620 5.63680764 0.31263186
C 2.40012004 2.79480432 1.76436808
C 2.38659439 4.01759027 1.12523160
H 3.34731786 2.34464604 2.03727972
H 3.32868130 4.49863613 0.88061764
H 3.14830281 -3.86389775 -2.05225675
Mg -1.60116506 0.20866509 -2.31917978
C -2.02039241 -0.96225162 -0.38826565
C -3.36156549 -1.57804157 -0.82956924
H -2.23158711 -0.44964898 0.57446980
H -1.39231658 -1.83598401 -0.11204876
H -4.05800160 -0.79012452 -1.14821698
H -3.19909494 -2.20605608 -1.71481052
Nd 0.29529801 0.05007064 0.34913765
Mg -3.15789520 0.60890177 -4.63192308
C -1.77674180 -1.18616808 -4.14074239
C -2.65109957 -2.25474390 -4.82491111
H -1.20201906 -1.73615945 -3.36961803

H -0.99616699 -0.88137721 -4.85666019
H -3.41167797 -2.62720140 -4.12543353
H -3.21358815 -1.81393758 -5.66451706
C -4.04895320 -2.42266614 0.24907281
H -3.35167002 -3.20035570 0.58245699
H -4.24002272 -1.78960666 1.12388445
C -1.87765127 -3.45570401 -5.38048277
H -1.32369426 -3.92821524 -4.55874722
H -1.12181231 -3.09123428 -6.08724071
C -2.76285548 -4.49265119 -6.06438115
H -3.50684136 -4.90268625 -5.37207134
H -3.30471934 -4.05772183 -6.91157861
C -5.35202014 -3.06728981 -0.21143070
H -6.08259465 -2.31467101 -0.52722806
H -5.18645345 -3.74433452 -1.05634478
C 0.59066816 0.93066258 -2.18198521
C 1.38235568 0.17448703 -3.07501794
C 0.87490565 2.31409215 -2.15498931
C 2.36195634 0.74428256 -3.88642852
C 1.86556835 2.89832651 -2.94254754
C 2.60722350 2.11198593 -3.81880223
H 2.93502375 0.12082332 -4.56632856
H 2.05071538 3.96690783 -2.87954278
H -2.17581540 -5.33279599 -6.44865034
H -5.81166241 -3.65288254 0.59106393
C -2.87226726 1.33294848 -6.64758244
H -3.60181662 0.83792285 -7.31223000
H -3.15797143 2.39909819 -6.67489209
C -1.47935271 1.18798758 -7.27480387
H -1.19082987 0.12636714 -7.30467014
H -0.72261391 1.66946131 -6.63746977
C -1.33248066 1.75651435 -8.69199828
H -1.59576658 2.82264686 -8.67463684
H -2.07226915 1.27466450 -9.34538911
C 0.06251580 1.58387815 -9.28676190
H 0.34134978 0.52542520 -9.34419289
H 0.12851725 1.99640986 -10.29940647
H 0.82049129 2.08792561 -8.67650271
C -2.91514215 2.02474549 -2.74251007
C -2.36996607 3.20398643 -3.29757978
C -3.97050434 2.23181847 -1.82805444
C -2.83953779 4.47974291 -2.98471273
C -4.44600743 3.49859020 -1.49028084
C -3.88209581 4.62949613 -2.07471582
H -2.39092864 5.35478062 -3.44700351
H -5.25750507 3.60474541 -0.77513334
O -5.31141253 0.43205293 -4.52573954
C -6.11910929 -0.60201363 -5.18127922
C -5.98625972 1.70992305 -4.63809883
C -7.29648898 0.14467205 -5.81782980
H -5.47889904 -1.03659044 -5.95523235
C -6.52197506 -1.65775911 -4.17666041
C -6.81860527 1.59274715 -5.89833405
H -6.60760695 1.86041746 -3.74904004
H -5.22747063 2.49329987 -4.67245520
H -8.17759233 0.06962107 -5.17168752

H -7.55768041 -0.27708784 -6.79026956
H -7.11330544 -2.43418548 -4.67259848
H -5.64977273 -2.13627196 -3.72750753
H -7.13016938 -1.22147155 -3.37901175
H -7.63822590 2.31417852 -5.92104846
H -6.19151529 1.75218011 -6.77948813
H 0.30500677 2.97354714 -1.50269006
H -4.25171195 5.61915007 -1.82247435
H -1.54616417 3.13229667 -4.00563856
H -4.44941734 1.37613324 -1.35476960
H 3.37226818 2.56222603 -4.44432753
H 1.23510140 -0.90119378 -3.15572835

SiFlu2_BuBu_Mg_PhBu_Mg_PhMeTHF
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E: -2726.29703076 ; H: -2725.130227 ; G: -
2725.310987 ; D: -0.3784538

C 2.86989235 -1.76836424 0.81628287
C 2.07558442 -1.80226822 2.02560896
C 1.07912723 -2.82664050 1.79077225
C 1.22552288 -3.36733058 0.46332758
C 2.35073997 -2.70910238 -0.14537932
C -0.44586265 0.76834096 3.14526574
C 0.99653903 0.75890803 3.03475025
C 1.31485396 1.89841127 2.20547700
C 0.10548838 2.53833805 1.75113951
C -0.99900513 1.82666314 2.33675687
Si 2.17371919 -0.64612266 3.52281856
C 4.00207168 -1.00242902 0.44063715
C 4.59952713 -1.20656848 -0.78819186
H 4.43236903 -0.28301035 1.12626774
H 5.48062287 -0.62909956 -1.05102094
C 2.97915960 -2.89816864 -1.38699552
C 4.10066734 -2.15601066 -1.70210980
H 4.60116113 -2.30117411 -2.65361670
C 0.04267882 -3.34723597 2.60372800
C -0.77018668 -4.35649354 2.12714058
H -0.10048572 -2.98080862 3.61217624
H -1.54940374 -4.75732009 2.76812680
C 0.38643912 -4.39505149 0.00296623
C -0.60420451 -4.88548063 0.83155390
H 0.52514169 -4.81004080 -0.99120632
H -1.25240202 -5.68618458 0.49096392
C 1.67662804 -1.49687907 5.14050661
H 2.35764637 -2.33559429 5.32193715
H 1.79548697 -0.78489191 5.96485032
H 0.65999671 -1.88590280 5.19054726
C 3.93140740 -0.04018384 3.88503926
H 4.52994679 -0.89088718 4.22872355
H 4.46914724 0.41654066 3.05436869
H 3.89566342 0.69335622 4.69796172
C -1.34908402 -0.04168028 3.88119622
C -2.70345222 0.20722884 3.82154331
H -0.97809585 -0.82824575 4.52616441
H -3.38167363 -0.40452866 4.40856711
C -2.38800506 2.05245697 2.28700556

C	2.90382900	-2.92035135	-1.21961543	C	-4.59826194	3.03090269	-1.75151946
C	4.15416201	-2.37550531	-1.41619590	C	-3.91786823	4.22907263	-1.94791539
H	4.69746644	-2.57609364	-2.33359959	H	-2.11394988	5.13578610	-2.69318041
C	-0.21528088	-3.19242235	2.64843724	H	-5.58435262	3.03465813	-1.29541484
C	-1.09543837	-4.10808412	2.11340487	C	0.73119482	1.05309550	-1.82094288
H	-0.33268556	-2.87423041	3.67657563	H	0.69568249	1.98930196	-1.23421552
H	-1.91003176	-4.48206352	2.72597126	H	0.30042729	1.39024770	-2.78253059
C	0.08391815	-4.14149555	-0.00013533	C	2.20084433	0.72584715	-2.12839451
C	-0.95335277	-4.58503416	0.79141225	H	2.76589736	0.51810971	-1.20427520
H	0.20575390	-4.52040878	-1.01038331	H	2.26670213	-0.20085317	-2.71062202
H	-1.65987924	-5.31229310	0.40558207	C	2.94647433	1.83518155	-2.88062643
C	1.32552924	-1.24035737	5.22861805	H	2.88877226	2.76133437	-2.29644033
H	1.97381037	-2.05920360	5.55953328	H	2.40971744	2.03715022	-3.81768103
H	1.36948815	-0.45030913	5.98643791	C	4.40402641	1.51062091	-3.18993522
H	0.30310799	-1.61758772	5.21487330	H	4.49352348	0.59092387	-3.77821704
C	3.73494626	0.02264966	4.03667939	H	4.88052387	2.31512426	-3.75979232
H	4.29518597	-0.82983014	4.43605605	H	4.98469071	1.37019558	-2.27274398
H	4.32193354	0.44955480	3.22349354	C	-4.79039096	-0.48981194	-5.11599300
H	3.67087280	0.77981128	4.82576044	H	-4.63336025	-1.30287054	-5.84537331
C	-1.52680928	0.16647248	3.59846974	H	-5.23299367	-0.99314829	-4.23961823
C	-2.86058243	0.50803038	3.49574586	C	-5.82675864	0.48681938	-5.68665867
H	-1.24306080	-0.70009941	4.18219862	H	-5.43497021	0.95335003	-6.60383126
H	-3.60503181	-0.10335141	3.99650869	H	-5.98868279	1.32017315	-4.98621174
C	-2.34507461	2.42841081	2.11814589	C	-7.19584180	-0.11975113	-6.02024747
C	-3.27646882	1.63377891	2.75797448	H	-7.05575110	-0.94401132	-6.73212677
H	-2.66310725	3.29767223	1.55085608	H	-7.61205414	-0.57413823	-5.11133202
H	-4.33211098	1.87717605	2.69775046	C	-8.19355628	0.88446814	-6.59095370
C	0.34482944	3.92697803	0.93477544	H	-7.82263642	1.32998440	-7.52135860
C	1.61372274	4.34919075	0.58673195	H	-9.15971348	0.41914870	-6.81359377
H	-0.52669632	4.50000374	0.63319592	H	-8.37911207	1.70455811	-5.88785047
H	1.74700650	5.25913788	0.01092285	C	-1.14845063	-1.23500965	-4.11162838
C	2.61605715	2.44753428	1.73033471	C	-1.70508641	-2.52692221	-4.24712475
C	2.74115195	3.60389726	0.98399981	C	0.12914050	-1.07791799	-4.69367842
H	3.50808754	1.91761514	2.04044764	C	-1.05145992	-3.57171900	-4.89906564
H	3.73204068	3.95105174	0.70714548	C	0.80335594	-2.11050587	-5.34610276
H	2.45637775	-3.55835438	-1.97572639	C	0.21036319	-3.36509434	-5.45008645
Mg	-1.29856032	0.01761612	-2.18894961	H	-1.52704194	-4.54527595	-4.98044752
C	-2.02468823	-0.92599972	-0.24408123	H	1.78781672	-1.93775411	-5.77266948
C	-3.15822992	-1.72111781	-0.92037377	O	-2.09683054	1.48259576	-6.18681432
H	-2.48734966	-0.09792596	0.32318037	C	-1.25846049	1.03766284	-7.30765084
H	-1.65135762	-1.61959925	0.53646926	C	-2.63002170	2.79950104	-6.46437630
H	-3.58682013	-1.15850840	-1.76567636	C	-1.24661612	2.21964422	-8.28008896
H	-2.74409313	-2.63725335	-1.35783013	H	-0.26265686	0.87762297	-6.88484814
Nd	0.43941857	-0.27993828	0.50431369	C	-1.78993884	-0.25452014	-7.88622650
Mg	-2.85878879	0.30891036	-4.58553406	C	-1.62196881	3.41797256	-7.41013036
C	-4.30993300	-2.09555746	0.01829252	H	-3.61439560	2.69726010	-6.93390691
H	-3.89465262	-2.63620732	0.87735911	H	-2.74122176	3.31973935	-5.51238455
H	-4.75058720	-1.17616125	0.42308770	H	-1.99974859	2.06800220	-9.06054473
C	-5.39268141	-2.93919835	-0.64649117	H	-0.27519612	2.32612522	-8.76691778
H	-5.84568302	-2.41675212	-1.49574766	H	-1.16422891	-0.55940132	-8.73122964
H	-4.98753331	-3.88552429	-1.02147158	H	-1.76949720	-1.06362542	-7.15224429
H	-6.19696156	-3.18160831	0.05558509	H	-2.81539958	-0.13005580	-8.24506718
C	-2.73715059	1.74692937	-2.74310653	H	-2.04432641	4.24824399	-7.97970598
C	-2.09180472	2.99138962	-2.92079918	H	-0.75476392	3.78647940	-6.85366355
C	-4.01420871	1.82728667	-2.14386931	H	0.72542305	-4.17464911	-5.95877636
C	-2.65684065	4.20745847	-2.53592324	H	-2.69432691	-2.73022067	-3.84218310

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 H -4.58859268 0.91764932 -1.97973289
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 C -0.32247164 3.46363131 3.01759889
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SiFlu2_PhE_product

69
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 1427.409542 ; D: -0.21573672
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 C -0.44753686 -2.72969795 -1.13927434
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 H 0.15014750 1.97297880 -3.53761683
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 H 3.74929140 3.77414271 -2.05919538
 C 1.98998752 2.84738228 -2.90953096
 H 2.41687719 2.80501448 -3.90687460
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 H 1.32059376 3.90349800 2.38707458
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 C -1.85100187 2.72813092 2.79235399
 H -2.61332611 2.64524810 3.56109663
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C	-3.14018533	-1.34842563	0.89734714	C	1.17789281	3.46342791	-1.16319393
H	-3.83991181	-0.52549973	0.82041718	H	1.78059850	3.91244541	-0.37901768
C	-2.36196431	-3.32559547	2.08769241	C	-0.40165875	2.33832539	-3.21915355
H	-2.46014560	-3.99279812	2.93751896	H	-0.99275046	1.94128670	-4.03501989
C	-3.22224301	-2.21356363	1.96959254	C	1.65204193	3.40191008	-2.45746455
H	-3.97592197	-2.04368830	2.73252814	H	2.63431731	3.79520705	-2.69736932
C	0.54239947	-3.64019824	-1.54692404	C	0.85676497	2.84073887	-3.47844162
H	0.78070497	-4.50084373	-0.92878721	H	1.24042590	2.81327471	-4.49360522
C	1.19761715	-3.43794974	-2.74405855	C	-3.06286136	2.19030671	1.11407756
H	1.96011296	-4.13590696	-3.07348191	H	-4.03353486	1.74191692	0.94359703
C	-0.09587370	-1.42112202	-3.17467502	C	-0.57990466	3.43362049	1.63266919
H	-0.33192553	-0.59291203	-3.83026598	H	0.36589950	3.92997897	1.82981809
C	0.87796510	-2.32461005	-3.54701324	C	-1.51974593	3.30384679	2.63377153
H	1.40527900	-2.17856863	-4.48464291	H	-1.31601241	3.68831772	3.62754178
C	3.55994942	-0.44229027	0.65402357	C	-2.75073100	2.66815553	2.37041603
C	2.58876764	-0.50362333	-0.54369389	H	-3.47768843	2.56795917	3.17063551
H	3.87700944	0.59361629	0.81861882	C	-2.31841034	-3.78328098	0.39462024
H	4.48164789	-1.01696784	0.47691599	H	-1.66367281	-4.64980113	0.38636982
H	2.57981675	-1.52307741	-0.95905240	C	-4.06195440	-1.55887465	0.39437018
H	2.95317003	0.14713228	-1.34974820	H	-4.76731321	-0.73712796	0.40214646
C	-2.48786075	1.20226348	-3.65734956	C	-3.25269534	-3.62612569	1.39623820
H	-3.26468707	0.56057545	-4.08767580	H	-3.33284966	-4.36367110	2.18774491
H	-2.76732928	2.24352424	-3.85132864	C	-4.11522956	-2.50946133	1.39247205
H	-1.56541261	1.00381963	-4.20296381	H	-4.84932516	-2.40500223	2.18557296
C	-4.21246182	1.27063370	-1.24151776	C	-0.40553491	-3.60667846	-2.29633987
H	-4.49131068	2.26900187	-1.59619939	H	-0.12164424	-4.49277761	-1.73601743
H	-4.88453371	0.54719075	-1.71574390	C	0.19913570	-3.32266570	-3.50375128
H	-4.40393269	1.24416189	-0.16856867	H	0.96858226	-3.97960100	-3.89552148
C	2.71684374	-2.31601794	2.14461427	C	-1.16896988	-1.32762208	-3.78178180
H	3.08208754	-3.02724210	1.40930583	H	-1.45519346	-0.47719754	-4.38789459
C	2.07881743	-2.77657077	3.29196849	C	-0.18679611	-2.18259221	-4.23893859
H	1.94898677	-3.84352085	3.44435228	H	0.29505303	-1.97711143	-5.18986970
C	1.61016856	-1.87720403	4.24814464	C	2.12730673	-0.67137493	-0.03882204
H	1.11324750	-2.23890551	5.14221073	C	1.69430634	-0.39491303	-1.32519775
C	1.79500694	-0.51341360	4.04986144	H	2.64108840	0.09271357	0.53441868
C	2.44424597	-0.05519890	2.90221558	H	2.38694093	-1.68675791	0.23715534
H	1.44742835	0.19844532	4.79212039	H	1.53686102	-1.20548400	-2.03383721
H	2.61573294	1.01076190	2.77419621	H	1.82614714	0.60222966	-1.74133257

SiFlu2_PhE_TS

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C	-0.92903253	2.38606923	-1.90400637
C	-2.19871461	1.96087268	-1.34935919
C	-2.13786953	2.33460663	0.04664029
C	-0.86174218	2.93545118	0.34735397
C	-0.10179437	2.95898626	-0.87184070
C	-3.12994813	-1.69475412	-0.66643646
C	-2.87763609	-0.89104529	-1.84256845
C	-1.82862490	-1.59021088	-2.55355830
C	-1.40954413	-2.75177230	-1.80616555
C	-2.23323678	-2.82274320	-0.63010899

Si	-3.50300913	0.86684522	-2.18741192
C	1.17789281	3.46342791	-1.16319393
H	1.78059850	3.91244541	-0.37901768
C	-0.40165875	2.33832539	-3.21915355
H	-0.99275046	1.94128670	-4.03501989
C	1.65204193	3.40191008	-2.45746455
H	2.63431731	3.79520705	-2.69736932
C	0.85676497	2.84073887	-3.47844162
H	1.24042590	2.81327471	-4.49360522
C	-3.06286136	2.19030671	1.11407756
H	-4.03353486	1.74191692	0.94359703
C	-0.57990466	3.43362049	1.63266919
H	0.36589950	3.92997897	1.82981809
C	-1.51974593	3.30384679	2.63377153
H	-1.31601241	3.68831772	3.62754178
C	-2.75073100	2.66815553	2.37041603
H	-3.47768843	2.56795917	3.17063551
C	-2.31841034	-3.78328098	0.39462024
H	-1.66367281	-4.64980113	0.38636982
C	-4.06195440	-1.55887465	0.39437018
H	-4.76731321	-0.73712796	0.40214646
C	-3.25269534	-3.62612569	1.39623820
H	-3.33284966	-4.36367110	2.18774491
C	-4.11522956	-2.50946133	1.39247205
H	-4.84932516	-2.40500223	2.18557296
C	-0.40553491	-3.60667846	-2.29633987
H	-0.12164424	-4.49277761	-1.73601743
C	0.19913570	-3.32266570	-3.50375128
H	0.96858226	-3.97960100	-3.89552148
C	-1.16896988	-1.32762208	-3.78178180
H	-1.45519346	-0.47719754	-4.38789459
C	-0.18679611	-2.18259221	-4.23893859
H	0.29505303	-1.97711143	-5.18986970
C	2.12730673	-0.67137493	-0.03882204
C	1.69430634	-0.39491303	-1.32519775
H	2.64108840	0.09271357	0.53441868
H	2.38694093	-1.68675791	0.23715534
H	1.53686102	-1.20548400	-2.03383721
H	1.82614714	0.60222966	-1.74133257
C	-3.68827538	1.23240091	-4.03577841
H	-4.49520782	0.60853248	-4.43568575
H	-3.97864834	2.28059828	-4.16565536
H	-2.80737770	1.05553207	-4.65241311
C	-5.24941357	1.16014716	-1.51760755
H	-5.57635797	2.16190227	-1.81724090
H	-5.93250383	0.43529889	-1.97380338
H	-5.37146011	1.09212263	-0.43663025
C	0.48245642	-2.11495296	2.09985103
H	0.38747821	-2.92085408	1.37381066
C	0.40524775	-2.43975377	3.45249493
H	0.23823287	-3.46953890	3.75591493
C	0.55160597	-1.44391857	4.41458710
H	0.49973191	-1.69215811	5.47016575
C	0.77265489	-0.12943192	4.01371191
C	0.84643112	0.18243743	2.65689696
H	0.89296333	0.65285673	4.75808093

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