Electronic Supplementary Material (ESI) for ChemComm.

Kinetically controlled asymmetric synthesis of silicon-stereogenic methoxy silanes using a planar chiral ferrocene backbone

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Abstract: We present asymmetric syntheses of monomethoxy silanes starting from prochiral dimethoxy silanes by nucleophilic substitution with alkyllithium reagents. The stereoinduction is performed by a planar chiral ferrocene species, which leads to extremely high diastereomeric ratios in the Si-stereogenic product both as a reagent and as part of the prochiral silane itself. Experimental and quantum chemical calculation data support the mechanism hypothesis, in which the desymmetrization of dimethoxy silane takes place under kinetic control and the metal lithium plays a central role. Only the energy barrier of the nucleophilic attack determines the resulting configuration. The stereochemical pathway is highly defined, since a reversible conversion of various pentavalent intermediates is suppressed by coordination with the metal lithium.

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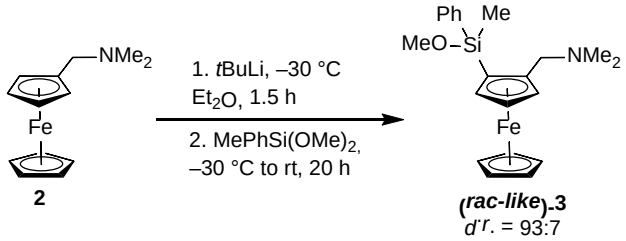
1 General Remarks

All experiments were performed under an atmosphere of argon by using standard Schlenk techniques. Diethyl ether and pentane were refluxed over sodium and distilled under an atmosphere of argon prior to use. All commercially available reagents and deuterated solvents were used without further purification. NMR spectra were recorded on a Bruker AV Avance III HD spectrometer. All NMR spectra were recorded at room temperature (ca. 22 °C). ^{1}H-NMR and {^{1}H}^{13}C-NMR chemical shifts (δ) are reported in parts per million (ppm) and referred to tetramethylsilane (TMS, δ = 0.0 ppm) with the deuterium signal of the solvent serving as internal lock and residual solvent signals as an additional reference. {^{1}H}^{29}Si-NMR chemical shifts are reported in ppm, referenced to an external standard of TMS (δ = 0.0 ppm), and measured via the INEPT puls sequence. The signals were assigned with the help of DEPT-135 and ^{13}C,^{1}H-HSQC. Spin-spin coupling constants (J) are reported in Hertz (Hz). For the assignment of the multiplicities the following abbreviations were used: brs = broad singlet, s = singlet, d = doublet, dd = dublet of dublets, brd = broad dublet, t = triplet, q = quartet, m = multiplet. Carbon and hydrogen atoms of the aromatic core are assigned as *ipso*, *ortho*, *meta*, and *para*. Major and minor diastereomers are denoted as D_{maj} and D_{min}, respectively. GC/EI-MS analyses were carried out on an Agilent Technologies 7890B GC system with an Agilent Technologies 5977A Series Mass Selective Detector equipped with an Agilent HP-5MS column (30 m, 0.25 mm, 0.25 µm) and helium as carrier gas. The m/z values of the molecular ions and selected fragment ions are based on the isotops with the highest natural abundance (^{1}H, ^{12}C, ^{14}N, ^{16}O, ^{28}Si, ^{56}Fe). Elemental analyses were performed on an *elementar vario MICRO cube* apparatus.

2 Syntheses of the Compounds

2.1 Synthesis of *rac-like* 3



To a stirred solution of *N*,*N*-dimethylaminomethylferrocene (**2**) (1.00 g, 4.11 mmol, 1.0 eq) in Et_2O (10 mL) at –30 °C *t*BuLi (1.9 M in pentane, 2.40 mL, 4.50 mmol, 1.1 eq) was added and stirred for 1.5 h. Then phenylmethyldimethoxysilane (1.12 g, 6.14 mmol, 1.5 eq) was added at –30 °C. The reaction mixture was allowed to warm to room temperature and stirred for further 20 h. After the reaction was stopped by adding H_2O (ca. 5 mL), the organic layer was separated and the auqeous layer was extracted with Et_2O (3 x 10 mL). The combined organic layers were dried with Na_2SO_4 and the solvent removed. The crude product was purified by column chromatography (*n*pentane/Et_2O = 5/1 + 10% Vol. Et_3N). The resulting highly viscous red brown oil yielded in 969 mg (2.46 mmol, 60%) of methoxyferrocenylsilane **3**.

^{1}H-NMR	(400.25 MHz, C_6D_6): δ = D_{maj} 0.70, D_{min} 0.73 (s, 3H; SiCH_3), D_{min} 1.97, D_{maj} 2.07 [s, 6H; N(CH_3)$_2$], D_{min} 2.70, D_{maj} 2.82 (AB-system, $^2J_{HH}$ =12.23, 1H; CpCH_2N), D_{min} 3.48, D_{maj} 3.49 (s, 3H; OCH_3), 3.63 (AB-system, $^2J_{HH}$ =12.23, 1H; CpCH_2N), D_{maj} 4.00, D_{min} 4.09 (s, 5H; Cp-C*H*), D_{maj} 4.05–4.07, D_{min} 4.13–4.15, 4.24 (m, 1H; Cp-C*H*), 4.10–4.12 (m, 1H; Cp-C*H*), D_{min} 4.18–4.20, D_{maj} 4.23–4.24 (m, 1H; Cp-C*H*), 7.21–7.31 (m, 3H; Ph-$H_{ortho,para}$), D_{min} 7.78–7.82, D_{maj} 7.87–7.91 (m, 2H; Ph-H_{meta}) ppm.
{^{1}H}^{13}C-NMR	(100.6 MHz, C_6D_6): δ = D_{min} –1.9, D_{maj} –1.7 (1C; Si*C*H$_3$), D_{min} 45.2, D_{maj} 45.5 [2C; N(*C*H$_3$)$_2$], 51.5 (1C; O*C*H$_3$), 60.0 (1C; Cp*C*H$_2$N), 69.2 (1C, Si*C*CCH$_2$), 70.0 (5C; Cp-*C*H), 70.9 (1C; Cp-*C*H), 74.7 (1C; Cp-*C*H), 76.1 (1C, Cp-*C*H), 91.0 (1C, Cp-*C*CH$_2$N), 128.2 (2C; Ph-C_{meta}), 130.0 (1C; Ph-C_{para}), 135.2 (2C; Ph-C_{ortho}), 138.7 (1C; Ph-C_{ipso}) ppm.
{^{1}H}^{29}Si-NMR	(79.52 MHz, C_6D_6): δ = 1.42 (s, 1Si; *Si*MePh) ppm.
GC/EI-MS:	D_{min} t_R = 7.46 min [80 °C (1 min) – 40 °C·min^{-1} – 270 °C (5.5 min)]; m/z (%): 393 (100) [M$^+$], 349 (8) [(M-NMe$_2$)$^+$], 317 (69) [M-Ph)$^+$], 242 (90) [(M-Ph-MeSiOMe)$^+$].
	D_{maj} t_R = 7.54 min [80 °C (1 min) – 40 °C·min^{-1} – 270 °C (5.5 min)]; m/z (%): 393 (95) [M$^+$], 349 (7) [(M-NMe$_2$)$^+$], 317 (67) [(M-Ph)$^+$], 242 (100) [(M-PhMeSiOMe)$^+$], 121 (59) [(FeCp)$^+$].

CHN-Analysis:				
	calculated:	C: 64.12%	H: 6.92%	N: 3.56%
	measured:	C: 64.2%	H: 7.0%	N: 3.6%

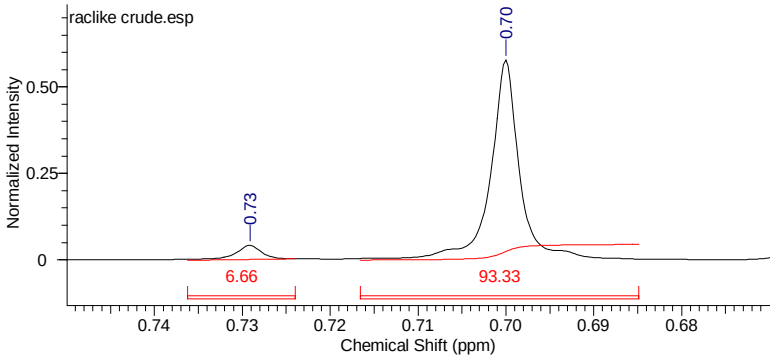


Figure 1: Integration of the diastereomeric ^{1}H-NMR signals caused by the SiCH$_3$ groups to quantify the *d.r.* value.

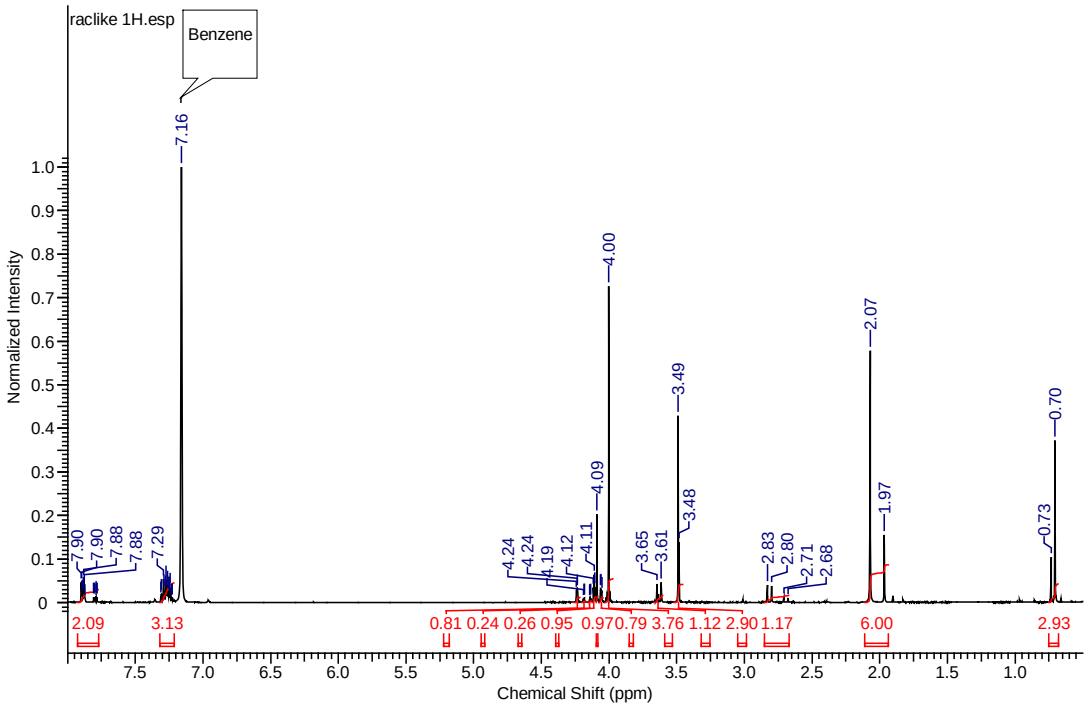


Figure 2: ^{1}H-NMR spectrum of ***(rac-like)*-3**.

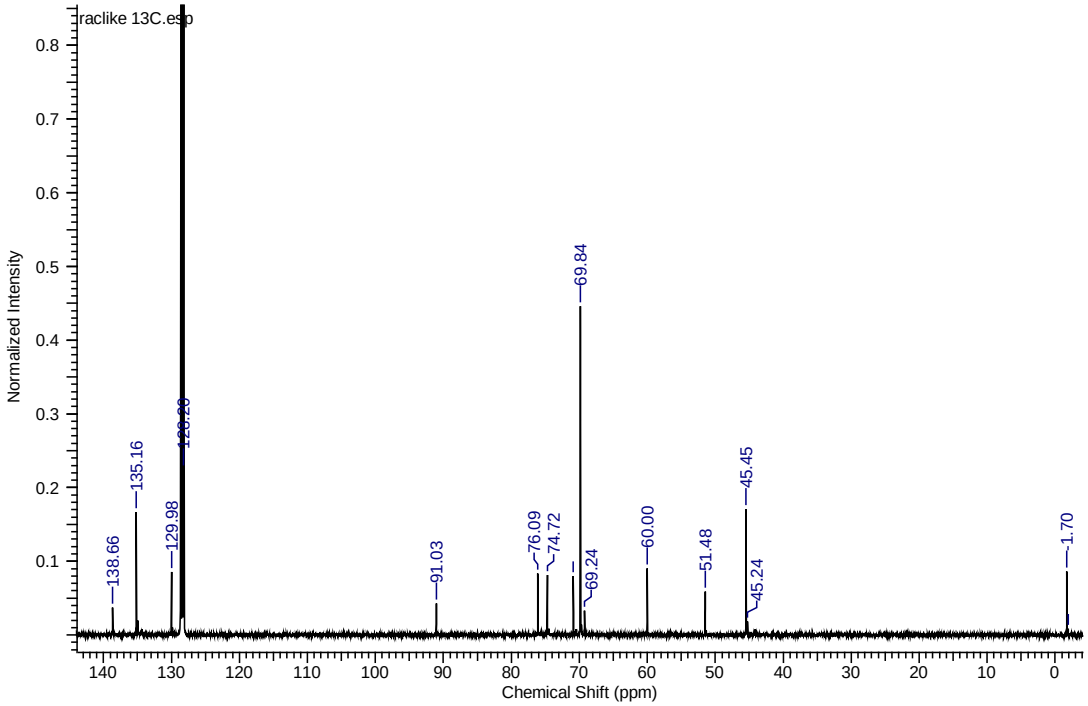


Figure 3: ^{13}C-NMR spectrum of ***(rac-like)*-3**.

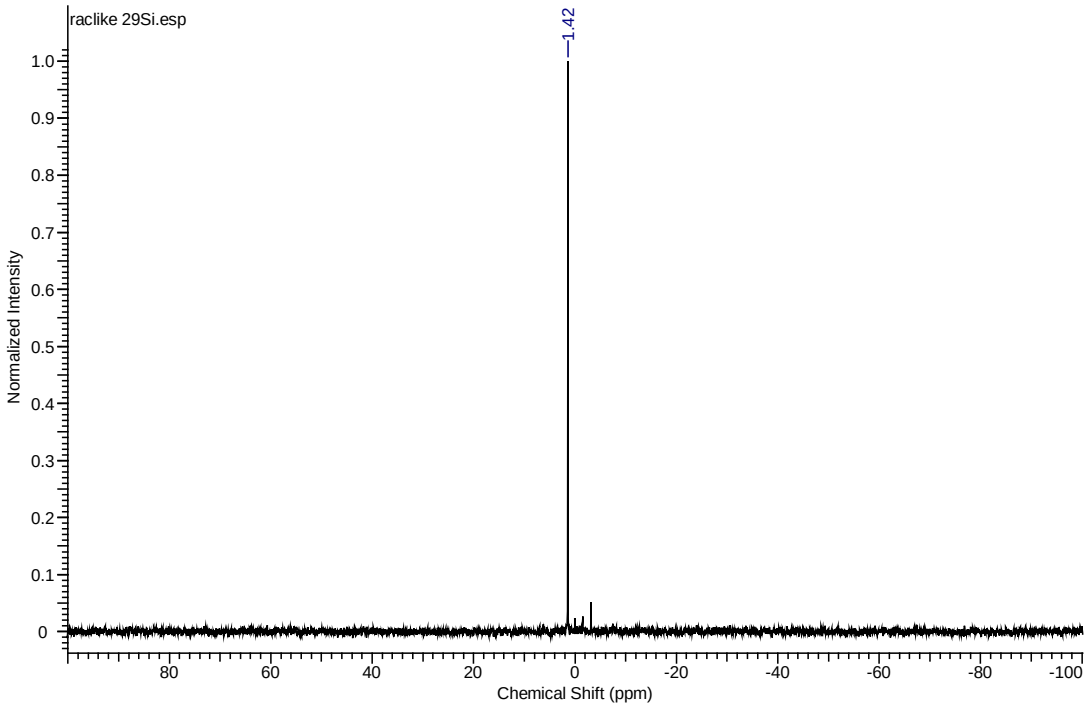
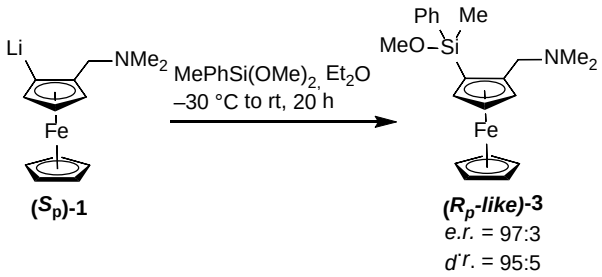


Figure 4: ^{29}Si-NMR spectrum of **(*rac-like*)-3**.

2.2 Synthesis of (*R*$_p$-*like*)-3



(*S*$_p$)-1 **(*R*$_p$-*like*)-3**
e.r. = 97:3
d.r. = 95:5

Highly enantio enriched lithiated ferrocene **(*S*$_p$)-1** was prepared according to the procedure published by our group.[1] After removal of the mother layer, the enantiomeric pure lithiated crystals were washed with cold *n*pentane (2 x 5 mL) and Et_2O (1 x 5 mL) and redissolved in Et_2O (5 mL). Then phenylmethyldimethoxysilane (974 mg, 5.34 mmol, 1.3 eq) was added at –65 °C. The reaction mixture was allowed to warm to room temperature and stirred for further 20 h. After the reaction was stopped by adding H_2O (ca. 5 mL), the organic layer was separated and the auqeous layer was extracted with Et_2O (3 x 10 mL). The combined organic layers were dried with Na_2SO_4 and the solvent removed. The crude product was purified by column chromatography (*n*pentane/Et_2O = 5/1 + 10% Vol. Et_3N). The resulting highly viscous red brown oil yielded in 635 mg (1.61 mmol, 39%) of methoxyferrocenylsilane **(*R*$_p$-*like*)-3**.

The spectroscopic data correspond to **(*rac-like*)-3**.

$[\alpha]_D^{20}$ = +48.0° mL g^{-1} dm^{-1} (C_6H_6, 56.5 mg/10mL)

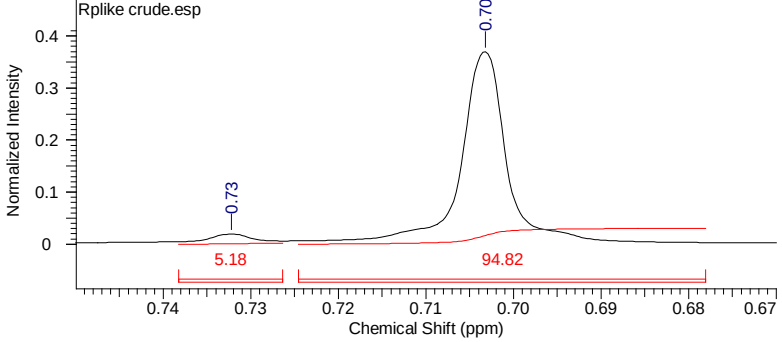


Figure 5: Integration of the diastereomeric ^{1}H-NMR signals caused by the $SiCH_3$ groups to quantify the *d.r.* value of **(*R*$_p$)-*like*-3**.

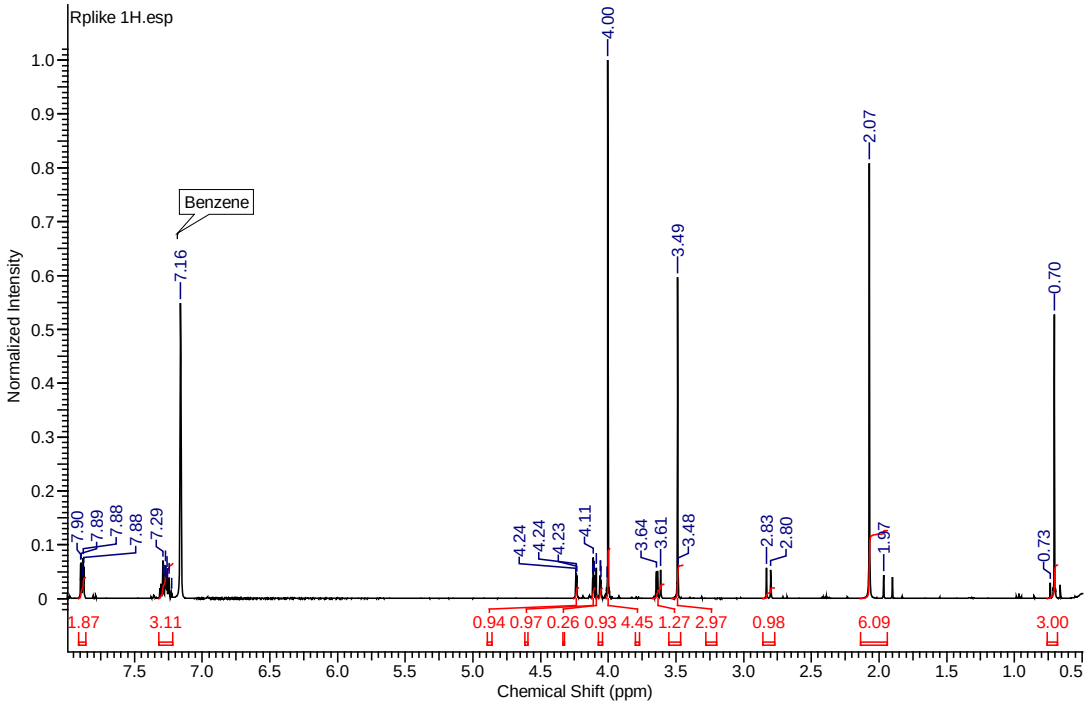


Figure 6: ^{1}H-NMR spectrum of **(R_p-*like*)-3**.

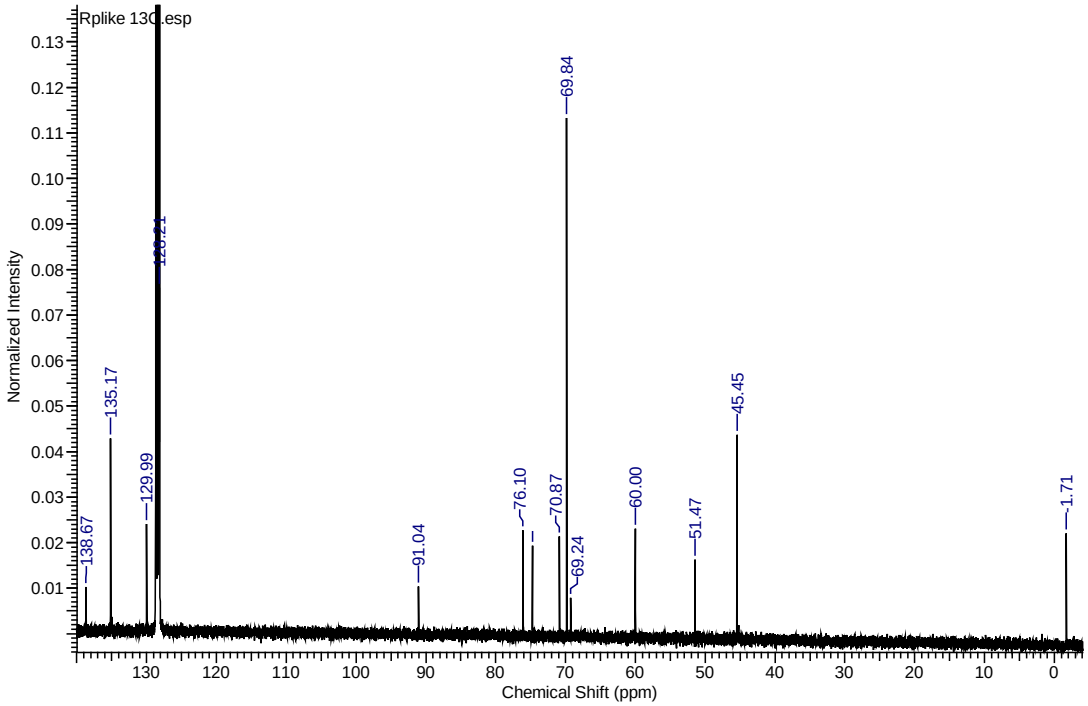


Figure 7: ^{13}C-NMR spectrum of **(R_p-*like*)-3**.

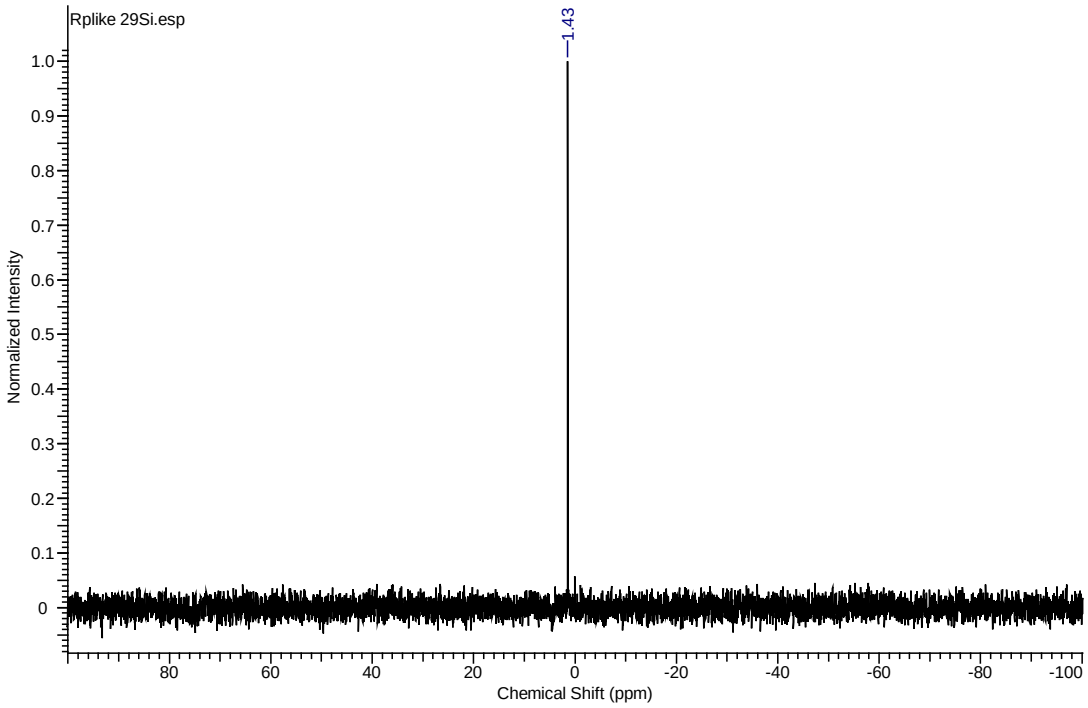


Figure 8: ^{29}Si-NMR spectrum of **(R_p-*like*)-3**.

The enantiomeric purity of **(R_p-*like*)-3** was determined by the addition of (*R*)-anthryltrifluorethanol to the ^{1}H-NMR samples of **(R_p-*like*)-3** and **(*rac*-*like*)-3** and comparison of their spectra as well as the spectrum of the remixed samples.

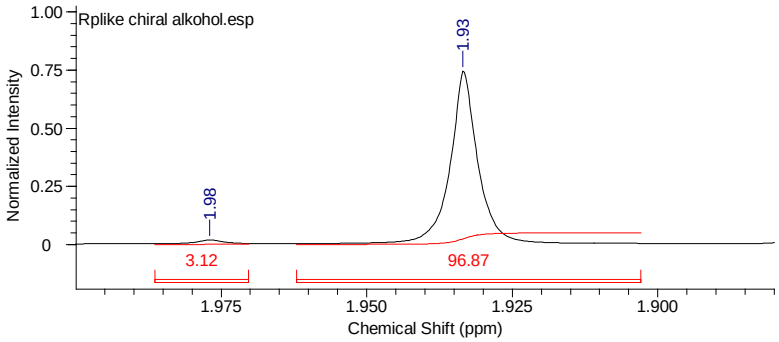


Figure 9: ^{1}H-NMR spectrum of **(R_p-*like*)-3** with (*R*)-anthryltrifluorethanol. Integration of the diastereomeric ^{1}H-NMR signals caused by the NCH_3 groups to quantify the *e.r.* value.

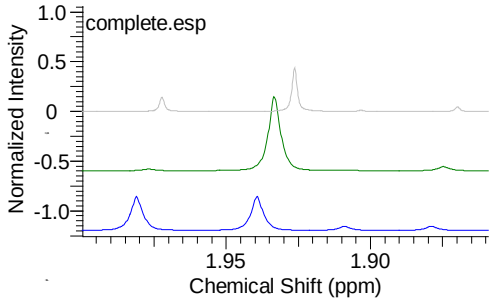
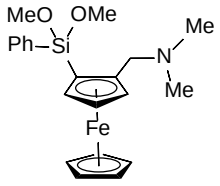


Figure 10: ^{1}H-NMR spectra of **(R_p-*like*)-3** with (*R*)-anthryltrifluorethanol (green), **(*rac*-*like*)-3** with (*R*)-anthryltrifluorethanol (blue), as well as a 1:1 mixture of them both (grey). The extract shows the signals caused by the diastereomeric NCH_3 groups.

2.3 Synthesis of 5



5

Compound **5** was prepared according to a procedure from our group.[2]

^{1}H-NMR	(400.25 MHz, C_6D_6): δ = 2.09 [s, 6H; N(CH_3)$_2$], 2.84 (AB-system, 1H, $^2J_{HH}$ = 12.29; CpCH_2N), 3.59 [s, 3H; SiOCH_3], 3.62 [s, 3H; SiOCH_3], 3.71 (AB-system, 1H, $^2J_{HH}$ = 12.29; CpCH_2N), 4.06 (s, 5H; Cp-CH), 4.11-4.13 (m, 1H; Cp-CH), 4.18–4.20 (m, 1H; Cp-CH), 4.24–4.25 (m, 1H; Cp-CH), 7.24–7.30 (m, 3H; Ph-$H_{ortho,para}$), 7.99–8.01 (m, 2H; Ph-H_{meta}) ppm.
{^{1}H}^{13}C-NMR	(100.6 MHz, C_6D_6): δ = 45.5 [2C; N(CH_3)$_2$], 51.3 [1C; SiOCH_3], 51.5 [1C; SiOCH_3], 59.8 (1C; CpCH_2N), 66.0 (1C; Cp-CSi), 70.1 (5C; Cp-CH), 71.1 (1C; Cp-CH), 74.7 (1C; Cp-CH), 76.2 (1C; Cp-CH), 91.2 (1C; Cp-CCH$_2$N), 128.3 (2C; Ph-C_{meta}), 130.5 (1C; Ph-C_{para}), 135.4 (1C; Ph-C_{ipso}), 135.8 (2C; Ph-C_{ortho}) ppm.
{^{1}H}^{29}Si-NMR	(79.52 MHz, C_6D_6): δ = –23.19 [s, 1Si; SiPh(OMe)$_2$] ppm.
GC/EI-MS:	t_R = 7.65 min [80 °C (1 min) – 40 °C·min^{-1} – 270 °C (5.5 min)]; m/z (%): 409 (100) [M$^+$], 394 (2) [(M-Me)$^+$], 365 (15) [(M-NMe$_2$)$^+$], 333 (58) [(M-CH$_2$NMe$_3$)$^+$], 242 (60) [(M-PhSi(OMe)$_2$)$^+$], 121 (21) [FeCp$^+$].

CHN-Analysis:			
calculated:	C: 61.61%	H: 6.65%	N: 3.42%
measured:	C: 61.6%	H: 6.5%	N: 3.5%

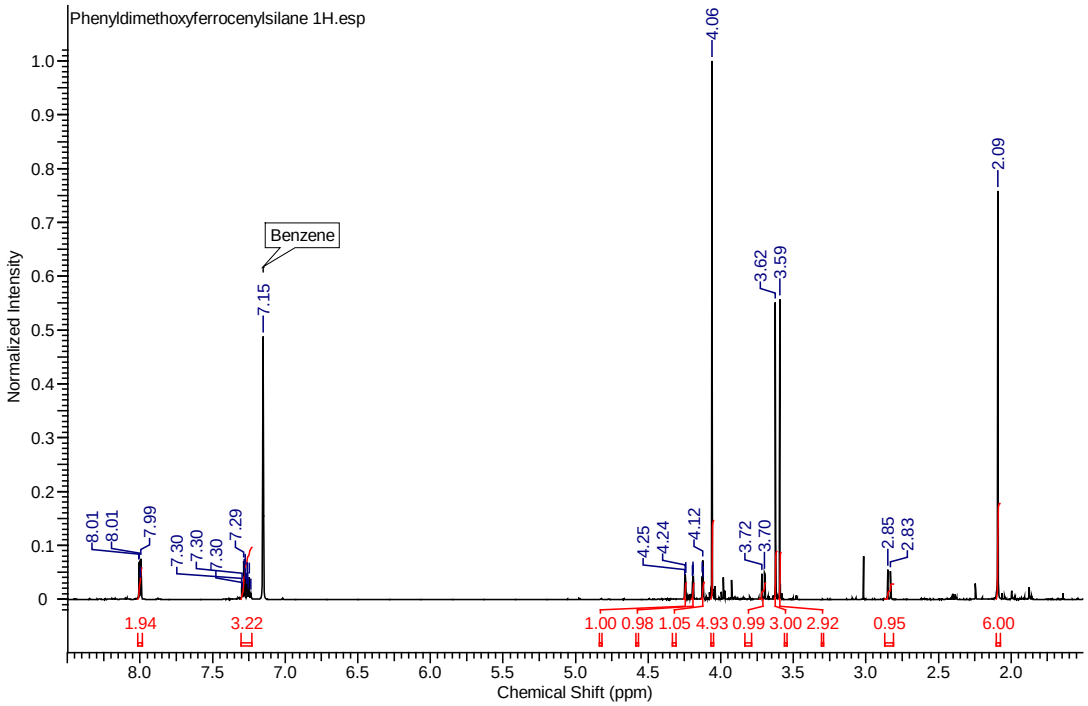


Figure 11: ^{1}H-NMR spectrum of **5.**

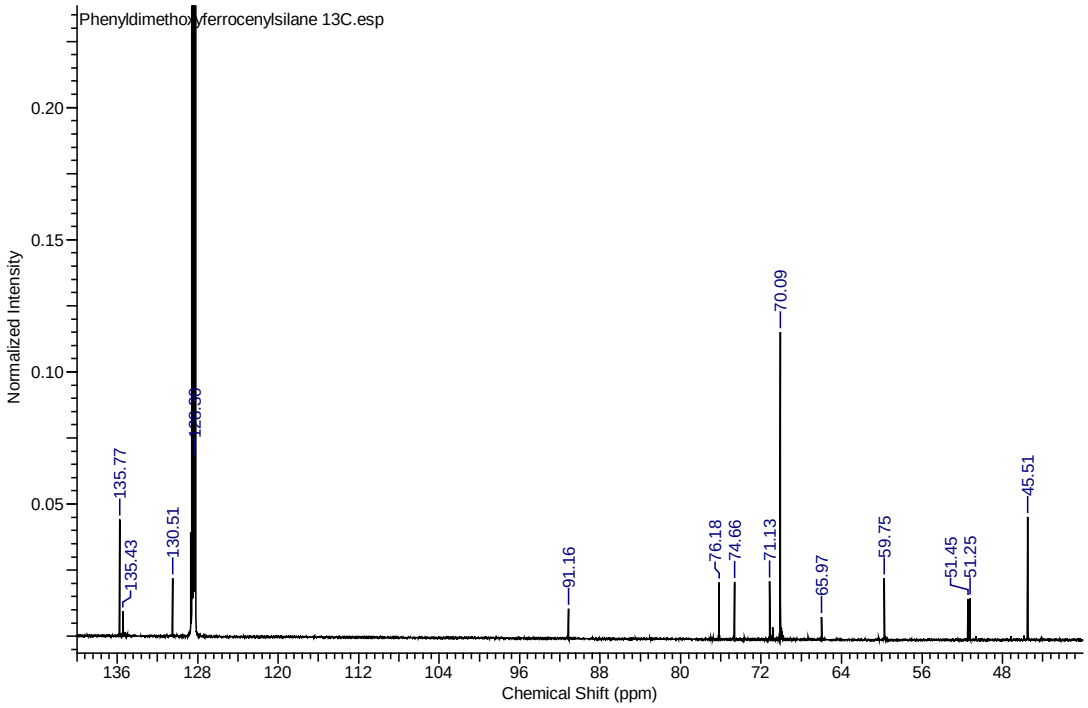


Figure 12: ^{13}C-NMR spectrum of **5.**

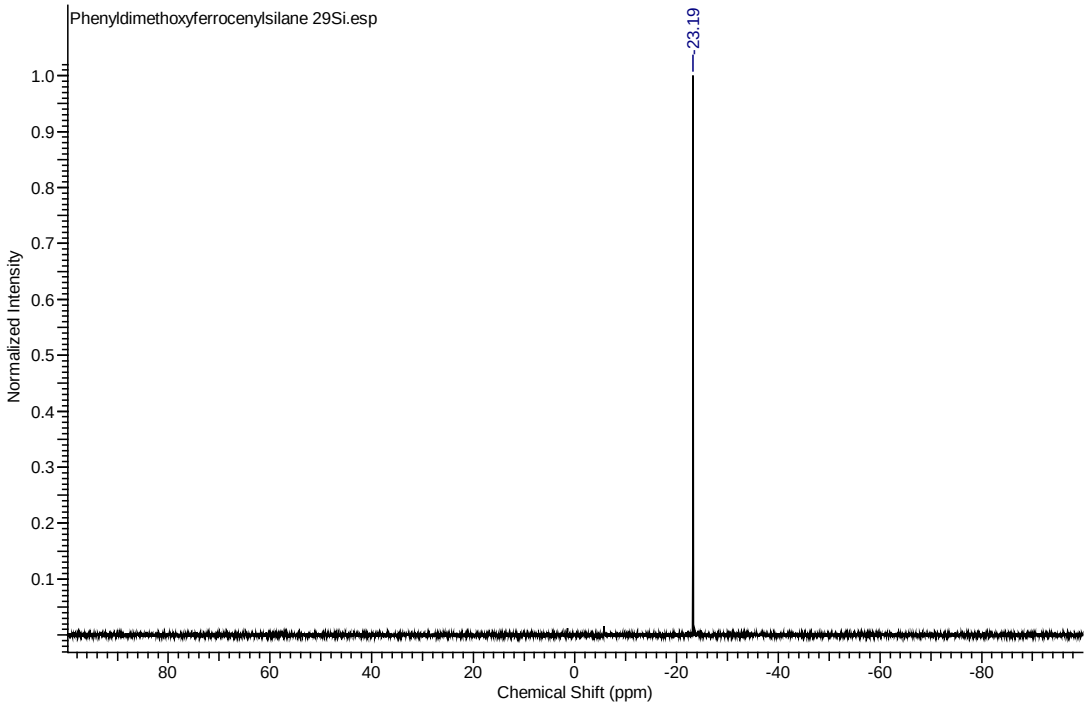
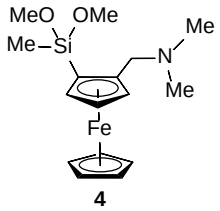


Figure 13: ^{29}Si-NMR spectrum of **5.**

2.4 Synthesis of 4



4

Compound **4** was prepared according to a procedure from our group.[2]

^{1}H-NMR	(400.25 MHz, C_6D_6): δ = 0.47 [s, 3H; SiCH_3], 2.12 [s, 6H; N(CH_3)$_2$], 2.87 (AB-system, 1H, $^{2}J_{HH}$ = 12.23; CpCH_2N), 3.53 [s, 3H; SiOCH_3], 3.55 [s, 3H; SiOCH_3], 3.74 (AB-system, 1H, $^{2}J_{HH}$ = 12.23; CpCH_2N), 4.08 (s, 5H; Cp-CH), 4.13–4.15 (m, 1H; Cp-CH), 4.20–4.22 (m, 1H; Cp-CH), 4.23–4.25 (m, 1H; Cp-CH) ppm.
{^{1}H}^{13}C-NMR	(100.6 MHz, C_6D_6): δ = –3.0 (1C; SiCH_3), 45.5 [2C; N(CH_3)$_2$], 51.7 [1C; Si(OCH_3)$_2$], 50.8 [1C; Si(OCH_3)$_2$], 60.0 (1C; CpCH_2N), 67.0 (1C; Cp-CSi), 70.0 (5C; Cp-CH), 70.8 (1C; Cp-CH), 74.5 (1C; Cp-CH), 75.5 (1C; Cp-CH), 91.1 (1C; Cp-CCH$_2$N) ppm.
{^{1}H}^{29}Si-NMR	(79.52 MHz, C_6D_6): δ = –9.56 [s, 1Si; Si(OMe)$_2$] ppm.
GC/EI-MS	t_R = 5.86 min [80 °C (1 min) – 40 °C·min^{-1} – 270 °C (5.5 min)]; m/z (%): 347 (100) [M$^+$], 303 (44) [(M-NMe$_2$)$^+$], 273 (73) [(M-CH$_2$NMe$_3$)$^+$], 242 (89) [(M-MeSi(OMe)$_2$)$^+$], 121 (31) [FeCp$^+$].

CHN-Analysis:				
	calculated:	C: 55.33%	H: 7.26%	N: 4.03%
	measured:	C: 55.3%	H: 7.1%	N: 3.9%

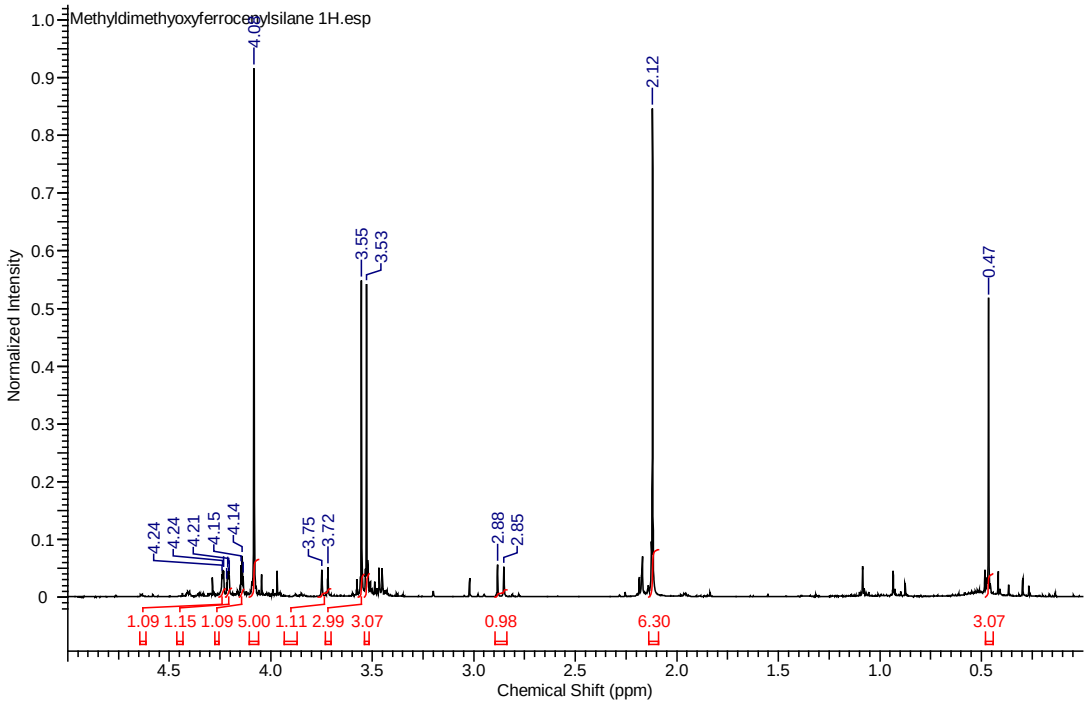


Figure 14: ^{1}H-NMR spectrum of **4**.

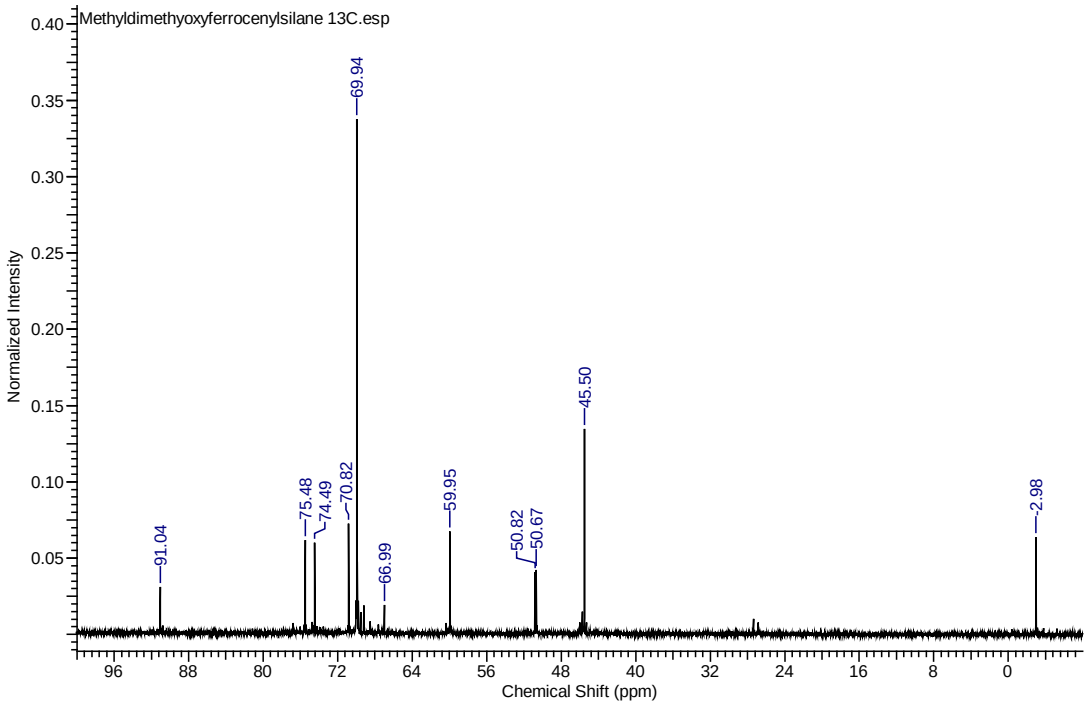


Figure 15: ^{13}C-NMR spectrum of **4**.

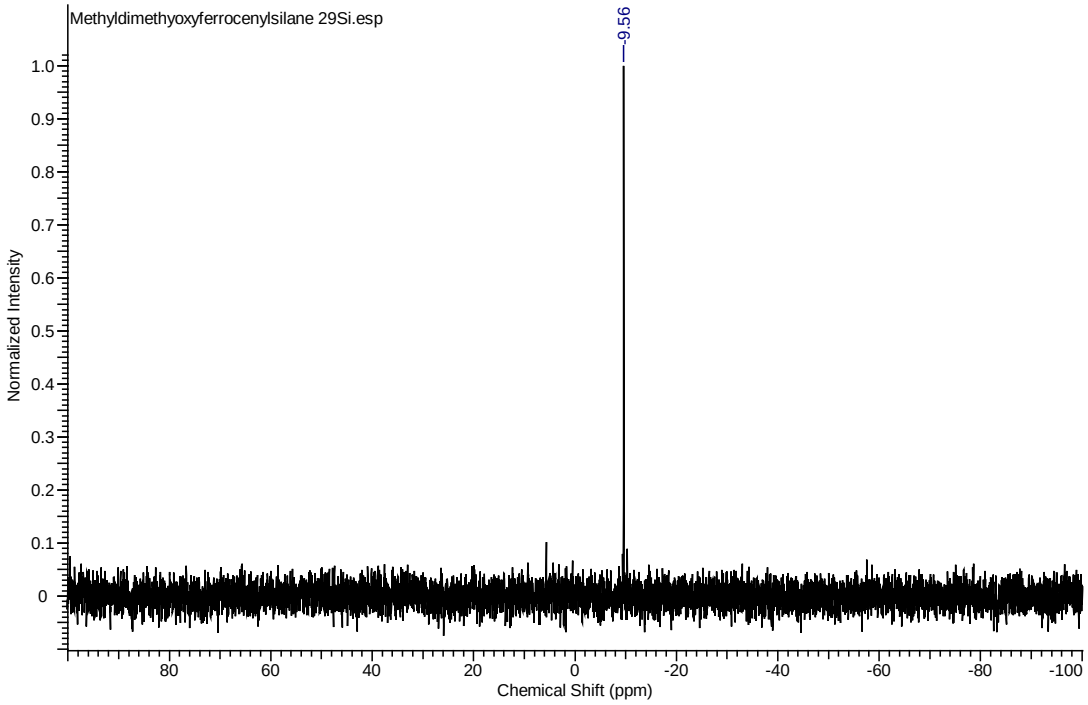
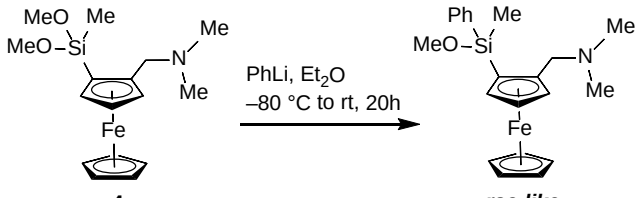


Figure 16: ^{29}Si-NMR spectrum of **4**.

2.5 Stereodivergent synthesis of (*rac-like*)-3



4 **(*rac-like*)-3**
d.r. > 99:1

To a stirred solution of methyldimethoxyferrocenylsilane (**4**) (241 mg, 0.69 mmol, 1.0 eq) in Et_2O (7 mL) at –80 °C PhLi (1.9 M in Bu_2O, 0.36 mL, 0.69 mmol, 1.0 eq) was added. The reaction mixture was allowed to warm to room temperature and stirred for further 20 h. After the reaction was stopped by adding H_2O (ca. 5 mL), the organic layer was separated and the auqeous layer was extracted with Et_2O (3 x 5 mL). The combined organic layers were dried with Na_2SO_4 and the solvent removed. The crude product was purified by column chromatography (*n*pentane/Et_2O = 5/1 + 10% Vol. Et_3N). The resulting highly viscous red brown oil yielded in 119 mg (0.30 mmol, 44%) of methoxyferrocenylsilane **(*rac-like*)-3**.

The spectroscopic data correspond to **(*rac-like*)-3**. The diastereomeric ratio was determined from the 1H NMR of the crude product.

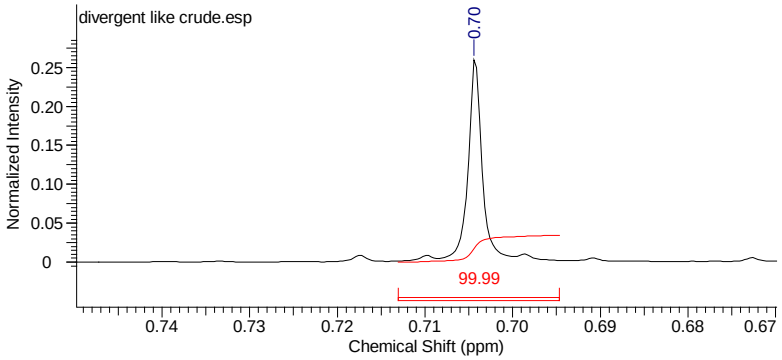
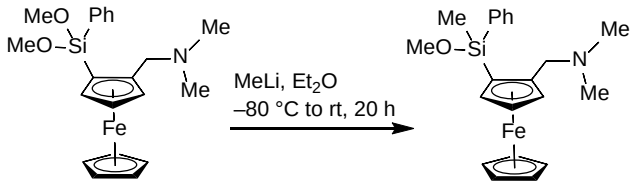


Figure 17: Integration of the diastereomeric ^{1}H-NMR signals caused by the $SiCH_3$ groups to quantify the *d.r.* value.

2.6 Stereodivergent synthesis of (*rac-unlike*)-3



5 **(*rac-unlike*)-3**
d.r. = 96:4

To a stirred solution of phenyldimethoxyferrocenylsilane (**5**) (265 mg, 0.65 mmol, 1.0 eq) in Et_2O (5 mL) at –80 °C MeLi (1.6 M in Et_2O, 0.40 mL, 0.65 mmol, 1.0 eq) was added. The reaction mixture was allowed to warm to room temperature and stirred for further 20 h. After the reaction was stopped by adding H_2O (ca. 5 mL), the organic layer was separated and the auqeous layer was extracted with Et_2O (3 x 5 mL). The combined organic layers were dried with Na_2SO_4 and the solvent removed. The crude product was purified by column chromatography (*n*pentane/Et_2O = 5/1 + 10% Vol. Et_3N). The resulting highly viscous red brown oil yielded in 126 mg (0.32 mmol, 49%) of methoxyferrocenylsilane **(*rac-unlike*)-3**.

The diastereomeric ratio was determined from the ^{1}H-NMR of the crude product.

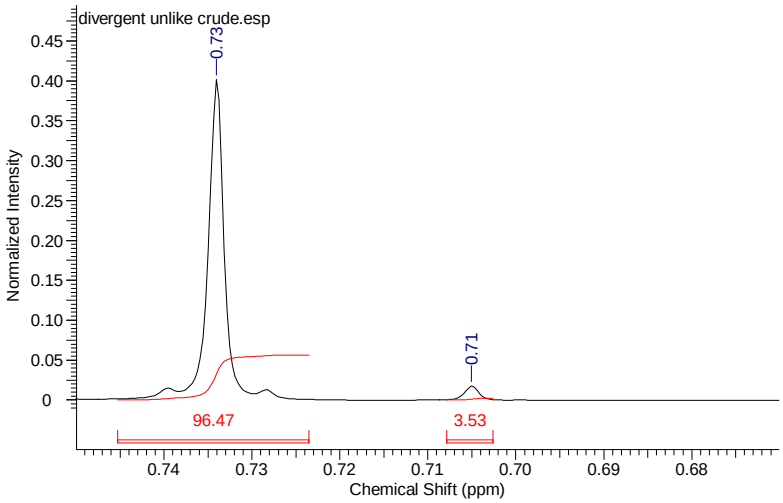


Figure 18: Integration of the diastereomeric ^{1}H-NMR signals caused by the $SiCH_3$ groups to quantify the *d.r.* value.

^{1}H-NMR	(400.25 MHz, C_6D_6): δ = 0.73 (s, 3H; SiCH_3), 1.97 [s, 6H; N(CH_3)$_2$], 2.70, (AB-system, $^{2}J_{HH}$ =12.23, 1H; CpCH_2N), 3.48 (s, 3H; OCH_3), 3.63 (AB-system, $^{2}J_{HH}$ =12.23, 1H; CpCH_2N), 4.09 (s, 5H; Cp-C*H*), 4.10-4.12 (m, 1H; Cp-C*H*), 4.13–4.15 (m, 1H; Cp-C*H*), 4.18–4.20 (m, 1H; Cp-C*H*), 7.23–7.29 (m, 3H; Ph-$H_{ortho,para}$), 7.78–7.82 (m, 2H; Ph-H_{meta}) ppm.
{^{1}H}^{13}C-NMR	(100.6 MHz, C_6D_6): δ = –2.0 (1C; SiCH_3), 45.2 [2C; N(CH_3)$_2$], 51.4 (1C; OCH_3), 60.0 (1C; CpCH_2N), 69.6 (1C, SiCCCH$_2$), 69.9 (5C; Cp-*C*H), 70.5 (1C; Cp-*C*H), 74.5 (1C; Cp-*C*H), 76.1 (1C, Cp-*C*H), 91.0 (1C, Cp-*C*CH$_2$N), 128.3 (2C; Ph-C_{meta}), 129.9 (1C; Ph-C_{para}), 134.9 (2C; Ph-C_{ortho}), 138.7 (1C; Ph-C_{ipso}) ppm.
{^{1}H}^{29}Si-NMR	(79.52 MHz, C_6D_6): δ = 1.47 (s, 1Si; *Si*MePh) ppm.
GC/EI-MS	t_R = 7.46 min [80 °C (1 min) – 40 °C·min^{-1} – 270 °C (5.5 min)]; m/z (%): 393 (100) [M$^+$], 349 (8) [(M-NMe$_2$)$^+$], 317 (69) [(M-Ph)$^+$], 242 (90) [(M-PhMeSiOMe)$^+$], 121 (49) [(FeCp)$^+$].

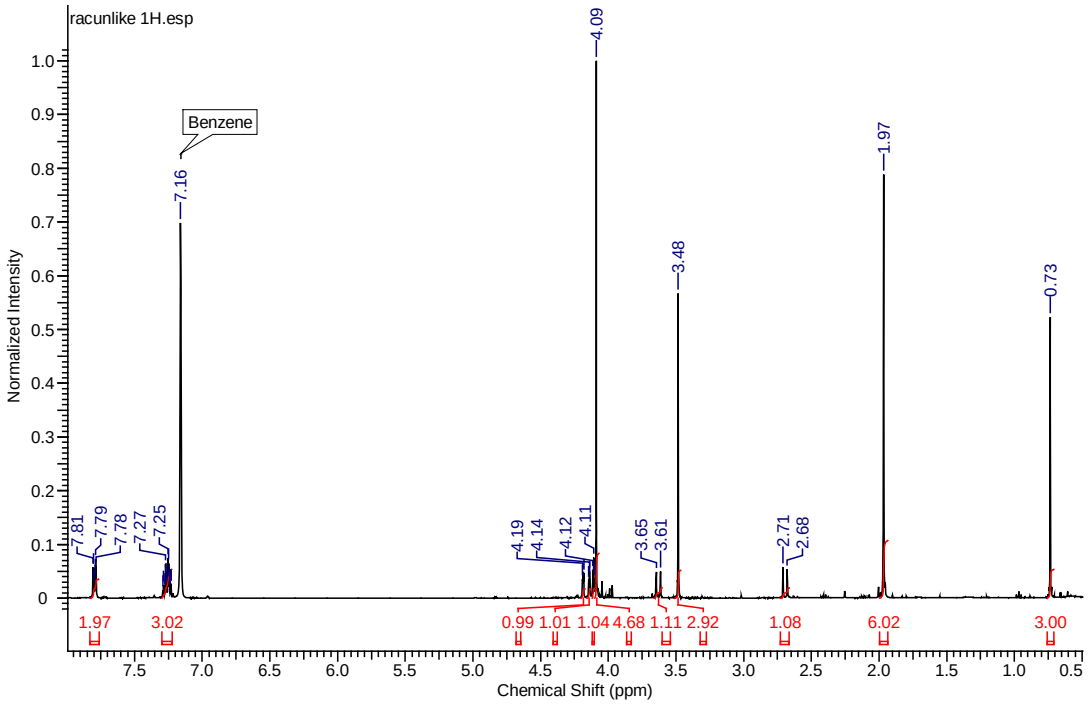


Figure 19: ^{1}H-NMR spectrum of ***(rac-unlike)*-3**.

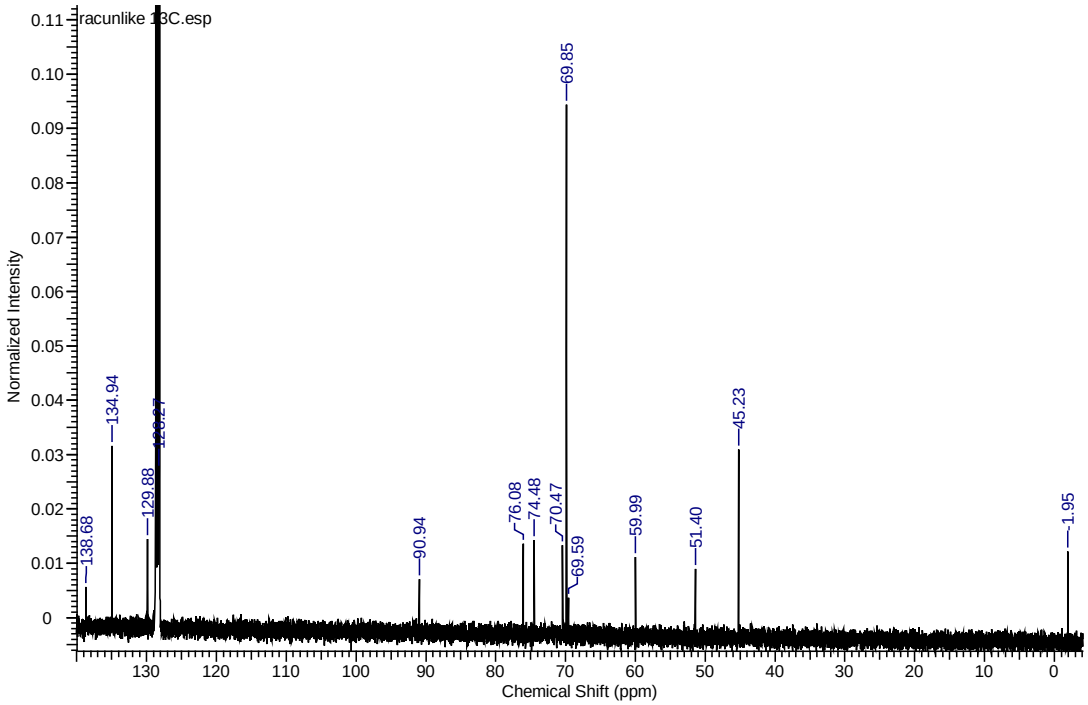


Figure 20: ^{13}C-NMR spectrum of **(*rac-unlike*)-3**.

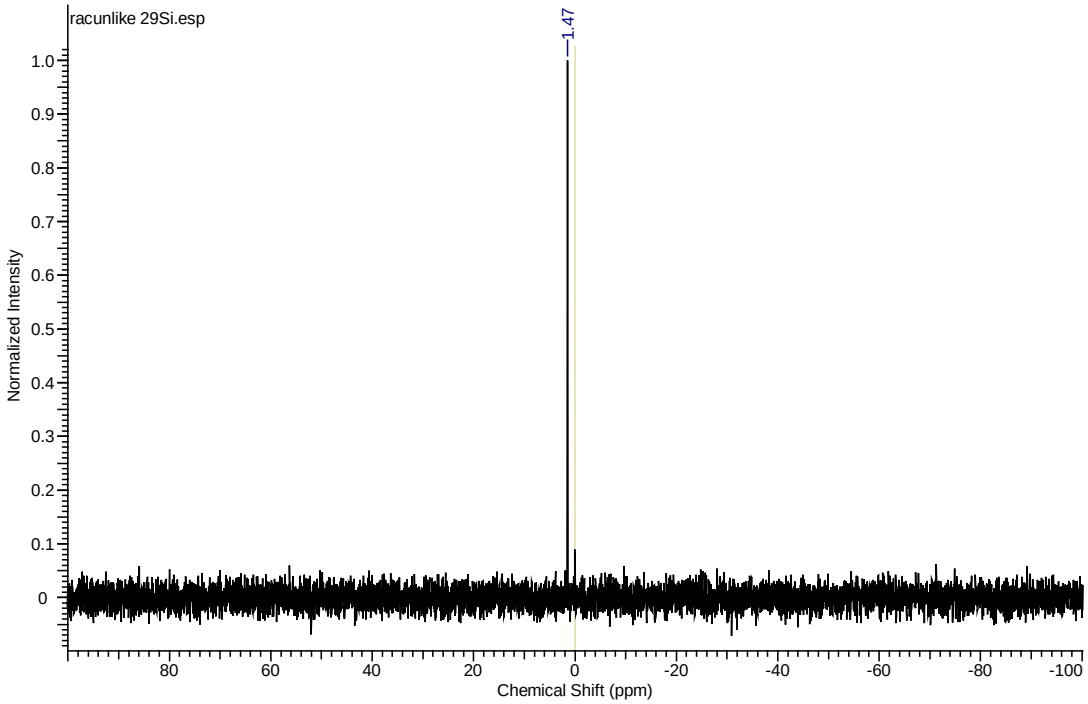


Figure 21: ^{29}Si-NMR spectrum of **(*rac-unlike*)-3**.

3 Single-Crystal X-ray Diffractional Analysis of (R_p,R_{Si})-3 and Determination of the Configurations of the Diastereomers

Data collection was conducted on *Bruker D8 Venture* four-circle diffractometer by *Bruker AXS GmbH* using a *PHOTON II* CPAD detector by *Bruker AXS GmbH.* X-ray radiation was generated by microfocus sources *IμS 3.0* Mo (λ = 0.71073) by *Incoatec GmbH* with HELIOS mirror optics and a single-hole collimator by *Bruker AXS GmbH*.
For the data collection, the programs APEX 3 Suite (v.2017.3-0) with the integrated programs SAINT (integration) and SADABS (adsorption correction) by Bruker AXS GmbH were used. Using Olex2[3], the structures were solved with the ShelXT[4] structure solution program using Intrinsic Phasing and refined with the XL[5] refinement package using Least Squares minimization. Crystallographic data have been deposited at the CCDC (Cambridge Crystallographic Data Centre). These data can be obtained free of charge from the CCDC, Union Road, Cambridge, CB2 IEZ, UK (Fax: +44-1223-336033; e-mail: deposit@ccdc.cam.ac.uk or www: http://www.ccdc.cam.ac.uk). CCDC deposition number is 1900067.

Table 1: Crystal data and structure refinement for **(R_pR_{Si})-3**.

Compound	**(R_p,R_{Si})-3**
Empirical formula	$C_{21}H_{27}FeNOSi$
Formula weight [g·mol^{-1}]	393.37
Temperature [K]	100.0
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	7.5129(8)
b/Å	10.4560(7)
c/Å	24.907(2)
α/°	90
β/°	90
γ/°	90
Volume [Å^3]	1956.6(3)
Z	4
Density (calculated) ρ [g·cm^{-3}]	1.335
Absorption coefficient μ [mm^{-1}]	0.840
F(000)	832.0
Crystal size [mm^3]	0.577 × 0.512 × 0.346
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.664 to 69.996
Index ranges	-11 ≤ h ≤ 12, -15 ≤ k ≤ 16, -40 ≤ l ≤ 39
Reflections collected	38690
Independent reflections	8597 [R_{int} = 0.0249, R_{sigma} = 0.0203]
Data/restraints/parameters	8597/0/230
Goodness-of-fit on F^2	1.083
Final R indexes [I > 2σ (I)]	R_1 = 0.0238, wR_2 = 0.0626
Final R indexes [all data]	R_1 = 0.0241, wR_2 = 0.0627
Largest diff. peak and hole [e·Å^{-3}]	0.81/-0.45
Flack parameter	0.002(3)

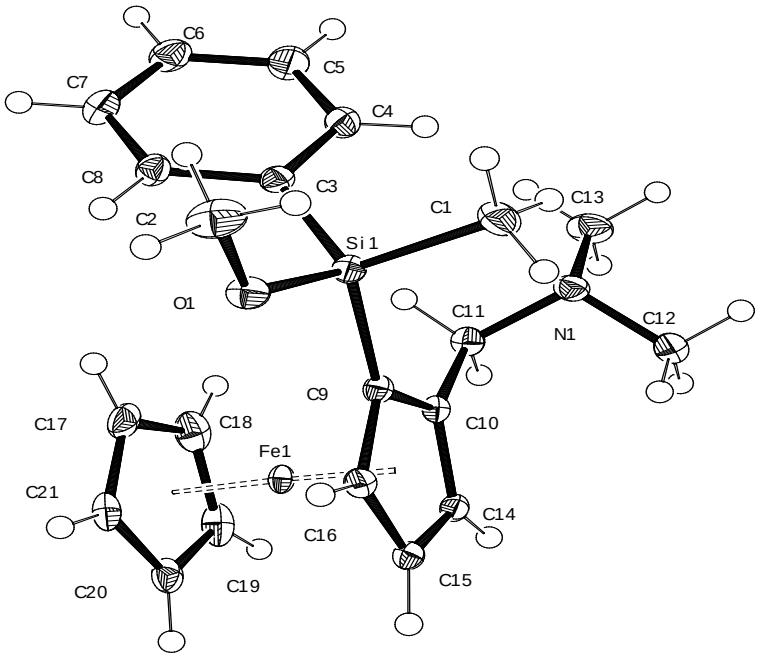


Figure 22: Ortep[6] plot of the molecular structure of **(R_pR_{Si})-3** in the crystal, with displacement ellipsoids drawn at the 50% probability level. Numbering scheme of hydrogen atoms omitted for clarity. Selected bondlengths [Å] and –angles [°]:Si1–C1 1.8610(16), Si1–C3 1.8801(14), Si1–C9 1.8473(13), O1–C2 1.4166(19), C9–C10 1.4457(18), C9–C16 1.4431(18), C10–C14 1.4305(18), C14–C15 1.4263(18), N1–C12 1.460(2), O1–Si1–C1 110.67(7), C9–Si1–C1 108.23(7), C12–N1–C13 109.64(13), C16–C15–C14 107.96(11).

Comparison of the retention times of the measured crystal with the diastereomeric mixture in the gas chromatogram shows, that (R_p,R_{Si})-*like* configuration determined from the crystal structure corresponds to the major diastereomer. As the crystallization took place from the substance, small adhesions of the minor diastereomer remained at the measured one and lead to the low peak in the gas chromatogram.

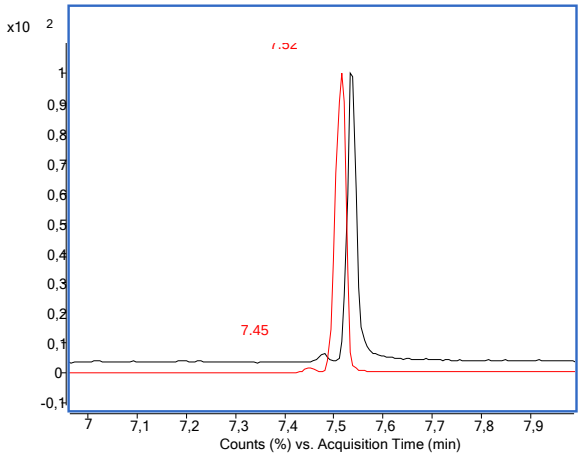


Figure 23: Overlay of the gas chromatograms of the measured **(R_p,R_{Si})-3** crystal (red curve) and the mixture from the synthesis (black courve).

4 Quantum Chemical Calculations

Optimization and additional harmonic vibrational frequency analyses were performed with the software package Gaussian 09 (Revision E.01)[7]. The GJF input files were created with the program GaussView 5.0. The ground state structures were optimized without symmetry restrictions. Vibrational frequency analysis was used to confirm the characteristics of ground states and transition states. The calculated standard orientations of the optimized structures can be found in Tables 3–40. The visualization of the optimized structures was performed with the program Molekel[8] V. 4.3 (Figures 25–36).

4.1 Comparison of the possible starting structures according to the different precoordination patterns

The precoordination of the MeLi dimer should be possible either in a bidentate pattern, or in a monodentate one. In case of a bidentate coordination one Li center can be addressed by both OMe groups. Furthermore both Li can have a contact to one OMe respectively. The figure below show these precoordinations and the resulting trajectories for the nucleophilic attack of a methanide to the silicon center. The bidentate versions go along with the formation of many small rings, long moving distances for the methanide and hinderence for a clear backside attack. Thus, the monodentate precoordination was used as starting structure for the calculation of the substitution mechanism.

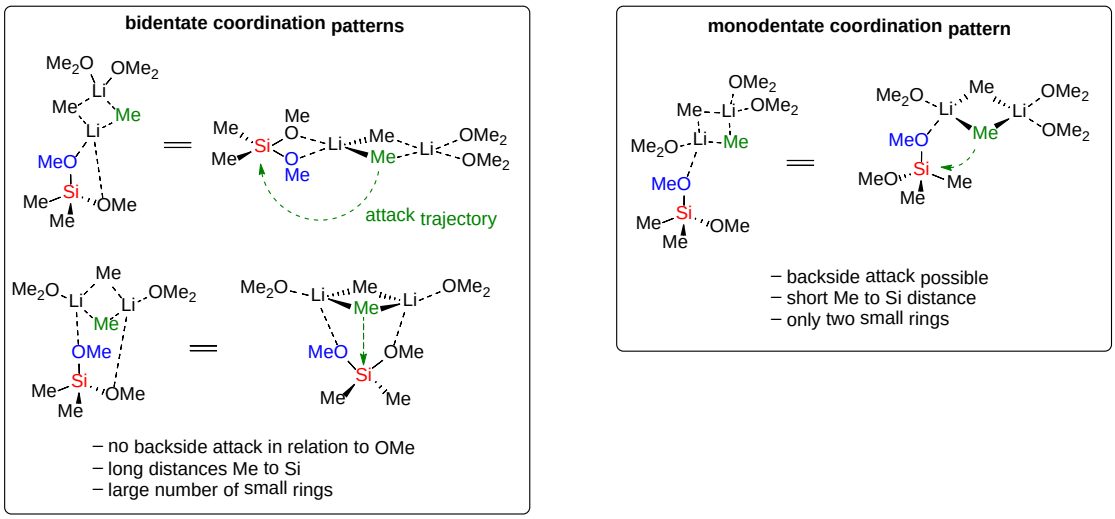


Figure 24: Precoordination patterns of dimethyldimethoxysilane to a MeLi dimer and the resulting possibilities for nucleopihilic attack.

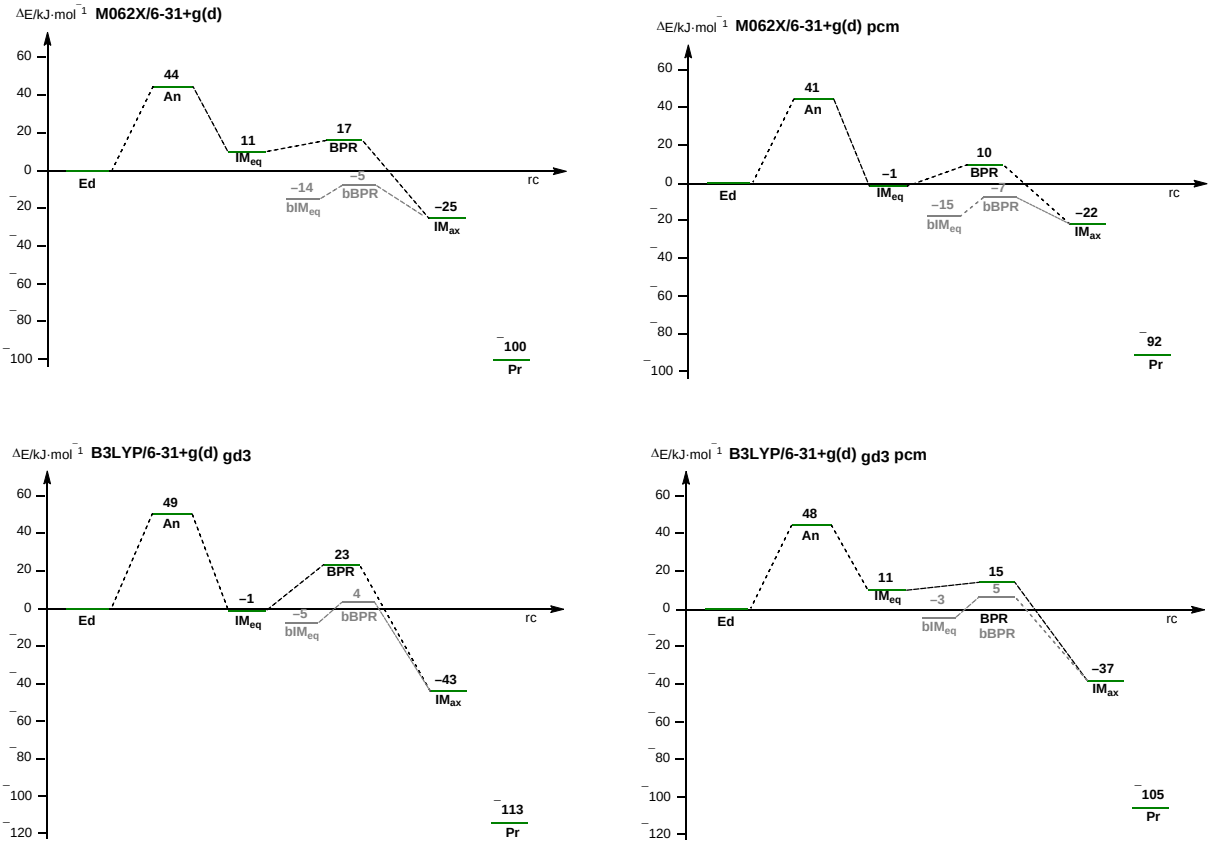
4.1 Overview of all calculated stationary points

Table 2: Total (SCF) and zero-point-corrected (ZPE) energies of the optimized structures. [a]: In order to avoid numerical artifacts, the integration mesh was set to ultrafine; [b]: The polar environment was described with a polarizable continuum of diethyleter; [c]: Calculations were done with the use of empirical dispersion correction (gd3).

Block	Optimized structure	Method/Basis	SCF [Hartree]	ZPE [Hartree]
Diastereomers of **3**	**like**	M062X/6-31+G(d)[a]	–2499.11766160	–2498.679625
	unlike	M062X/6-31+G(d)[a]	–2499.11795529	–2498.680119
Mechanism M062X	**Ed**	M062X/6-31+G(d)	–1159.26382151	–1158.779692
	At	M062X/6-31+G(d)	–1159.24939442	–1158.763078
	IM$_{eq}$	M062X/6-31+G(d)	–1159.26320212	–1158.775598
	bIM$_{eq}$	M062X/6-31+G(d)	–1159.27200503	–1158.785038
	BPR	M062X/6-31+G(d)	–1159.26031304	–1158.773208
	bBPR	M062X/6-31+G(d)	–1159.26965448	–1158.78167
	IM$_{ax}$	M062X/6-31+G(d)	–1159.27672587	–1158.789196
	Pr	M062X/6-31+G(d)	–1159.30425033	–1158.817590
Mechanism M062X pcm	**Ed**	M062X/6-31+G(d)[b]	–1159.27282822	–1158.789399
	At	M062X/6-31+G(d)[b]	–1159.2589575	–1158.773748
	IM$_{eq}$	M062X/6-31+G(d)[b]	–1159.27660864	–1158.789905

	bIM$_{eq}$	M062X/6-31+G(d)[b]	–1159.28072073	–1158.795091
	BPR	M062X/6-31+G(d)[b]	–1159.27269962	–1158.785705
	bBPR	M062X/6-31+G(d)[b]	–1159.27867452	–1158.791989
	IM$_{ax}$	M062X/6-31+G(d)[b]	–1159.28477428	–1158.79786
	Pr	M062X/6-31+G(d)[b]	–1159.30967163	–1158.824335
Mechanism B3LYP	**Ed**	B3LYP/6-31+G(d)[c]	–1159.80045462	–1159.322876
	At	B3LYP/6-31+G(d)[c]	–1159.78420369	–1159.30419
	IM$_{eq}$	B3LYP/6-31+G(d)[c]	–1159.80417809	–1159.323242
	bIM$_{eq}$	B3LYP/6-31+G(d)[c]	–1159.80662244	–1159.324911
	BPR	B3LYP/6-31+G(d)[c]	–1159.79472913	–1159.314109
	bBPR	B3LYP/6-31+G(d)[c]	–1159.80227427	–1159.321472
	IM$_{ax}$	B3LYP/6-31+G(d)[c]	–1159.82022657	–1159.339229
	Pr	B3LYP/6-31+G(d)[c]	–1159.844911	–1159.365799
Mechanism B3LYP pcm	**Ed**	B3LYP/6-31+G(d)[b,c]	–1159.81016125	–1159.333445
	At	B3LYP/6-31+G(d)[b,c]	–1159.7942394	–1159.315352
	IM$_{eq}$	B3LYP/6-31+G(d)[b,c]	–1159.81012741	–1159.329436
	bIM$_{eq}$	B3LYP/6-31+G(d)[b,c]	–1159.81587693	–1159.334745
	BPR	B3LYP/6-31+G(d)[b,c]	–1159.80844712	–1159.327906
	bBPR	B3LYP/6-31+G(d)[b,c]	–1159.81168926	–1159.33169
	IM$_{ax}$	B3LYP/6-31+G(d)[b,c]	–1159.82740635	–1159.34741
	Pr	B3LYP/6-31+G(d)[b,c]	–1159.85104051	–1159.373335
Nucleophilic attack M062X	**EdFc**	M062X/6-31+G(d)	–2787.47915634	–2786.847693
	AnFc	M062X/6-31+G(d)	–2787.46487477	–2786.8323
Nucleophilic attack B3LYP	**EdFc**	B3LYP/6-31+G(d)[c]	–2788.29989508	–2787.676242
	AnFc	B3LYP/6-31+G(d)[c]	–2788.28199854	–2787.657387

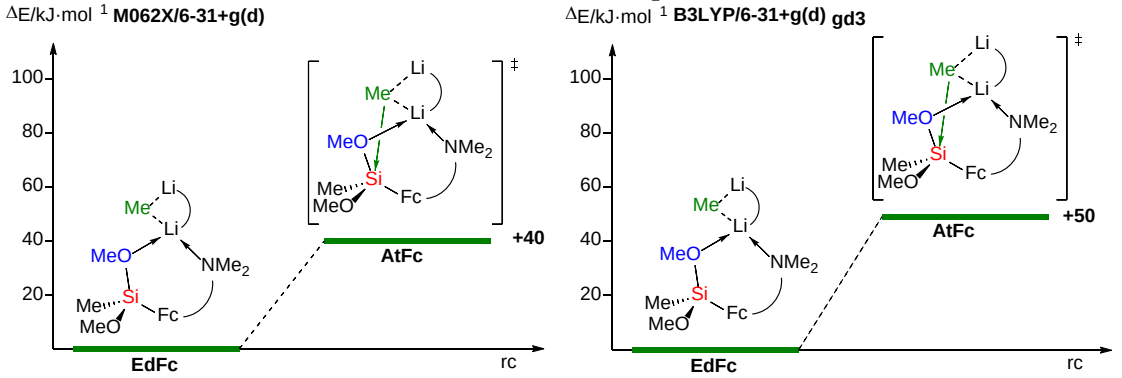
Reaction schemes for each theory level were created. Therefore the zero point corrected energies of all stationary points were convertet into relative energies regarding to the starting structure in kJ/mol.



Scheme 1: Reaction schemes of the calculated substitution of dimethyldimethoxysilane with a MeLi dimer with the use of different calculation methods.

The comparison of the reaction schemes point out, that both calculation methods (M062X, B3LYP plus dispersion correction) deliver the same results. There is no significant effect from the polar environment described as diethylether in a polarizable continuum on the relative energies of the stationary points.

To validate the fitting of the simplified model system to the ferrocenesilanes from the experiements, the rate determining step of the nucleophilic attack was calculated for a ferrocenic model system, too. The aminogroup replaces the coordinating ether molecule at the precoordinated Li center. The energy barriers are highly comparable to the corresponding steps of the simplified system for both methods (M062X and B3LYP plus dispersion correction gd3).



Scheme 2: Energy barriers for the nucleophilc attack of a MeLi dimer to the silicon center of a ferrocenic dimethoxysilane calculatet on M062X/6-31+g(d) and B3LYP/6-31+g(d) with dispersion correction gd3.

4.2 Visualization of the calculated molecular geometries

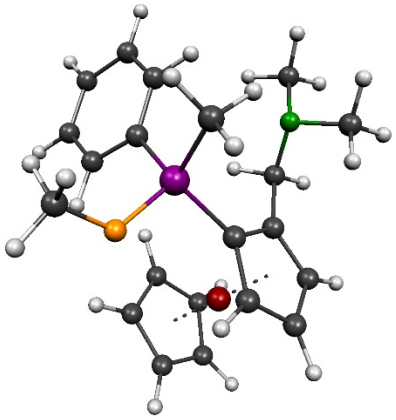


Figure 25 : Molekel plot of **like** [M062X/6-31+G(d)].

Table 3: Standard orientation of **like** [M062X/6-31+G(d)].

Atomic Symbol	x	y	z
Fe	2.149923	-0.032224	-0.203927
Si	-0.987641	-0.207922	1.465853
O	-0.405881	-1.534272	2.309342
N	-1.418073	2.541317	-0.535208
C	-2.085554	0.836433	2.569416
H	-3.005745	0.312054	2.851367
H	-2.364724	1.757035	2.045069
H	-1.551289	1.115695	3.484569
C	-1.289375	-2.39366	3.000593
H	-0.712376	-3.240105	3.381861
H	-2.079305	-2.776529	2.339277
H	-1.759559	-1.880396	3.849611

C	-1.995411	-0.876513	0.025577
C	-3.137387	-0.219735	-0.454425
H	-3.436083	0.725739	-0.006914
C	-3.887725	-0.748046	-1.504776
H	-4.7678	-0.220086	-1.863063
C	-3.510164	-1.954851	-2.092922
H	-4.092478	-2.368273	-2.911789
C	-2.389273	-2.635597	-1.618118
H	-2.097411	-3.58301	-2.063332
C	-1.646592	-2.100071	-0.566223
H	-0.78252	-2.646277	-0.191478
C	0.565637	0.695265	1.004802
C	0.793111	1.58571	-0.093107
C	-0.224615	1.94642	-1.136441
H	0.236512	2.635869	-1.872253
H	-0.549501	1.051242	-1.682911
C	-1.097811	3.735087	0.23284
H	-0.414205	3.485041	1.048796
H	-2.017253	4.145885	0.661815
H	-0.625334	4.517339	-0.391902
C	-2.393234	2.846691	-1.568328
H	-2.025887	3.616267	-2.273567
H	-3.31654	3.215395	-1.108983
H	-2.62617	1.940271	-2.135756
C	2.119865	2.082258	-0.001189
H	2.59081	2.74966	-0.713191
C	2.73382	1.501126	1.142292
H	3.760046	1.643154	1.455771
C	1.778702	0.655981	1.7624
H	1.946251	0.031827	2.631458
C	1.606402	-1.482279	-1.648499
H	0.605955	-1.549852	-2.057062
C	2.662174	-0.678843	-2.157568
H	2.607056	-0.033415	-3.024659
C	3.783962	-0.827711	-1.297477
H	4.732454	-0.315984	-1.394631
C	3.421522	-1.725665	-0.256888
H	4.043427	-2.013226	0.580557
C	2.076305	-2.128555	-0.471238
H	1.498038	-2.762306	0.188882

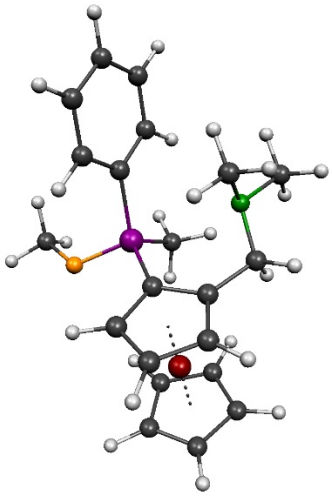


Figure 26: Molekel plot of **unlike** [M062X/6-31+G(d)].

Table 4: Standard orientation of **unlike** [M062X/6-31+G(d)].

Atomic Symbol	x	y	z
Fe	-2.451087	-0.069006	0.36895
Si	0.811079	0.954435	-0.423082
O	0.480377	2.548855	-0.014774
N	1.186595	-2.137666	-0.580937
C	1.235996	3.609324	-0.560672
H	0.898808	4.541339	-0.099696
H	1.089863	3.686527	-1.646999
H	2.308387	3.483739	-0.358726
C	-0.360198	0.042119	0.691946
C	-0.766529	-1.32899	0.618621
C	-0.251332	-2.307632	-0.402792
H	-0.508465	-3.34147	-0.098246
H	-0.726608	-2.13363	-1.377358
C	1.924616	-2.48485	0.625696
H	1.567617	-1.885035	1.467268
H	2.98686	-2.265016	0.477586
H	1.810626	-3.555464	0.879631
C	1.676572	-2.89923	-1.714498
H	1.542529	-3.989388	-1.580961
H	2.744531	-2.699386	-1.850383
H	1.147923	-2.598671	-2.625698
C	-1.693761	-1.581115	1.661499
H	-2.200988	-2.521575	1.840703
C	-1.880254	-0.372488	2.389819
H	-2.55873	-0.229178	3.220874
C	-1.056845	0.619863	1.799873
H	-0.997466	1.661495	2.089807
C	-3.089149	1.33677	-1.078107
H	-2.465617	2.168397	-1.381102
C	-3.090721	0.033098	-1.647297
H	-2.479929	-0.301373	-2.476478
C	-3.997134	-0.769899	-0.903373
H	-4.196556	-1.821083	-1.06649
C	-4.556163	0.036276	0.125061
H	-5.254515	-0.293672	0.882797
C	-3.995731	1.338102	0.015127

H	-4.187476	2.17163	0.677738
C	2.615526	0.63882	-0.001217
C	3.06941	0.854813	1.307442
C	3.534509	0.159784	-0.944438
C	4.390846	0.589898	1.66777
H	2.375252	1.225148	2.061171
C	4.858892	-0.103736	-0.595857
H	3.208149	-0.028245	-1.966132
C	5.287733	0.107937	0.714852
H	4.720574	0.756739	2.689597
H	5.555246	-0.476359	-1.342569
H	6.317509	-0.100561	0.991583
C	0.509728	0.728267	-2.26188
H	-0.465075	1.147674	-2.533641
H	1.271558	1.247466	-2.855713
H	0.523904	-0.32793	-2.548821

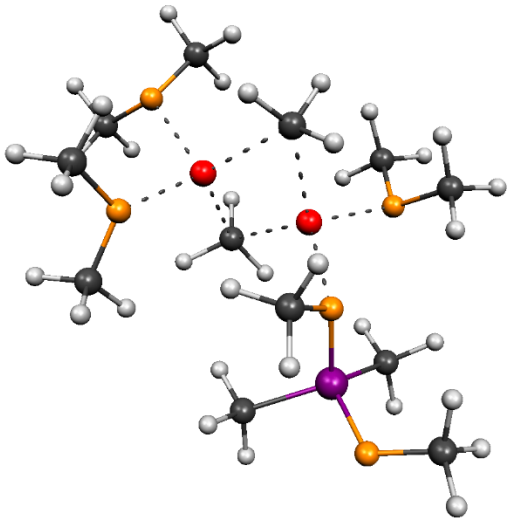


Figure 27: Molekel plot of **Ed** [M062X/6-31+G(d)].

Table 5: Standard orientation of **Ed** [M062X/6-31+G(d)].

Atomic Symbol	x	y	z
C	-1.277718	1.088987	1.871282
Li	0.057331	0.901161	0.175106
C	-0.940936	0.320538	-1.67158
Li	-1.968358	-0.044959	0.181889
O	1.592525	-0.248576	0.643
O	0.880199	2.646454	-0.020156
O	-3.860989	0.39463	-0.127981
O	-2.293991	-1.945973	0.471821
C	-1.772187	-3.018033	-0.283107
C	-3.234304	-2.347317	1.446347
C	-4.356101	-0.185201	-1.319661
C	-4.065576	1.795173	-0.081226
C	-0.048471	3.572471	-0.553113
C	1.434651	3.073771	1.210456
Si	2.60063	-0.697195	-0.628727
C	1.142492	-1.256599	1.551065
C	3.059269	0.881615	-1.499958

C	1.822568	-2.008561	-1.690197
O	3.938031	-1.420143	0.052075
C	4.751721	-0.722243	0.97459
H	-1.573697	2.156197	1.898078
H	-0.431791	1.023843	2.581509
H	-2.100436	0.57112	2.405217
H	-1.279953	-0.600691	-2.18377
H	-0.005799	0.586408	-2.200202
H	-1.658139	1.097685	-2.007255
H	-1.070938	-2.589046	-1.00057
H	-2.577381	-3.542322	-0.8171
H	-1.250973	-3.732597	0.369848
H	-4.093421	-2.841709	0.971042
H	-3.569539	-1.445912	1.960864
H	-2.772128	-3.036897	2.165316
H	-4.108666	-1.248712	-1.285758
H	-3.880112	0.267488	-2.199199
H	-5.445501	-0.058696	-1.380927
H	-3.534386	2.286264	-0.908354
H	-3.662417	2.145153	0.869868
H	-5.137812	2.024708	-0.146101
H	-0.41448	3.153216	-1.492221
H	0.441517	4.537844	-0.738662
H	-0.889528	3.711053	0.139683
H	2.020656	3.991366	1.063556
H	2.084094	2.268247	1.561813
H	0.643033	3.249884	1.950025
H	0.192641	-1.676446	1.200487
H	0.974134	-0.788605	2.522509
H	1.893213	-2.050422	1.650711
H	3.852813	0.688953	-2.230846
H	3.415874	1.636349	-0.790596
H	2.199611	1.311366	-2.022299
H	0.89674	-1.633529	-2.13828
H	1.593326	-2.899968	-1.094874
H	2.505156	-2.311959	-2.490971
H	4.158506	-0.321577	1.808052
H	5.280974	0.106937	0.487594
H	5.490434	-1.421614	1.373544

Table 6: Standard orientation of **Ed** [M062X/6-31+G(d) pcm].

Atomic Symbol	x	y	z
C	-1.238187	1.047775	1.904763
Li	0.072621	0.890349	0.183105
C	-0.935223	0.325031	-1.667147
Li	-1.970844	-0.06318	0.194454
O	1.606865	-0.27047	0.63736
O	0.830396	2.66365	-0.020688
O	-3.850749	0.426551	-0.122096
O	-2.316186	-1.959236	0.47977
C	-1.834359	-3.03493	-0.300939
C	-3.290067	-2.353615	1.427292
C	-4.38573	-0.190178	-1.279717
C	-4.050469	1.829326	-0.119378
C	-0.132909	3.585914	-0.500211
C	1.459652	3.105544	1.169389

Si	2.63732	-0.689697	-0.627816
C	1.130546	-1.317804	1.489379
C	3.104289	0.907144	-1.458688
C	1.865624	-1.980966	-1.71847
C	3.970647	-1.4241	0.052868
C	4.771881	-0.731726	0.997236
H	-1.603744	2.091191	1.959436
H	-0.326265	1.037124	2.532152
H	-1.974327	0.458194	2.486981
H	-1.237395	-0.612781	-2.170801
H	0.005732	0.619029	-2.170898
H	-1.673351	1.079839	-2.005103
H	-1.103072	-2.621784	-0.997534
H	-2.65569	-3.503224	-0.860533
H	-1.358201	-3.790726	0.338185
H	-4.161859	-2.792167	0.922666
H	-3.595009	-1.458092	1.970198
H	-2.869289	-3.087491	2.126374
H	-4.151665	-1.254978	-1.215759
H	-3.929369	0.228425	-2.186219
H	-5.473764	-0.050379	-1.31742
H	-3.546842	2.28937	-0.980532
H	-3.61662	2.213071	0.804781
H	-5.122724	2.061224	-0.157133
H	-0.547305	3.167595	-1.419235
H	0.339918	4.554236	-0.709327
H	-0.935111	3.71868	0.237789
H	2.03912	4.017666	0.976176
H	2.125214	2.302926	1.4959
H	0.712465	3.299805	1.949656
H	0.243205	-1.785427	1.046969
H	0.850705	-0.876071	2.44692
H	1.910622	-2.072019	1.646912
H	3.862474	0.720142	-2.227373
H	3.515057	1.621911	-0.736916
H	2.237232	1.379969	-1.928844
H	0.931214	-1.60386	-2.146983
H	1.646604	-2.889497	-1.145861
H	2.541685	-2.25439	-2.535471
H	4.164474	-0.344277	1.825483
H	5.302953	0.10367	0.525006
H	5.507032	-1.432892	1.398354

Table 7: Standard orientation of **Ed** [B3LYP/6-31+G(d)].

Atomic Symbol	x	y	z
C	-1.38892	1.123485	1.865359
Li	-0.040185	0.955207	0.166106
C	-1.052735	0.450268	-1.70414
Li	-2.038376	-0.052888	0.163071
O	1.561839	-0.222682	0.611388
O	0.801612	2.747015	0.028241
O	-3.994297	0.263648	-0.127518
O	-2.101334	-2.031288	0.470761
C	-1.683479	-3.059713	-0.416542
C	-2.597769	-2.513719	1.71404
C	-4.518798	-0.384813	-1.281679
C	-4.335162	1.647018	-0.061059
C	-0.071052	3.737654	-0.508065
C	1.45608	3.159621	1.22437
Si	2.577415	-0.664666	-0.667731
C	1.204219	-1.198212	1.607067
C	3.032249	0.925964	-1.537028
C	1.779525	-1.956131	-1.751675
O	3.9241	-1.404998	-0.006721
C	4.80097	-0.74833	0.900191

H	-1.654155	2.199343	1.795646
H	-0.556816	1.094142	2.59675
H	-2.238513	0.676373	2.421664
H	-1.348233	-0.469705	-2.247683
H	-0.128609	0.77302	-2.222883
H	-1.806732	1.203839	-2.015776
H	-1.308866	-2.568871	-1.315224
H	-2.525178	-3.721434	-0.671862
H	-0.879981	-3.661734	0.034073
H	-3.479832	-3.153033	1.56049
H	-2.872949	-1.640191	2.306995
H	-1.822733	-3.087013	2.244329
H	-4.212037	-1.431569	-1.221655
H	-4.112619	0.061066	-2.200347
H	-5.617176	-0.323776	-1.294115
H	-3.945408	2.185591	-0.936978
H	-3.872441	2.041927	0.844794
H	-5.427072	1.770465	-0.010786
H	-0.528762	3.304129	-1.399448
H	0.495068	4.641123	-0.778828
H	-0.855355	3.99794	0.216683
H	2.081647	4.044725	1.035355
H	2.084308	2.32407	1.541354
H	0.723809	3.383629	2.012275
H	0.353206	-1.794683	1.261694
H	0.903943	-0.661966	2.508983
H	2.054756	-1.854025	1.829758
H	3.746406	0.71989	-2.344076
H	3.490832	1.642758	-0.846346
H	2.14987	1.408634	-1.967657
H	0.849158	-1.561119	-2.172496
H	1.548658	-2.860787	-1.176798
H	2.445869	-2.243687	-2.573554
H	4.266519	-0.398109	1.795176
H	5.29751	0.11171	0.428596
H	5.567652	-1.466412	1.208353

Table 8: Standard orientation of **Ed** [B3LYP/6-31+G(d) pcm].

Atomic Symbol	x	y	z
C	-1.318902	1.112287	1.913505
Li	0.008948	0.961257	0.178541
C	-1.02618	0.48743	-1.696860
Li	-2.044533	0.010945	0.177517
O	1.574406	-0.277098	0.608245
O	0.865714	2.740325	0.014883
O	-4.002662	0.375829	-0.102856
O	-2.213004	-1.971634	0.459748
C	-1.752543	-3.001299	-0.408609
C	-3.0123	-2.454987	1.535473
C	-4.586899	-0.352454	-1.181191
C	-4.35912	1.757877	-0.112880
C	-0.000665	3.775274	-0.446266
C	1.709391	3.147869	1.088385
Si	2.618951	-0.721165	-0.647515
C	1.175129	-1.264552	1.579712
C	3.119184	0.869151	-1.491320
C	1.819237	-1.983371	-1.764757
O	3.939179	-1.492294	0.035206
C	4.803774	-0.849343	0.971461
H	-1.855003	2.082755	1.938739
H	-0.372081	1.303349	2.459011
H	-1.893015	0.444257	2.587570
H	-1.290279	-0.452785	-2.219954
H	-0.090011	0.822717	-2.185503
H	-1.790301	1.22299	-2.024538
H	-1.143582	-2.520149	-1.174212
H	-2.598797	-3.523004	-0.879452
H	-1.143812	-3.731986	0.143681
H	-3.918656	-2.948738	1.155681
H	-3.29345	-1.590656	2.139553

H	-2.443421	-3.165757	2.151564
H	-4.257046	-1.388014	-1.079407
H	-4.248986	0.045261	-2.148258
H	-5.683897	-0.306266	-1.128690
H	-4.019409	2.239434	-1.040985
H	-3.86065	2.21994	0.740683
H	-5.448013	1.874561	-0.018288
H	-0.60156	3.347127	-1.250905
H	0.584449	4.624164	-0.827553
H	-0.660928	4.118836	0.362528
H	2.375196	3.961953	0.767994
H	2.302333	2.275813	1.371883
H	1.112437	3.479801	1.949270
H	0.448446	-1.959412	1.144260
H	0.698038	-0.739602	2.408345
H	2.046077	-1.822077	1.943013
H	3.779504	0.648616	-2.339115
H	3.654582	1.535241	-0.804886
H	2.24471	1.413095	-1.861435
H	0.913962	-1.557972	-2.211025
H	1.541143	-2.885212	-1.206878
H	2.500627	-2.281136	-2.570542
H	4.250234	-0.501026	1.854213
H	5.318811	0.00738	0.516332
H	5.554102	-1.578087	1.292628

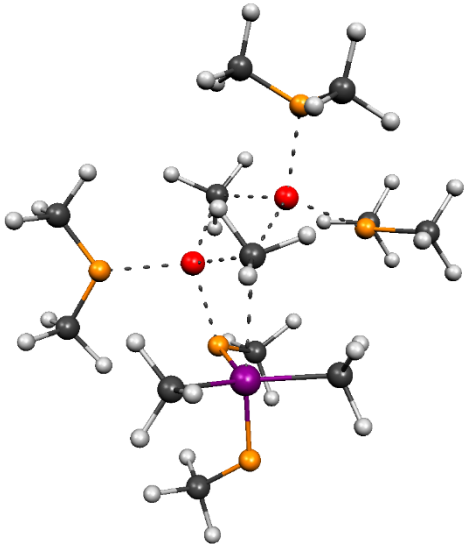


Figure 28: Molekel plot of **At** [M062X/6-31+G(d)].

Table 9: Standard orientation of **At** [M062X/6-31+G(d)].

Atomic Symbol	x	y	z
C	-1.308528	1.308828	1.880422
Li	0.260433	1.070375	0.461094
C	-0.434885	0.224906	-1.460174
Li	-1.883473	0.077308	0.271748
O	1.507226	-0.281545	0.785747
O	1.350384	2.657567	0.316152
O	-3.539582	0.816682	-0.522919
O	-2.221631	-1.759616	0.781378
C	-2.713052	-2.78721	-0.05615
C	-2.520547	-1.978399	2.15059
C	-3.964092	0.345357	-1.788254
C	-3.57446	2.233156	-0.453019
C	0.788742	3.952325	0.279028

C	2.727448	2.655494	0.644265
Si	1.744844	-0.941889	-0.784119
C	1.286102	-1.170062	1.868046
C	2.488306	0.338297	-1.953494
C	0.713775	-2.427208	-1.305424
O	3.137293	-1.883879	-0.392156
C	4.240527	-1.343023	0.277237
H	-1.195313	2.409401	1.892407
H	-0.683365	0.960774	2.724225
H	-2.347245	1.152188	2.232808
H	-1.290858	-0.478936	-1.516109
H	-0.042973	0.200814	-2.485748
H	-0.888771	1.240468	-1.395004
H	-2.388466	-2.564092	-1.074741
H	-3.809959	-2.83033	-0.00965
H	-2.297707	-3.75724	0.246447
H	-3.607067	-1.995587	2.307367
H	-2.078109	-1.153355	2.71121
H	-2.087846	-2.931466	2.482004
H	-3.937387	-0.745617	-1.759152
H	-3.290518	0.703151	-2.57783
H	-4.990333	0.678456	-1.991524
H	-2.905046	2.667518	-1.208702
H	-3.236037	2.517467	0.543418
H	-4.598047	2.591704	-0.623825
H	-0.268101	3.839927	0.028226
H	1.287849	4.564228	-0.48398
H	0.879584	4.440583	1.258266
H	3.300508	3.198848	-0.118855
H	3.045	1.612097	0.677986
H	2.885525	3.124355	1.624549
H	0.262547	-1.567751	1.831675
H	1.411959	-0.61421	2.801834
H	1.998329	-2.003443	1.835497
H	2.250207	0.045443	-2.983234
H	3.579676	0.379107	-1.87012
H	2.072786	1.337531	-1.7969
H	0.155188	-2.25089	-2.228915
H	-0.016916	-2.630175	-0.512198
H	1.355476	-3.30498	-1.423249
H	3.968371	-0.954375	1.271788
H	4.709293	-0.518845	-0.283901
H	4.993539	-2.127814	0.409024

Table 10: Standard orientation of **At** [M062X/6-31+G(d) pcm].

Atomic Symbol	x	y	z
C	-1.259131	1.319449	1.901124
Li	0.284753	1.084663	0.441235
C	-0.438417	0.266408	-1.477786
Li	-1.878098	0.101204	0.278539
O	1.508372	-0.305760	0.783258
O	1.404462	2.653485	0.294378
O	-3.512908	0.902661	-0.456129
O	-2.293898	-1.732294	0.730698

C	-2.720620	-2.780041	-0.121957
C	-2.582671	-1.992862	2.096413
C	-4.095908	0.339917	-1.618487
C	-3.477852	2.320479	-0.517032
C	0.860783	3.958636	0.239749
C	2.775357	2.640381	0.652635
Si	1.752818	-0.966733	-0.777266
C	1.221946	-1.189576	1.856937
C	2.521611	0.303144	-1.937765
C	0.688093	-2.415900	-1.323874
O	3.128308	-1.940086	-0.380508
C	4.216803	-1.407305	0.328495
H	-1.066736	2.408930	1.927977
H	-0.683615	0.905350	2.749954
H	-2.319345	1.227482	2.207925
H	-1.310093	-0.415755	-1.552757
H	-0.009558	0.223945	-2.488215
H	-0.870946	1.290799	-1.428371
H	-2.429056	-2.516252	-1.140520
H	-3.809939	-2.902574	-0.062755
H	-2.233777	-3.722116	0.160229
H	-3.664768	-2.097114	2.244470
H	-2.208749	-1.144575	2.672413
H	-2.079317	-2.913260	2.418460
H	-4.121470	-0.742577	-1.481791
H	-3.497275	0.585031	-2.505383
H	-5.118730	0.714687	-1.748818
H	-2.891163	2.650201	-1.385003
H	-3.006351	2.670985	0.401887
H	-4.497374	2.718420	-0.594630
H	-0.191080	3.862383	-0.037203
H	1.386852	4.559403	-0.512897
H	0.938069	4.448638	1.218709
H	3.368456	3.181851	-0.095763
H	3.085222	1.594698	0.690427
H	2.916540	3.105424	1.636641
H	0.179485	-1.529937	1.802956
H	1.365358	-0.648106	2.795988
H	1.889133	-2.059559	1.832031
H	2.261551	0.037009	-2.969236
H	3.614614	0.307154	-1.863209
H	2.141884	1.312016	-1.754282
H	0.130947	-2.206782	-2.240845
H	-0.046785	-2.618253	-0.534797
H	1.304535	-3.309053	-1.464183
H	3.923009	-1.070441	1.333905
H	4.672743	-0.549606	-0.189809
H	4.983654	-2.182196	0.434605

Table 11: Standard orientation of **At** [B3LYP/6-31+G(d)].

Atomic Symbol	x	y	z
C	-1.319311	1.405204	1.836623
Li	0.264567	1.110215	0.433364
C	-0.412474	0.253842	-1.503929
Li	-1.912082	0.092933	0.288353
O	1.475701	-0.292376	0.757353

O	1.376555	2.729579	0.312522
O	-3.604547	0.791459	-0.548040
O	-2.215679	-1.760473	0.874241
C	-2.724965	-2.826078	0.079139
C	-2.392745	-1.970585	2.276114
C	-4.132260	0.206424	-1.735616
C	-3.653369	2.219777	-0.578725
C	0.822296	4.033782	0.198908
C	2.713057	2.719179	0.808157
Si	1.728788	-0.957626	-0.821066
C	1.401756	-1.120971	1.913562
C	2.528644	0.309551	-1.981976
C	0.697319	-2.448268	-1.355313
O	3.111503	-1.931438	-0.402285
C	4.295229	-1.413055	0.152646
H	-1.241766	2.509158	1.785535
H	-0.658547	1.121891	2.680032
H	-2.342000	1.234650	2.230016
H	-1.299143	-0.411828	-1.520411
H	-0.061000	0.209179	-2.543429
H	-0.812003	1.289041	-1.421892
H	-2.474266	-2.603358	-0.959830
H	-3.815824	-2.910127	0.193895
H	-2.254786	-3.778182	0.361250
H	-3.461103	-2.047589	2.524209
H	-1.957297	-1.108800	2.783274
H	-1.877135	-2.888889	2.590423
H	-4.109093	-0.877250	-1.602428
H	-3.522314	0.478602	-2.608092
H	-5.171821	0.527781	-1.893268
H	-3.061890	2.606265	-1.421254
H	-3.227098	2.572712	0.360544
H	-4.693983	2.561400	-0.673865
H	-0.193233	3.918776	-0.186196
H	1.413506	4.645602	-0.497948
H	0.783319	4.529310	1.179683
H	3.380848	3.263197	0.124951
H	3.015271	1.672961	0.867867
H	2.758107	3.178250	1.806588
H	0.450140	-1.668979	1.934669
H	1.449890	-0.477181	2.798527
H	2.226340	-1.841999	1.936950
H	2.255651	0.067842	-3.016894
H	3.622696	0.287399	-1.915975
H	2.178932	1.327040	-1.783722
H	0.132449	-2.266915	-2.274784
H	-0.026702	-2.667530	-0.561626
H	1.341575	-3.323616	-1.487783
H	4.102186	-0.656463	0.932942
H	4.939619	-0.947548	-0.611581
H	4.862666	-2.234294	0.611537

Table 12: Standard orientation of **At** [B3LYP/6-31+G(d) pcm].

Atomic Symbol	x	y	z
C	-1.293250	1.363587	1.88296
Li	0.279851	1.107827	0.451433
C	-0.384311	0.378744	-1.527616
Li	-1.909179	0.082759	0.283869
O	1.480644	-0.330961	0.754205
O	1.399235	2.721036	0.337039
O	-3.589133	0.842121	-0.498579
O	-2.227029	-1.786719	0.820988
C	-2.755854	-2.832842	0.006921
C	-2.398473	-2.031363	2.220025
C	-4.278939	0.225314	-1.585239
C	-3.571127	2.26887	-0.606601
C	0.840723	4.01696	0.144425
C	2.704458	2.742677	0.911927
Si	1.748460	-0.94825	-0.831088

C	1.364337	-1.1914	1.886314
C	2.594620	0.341813	-1.928264
C	0.670801	-2.373572	-1.440321
O	3.102608	-1.978647	-0.435158
C	4.280651	-1.491071	0.172258
H	-1.173051	2.464701	1.855588
H	-0.655843	1.024587	2.723562
H	-2.331477	1.212018	2.239494
H	-1.304160	-0.234412	-1.61101
H	0.029912	0.337983	-2.544555
H	-0.731626	1.430124	-1.432484
H	-2.532721	-2.58106	-1.031604
H	-3.842592	-2.920335	0.145703
H	-2.279379	-3.790808	0.254547
H	-3.465512	-2.106008	2.47113
H	-1.953134	-1.186746	2.746979
H	-1.889207	-2.961005	2.508122
H	-4.296448	-0.848904	-1.392434
H	-3.760537	0.4203	-2.534171
H	-5.310236	0.598828	-1.646558
H	-3.063752	2.578159	-1.530964
H	-3.021773	2.64475	0.257161
H	-4.596962	2.662068	-0.601639
H	-0.145206	3.878091	-0.304526
H	1.471360	4.611931	-0.530889
H	0.733919	4.543003	1.103496
H	3.405386	3.275595	0.254276
H	3.015241	1.702316	1.01937
H	2.685761	3.23052	1.896842
H	0.423895	-1.755698	1.848682
H	1.360100	-0.568496	2.786378
H	2.200932	-1.897226	1.934485
H	2.351615	0.138139	-2.978812
H	3.685564	0.302363	-1.825317
H	2.251873	1.355079	-1.70077
H	0.123525	-2.127178	-2.354728
H	-0.071052	-2.599179	-0.665633
H	1.278372	-3.269604	-1.609391
H	4.075788	-0.707719	0.919675
H	4.978581	-1.072829	-0.570592
H	4.789972	-2.320549	0.681225

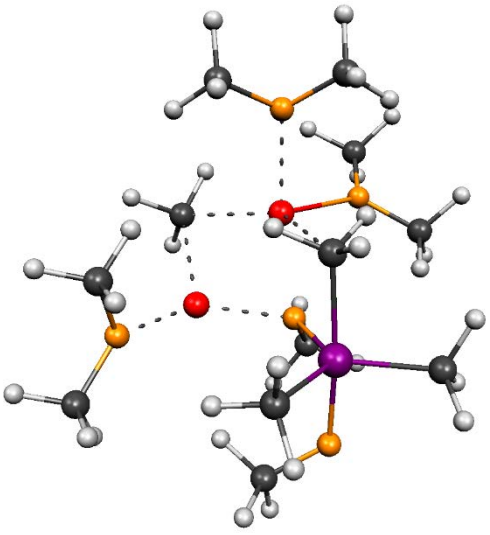


Figure 29: Molekel plot of **IM_{eq}** [M062X/6-31+G(d)].

Table 13: Standard orientation of **IM_{eq}** [M062X/6-31+G(d)].

Atomic Symbol	x	y	z
C	-0.911094	2.009978	1.856589

Li	0.823725	1.093513	1.215264
C	-0.228076	-0.279148	-1.79367
Li	-1.350853	0.422016	0.413876
O	0.366071	-0.664773	0.65867
O	2.177633	2.275007	0.565904
O	-2.797173	1.384586	-0.644667
O	-2.609262	-0.99542	0.854888
C	-2.447712	-2.37047	0.564209
C	-3.813085	-0.704933	1.537039
C	-3.552593	0.714558	-1.634353
C	-2.508323	2.719511	-1.016776
C	1.706504	3.056478	-0.522857
C	3.57433	2.405289	0.763586
Si	1.200469	-1.296134	-0.850896
C	0.354988	-1.399343	1.879344
C	2.59703	-0.342619	-1.770136
C	0.673328	-3.017881	-1.469244
O	2.383181	-2.086064	0.24381
C	3.337518	-1.353528	0.93214
H	-0.703637	3.082871	1.693481
H	-0.600395	1.834887	2.906868
H	-2.013853	1.951563	1.908694
H	-1.240017	-0.651354	-1.563708
H	-0.101997	-0.396664	-2.879262
H	-0.218075	0.811286	-1.604175
H	-1.498876	-2.482222	0.036992
H	-3.269779	-2.722566	-0.074593
H	-2.429671	-2.959976	1.490577
H	-4.678997	-1.036811	0.946922
H	-3.855796	0.376906	1.671973
H	-3.8294	-1.205111	2.514192
H	-3.700723	-0.311453	-1.291509
H	-3.012152	0.701515	-2.590123
H	-4.525351	1.207078	-1.766537
H	-1.898248	2.736248	-1.93149
H	-1.958558	3.170159	-0.189608
H	-3.438905	3.275045	-1.194209
H	0.621107	2.937392	-0.555015
H	2.150438	2.704861	-1.462689
H	1.954873	4.112828	-0.360758
H	4.122775	2.054229	-0.119753
H	3.846284	1.795671	1.625914
H	3.826831	3.454502	0.961009
H	0.310858	-2.47564	1.690374
H	-0.525159	-1.084921	2.454052
H	1.25633	-1.214152	2.47781
H	3.466572	-0.987189	-1.945591
H	2.946818	0.497116	-1.154044
H	2.263484	0.07355	-2.726685
H	-0.205237	-3.014147	-2.123233
H	0.486705	-3.687029	-0.61948
H	1.512125	-3.465141	-2.015909
H	2.947336	-0.38573	1.315156
H	4.216019	-1.110003	0.31114
H	3.690589	-1.922338	1.80427

Table 14: Standard orientation of **IM$_{eq}$** [M062X/6-31+G(d) pcm].

Atomic Symbol	x	y	z
C	0.956409	2.009595	-1.883895
Li	-0.816468	1.129685	-1.217904
C	0.183402	-0.210752	1.778267
Li	1.360737	0.426961	-0.419899
O	-0.383147	-0.6713	-0.664609
O	-2.199601	2.284065	-0.549707
O	2.781031	1.404897	0.648599
O	2.618683	-0.98717	-0.859507
C	2.508997	-2.347016	-0.481817
C	3.810037	-0.705288	-1.571471
C	3.578397	0.739403	1.609917
C	2.474314	2.72938	1.047103
C	-1.805348	3.113833	0.534005
C	-3.586638	2.380603	-0.830038
Si	-1.195944	-1.29326	0.846261
C	-0.320730	-1.44116	-1.862325
C	-2.631782	-0.369476	1.738506
C	-0.625331	-2.985535	1.521189
O	-2.361137	-2.162667	-0.227097
C	-3.322397	-1.458258	-0.945237
H	0.701554	3.072708	-1.719225
H	0.697662	1.819306	-2.94448
H	2.060691	1.984722	-1.866814
H	1.211055	-0.555568	1.57765
H	0.045904	-0.282051	2.866674
H	0.135383	0.866461	1.532188
H	1.577642	-2.454612	0.076736
H	3.356697	-2.634522	0.154676
H	2.486775	-2.992292	-1.369454
H	4.688820	-0.974748	-0.970467
H	3.821553	0.366473	-1.774556
H	3.831302	-1.265283	-2.514805
H	3.738606	-0.279355	1.2523
H	3.066212	0.708628	2.580747
H	4.543724	1.249872	1.721497
H	1.898617	2.722937	1.983369
H	1.881348	3.175612	0.247602
H	3.396593	3.306096	1.194682
H	-0.721737	3.021444	0.634834
H	-2.294498	2.786838	1.460135
H	-2.066405	4.15785	0.323525
H	-4.176645	2.056819	0.036539
H	-3.799408	1.731197	-1.679881
H	-3.846591	3.415348	-1.082845
H	-0.121751	-2.494497	-1.642304
H	0.495838	-1.039975	-2.47492
H	-1.256475	-1.391619	-2.429695
H	-3.498982	-1.021743	1.897986
H	-2.975015	0.471828	1.120636
H	-2.317817	0.046721	2.701854
H	0.245862	-2.929708	2.182789
H	-0.398234	-3.671557	0.694781
H	-1.452427	-3.445291	2.076392
H	-2.936438	-0.503822	-1.352908
H	-4.205434	-1.206319	-0.335105
H	-3.666191	-2.056758	-1.801026

Table 15: Standard orientation of **IM$_{eq}$** [B3LYP/6-31+G(d)].

Atomic Symbol	x	y	z
C	1.06975	2.654156	-0.658201
Li	-0.671529	1.584543	-0.364278
C	0.515642	-0.990843	1.779464
Li	1.510745	0.541098	-0.170778
O	-0.337038	-0.288031	-0.551449
O	-2.369426	2.407834	-0.34608
O	3.154361	0.836967	1.051991

O	2.554525	-0.602481	-1.417854
C	2.305223	-1.983207	-1.666025
C	3.617279	-0.062242	-2.195734
C	4.004621	-0.234893	1.443651
C	3.049982	1.844194	2.057493
C	-2.480506	3.828825	-0.288546
C	-3.633988	1.727055	-0.356719
Si	-1.143759	-1.321633	0.730949
C	-0.606619	-0.41055	-1.958467
C	-2.235846	-0.542657	2.119581
C	-0.888883	-3.219435	0.595671
O	-2.543711	-1.305725	-0.444343
C	-3.639325	-2.168968	-0.341109
H	0.972858	3.505129	0.044365
H	0.682466	3.047562	-1.621522
H	2.159808	2.578552	-0.830998
H	1.423556	-1.369174	1.28509
H	0.43757	-1.533299	2.732703
H	0.69104	0.065228	2.044665
H	1.473751	-2.278464	-1.025391
H	3.193741	-2.584547	-1.423317
H	2.033949	-2.145084	-2.718631
H	4.560642	-0.587089	-1.983789
H	3.713944	0.989018	-1.918527
H	3.391219	-0.142554	-3.268631
H	4.021029	-0.947453	0.617159
H	3.617391	-0.731389	2.344277
H	5.023582	0.132544	1.635512
H	2.638502	1.42117	2.9852
H	2.377218	2.609544	1.670222
H	4.036852	2.283636	2.262922
H	-1.466014	4.234091	-0.303824
H	-2.99069	4.136906	0.634884
H	-3.040177	4.204941	-1.156375
H	-4.188518	1.953823	0.563909
H	-3.415741	0.656278	-0.411506
H	-4.221167	2.048192	-1.228446
H	-0.648179	-1.461828	-2.259134
H	0.207698	0.0899	-2.49751
H	-1.567768	0.041312	-2.226693
H	-3.310872	-0.727833	2.020355
H	-2.09573	0.549844	2.086664
H	-1.914482	-0.86188	3.11921
H	-0.019666	-3.580555	1.157839
H	-0.754379	-3.492894	-0.461364
H	-1.768955	-3.775359	0.942602
H	-3.943162	-2.368659	0.703035
H	-3.441576	-3.146744	-0.814445
H	-4.508431	-1.724039	-0.853093

Table 16: Standard orientation of **IM_{eq}** [B3LYP/6-31+G(d) pcm].

Atomic Symbol	x	y	z
C	0.992866	1.961943	-2.004576
Li	-0.777447	1.138794	-1.228416
C	0.127343	-0.257705	1.865435
Li	1.417373	0.415529	-0.490172
O	-0.358006	-0.674355	-0.644614
O	-2.175587	2.295874	-0.547862
O	2.694859	1.481469	0.709414
O	2.746904	-1.008273	-0.848292
C	2.662748	-2.355878	-0.386405
C	3.935464	-0.741001	-1.590566
C	3.544834	0.868759	1.676219
C	2.323316	2.809397	1.075164
C	-1.850247	3.153351	0.549377
C	-3.539783	2.403537	-0.958021
Si	-1.231587	-1.305989	0.858844
C	-0.258403	-1.465750	-1.840600
C	-2.695109	-0.395338	1.738471

C	-0.670027	-3.022623	1.499157
O	-2.385958	-2.167389	-0.265819
C	-3.384068	-1.521167	-1.000582
H	0.782514	3.040016	-1.863572
H	0.703601	1.752093	-3.055906
H	2.097682	1.898792	-2.011009
H	1.160535	-0.575447	1.663083
H	-0.039128	-0.419065	2.941444
H	0.078522	0.832115	1.706735
H	1.734410	-2.446100	0.177022
H	3.514722	-2.592178	0.266619
H	2.649371	-3.054672	-1.233703
H	4.826456	-0.919548	-0.972042
H	3.902152	0.309107	-1.885862
H	3.981487	-1.375908	-2.485933
H	3.765667	-0.137033	1.316171
H	3.043032	0.806069	2.651532
H	4.479326	1.438002	1.780347
H	1.751142	2.805525	2.014412
H	1.705954	3.198423	0.264907
H	3.215479	3.439512	1.197452
H	-0.792693	3.001915	0.774536
H	-2.452533	2.893802	1.429375
H	-2.020957	4.203535	0.277896
H	-4.212406	2.120149	-0.137790
H	-3.682792	1.718498	-1.795751
H	-3.762518	3.429923	-1.278459
H	-0.017394	-2.506453	-1.603213
H	0.547127	-1.045961	-2.454452
H	-1.188934	-1.462209	-2.417211
H	-3.569067	-1.047343	1.863413
H	-3.018232	0.463411	1.135144
H	-2.403467	-0.005221	2.720993
H	0.185395	-2.975591	2.183844
H	-0.411157	-3.677885	0.656676
H	-1.503658	-3.511786	2.020354
H	-3.023332	-0.618832	-1.532602
H	-4.235098	-1.197486	-0.375571
H	-3.780078	-2.205046	-1.767999

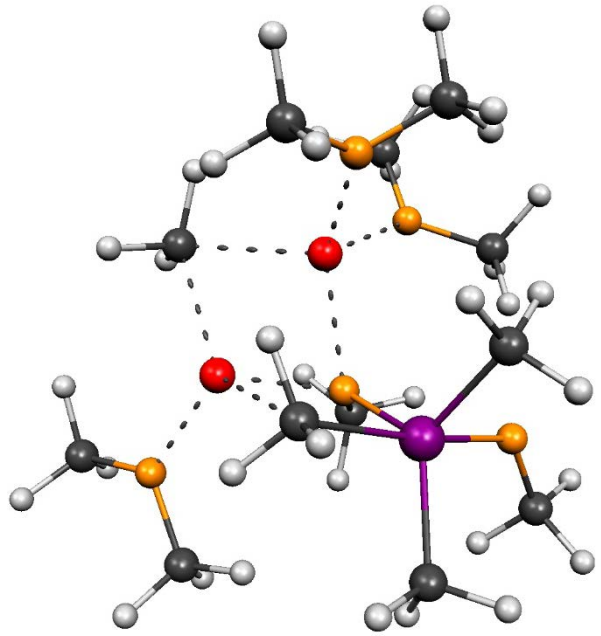


Figure 30: Molekel plot of **bIM$_{eq}$** [M062X/6-31+G(d)].

Table 17: Standard orientation of **bIM$_{eq}$** [M062X/6-31+G(d)].

Atomic Symbol	x	y	z
C	-0.222872	-2.989741	-0.070981

Li	1.154751	-1.490298	0.458562
C	0.997284	0.10193	2.179112
Li	-1.066687	-1.012311	-0.184978
O	0.58707	0.11458	-0.357554
O	2.936998	-1.8421	-0.067871
O	-2.459021	-0.997193	1.170517
O	-2.106821	-0.368748	-1.66628
C	-2.324375	0.974723	-2.07289
C	-2.96281	-1.294474	-2.304859
C	-3.622834	-0.195602	1.18226
C	-2.304841	-1.741792	2.366467
C	3.334186	-3.057993	-0.674905
C	3.92407	-0.830181	-0.135967
Si	0.590822	1.501965	0.791422
C	0.933812	0.189064	-1.729375
C	2.220695	2.457034	1.113095
C	-1.047948	2.001287	1.641223
O	0.103754	2.575372	-0.578103
C	0.916493	3.360263	-1.391499
H	0.246078	-3.682853	0.654744
H	0.104434	-3.361117	-1.060596
H	-1.293745	-3.26341	-0.015836
H	0.235068	-0.694161	2.261969
H	1.002731	0.593721	3.161884
H	1.988176	-0.383466	2.099281
H	-1.640496	1.612909	-1.502514
H	-3.368157	1.262029	-1.880443
H	-2.122594	1.075762	-3.14817
H	-4.012073	-1.084159	-2.054874
H	-2.691766	-2.290491	-1.947804
H	-2.834093	-1.246213	-3.393967
H	-3.635271	0.375543	0.252775
H	-3.607179	0.498155	2.032008
H	-4.51778	-0.830045	1.241498
H	-2.139848	-1.06473	3.215263
H	-1.438571	-2.391262	2.230221
H	-3.200166	-2.350544	2.550143
H	2.509211	-3.762554	-0.559072
H	4.234919	-3.450421	-0.185844
H	3.537048	-2.899779	-1.742057
H	4.813735	-1.125795	0.434357
H	3.492504	0.075486	0.296242
H	4.205517	-0.641564	-1.180436
H	0.316751	0.91703	-2.261915
H	0.79468	-0.806479	-2.169089
H	1.987812	0.47862	-1.842951
H	2.011802	3.525754	1.246857
H	2.9064	2.390095	0.257045
H	2.755091	2.098713	1.998812
H	-1.337983	1.354426	2.476827
H	-1.863874	2.041224	0.910173
H	-0.936866	3.025767	2.02082
H	1.823953	2.839356	-1.742726
H	1.247793	4.27996	-0.883672
H	0.350074	3.662422	-2.285373

Table 18: Standard orientation of **bIM$_{eq}$** [M062X/6-31+G(d) pcm].

Atomic Symbol	x	y	z
C	-0.311784	-3.004952	0.065197
Li	1.126225	-1.515079	0.514861
C	1.014518	0.180431	2.204661
Li	-1.11509	-1.004084	-0.143463
O	0.577221	0.091764	-0.33521
O	2.899009	-1.88551	-0.03169
O	-2.492356	-0.863933	1.21285
O	-2.105145	-0.441842	-1.688424
C	-2.302292	0.892844	-2.132796
C	-2.972277	-1.370966	-2.312703
C	-3.652086	-0.05481	1.153266

C	-2.374466	-1.540727	2.452834
C	3.296385	-3.126378	-0.591309
C	3.902411	-0.888716	-0.118353
Si	0.625245	1.517089	0.754173
C	0.922999	0.096184	-1.711679
C	2.271527	2.460943	1.04811
C	-1.00547	2.083407	1.579562
O	0.172056	2.571737	-0.650777
C	1.030226	3.244117	-1.520412
H	0.156801	-3.652715	0.831811
H	-0.003978	-3.442463	-0.903052
H	-1.390115	-3.236003	0.153283
H	0.239104	-0.593938	2.342287
H	1.047195	0.726964	3.158408
H	1.994577	-0.326236	2.129039
H	-1.625139	1.535914	-1.561482
H	-3.346071	1.195797	-1.971515
H	-2.073382	0.967276	-3.204319
H	-4.018252	-1.143155	-2.068276
H	-2.713815	-2.362791	-1.935785
H	-2.839254	-1.344852	-3.401354
H	-3.644775	0.458309	0.19091
H	-3.645492	0.687263	1.9613
H	-4.552092	-0.67801	1.234804
H	-2.22765	-0.818084	3.266373
H	-1.509407	-2.201521	2.378708
H	-3.277665	-2.132899	2.648343
H	2.466816	-3.822563	-0.45899
H	4.188059	-3.506166	-0.0779
H	3.512264	-3.007119	-1.660317
H	4.777599	-1.17598	0.476837
H	3.47599	0.036792	0.2749
H	4.203603	-0.740928	-1.163335
H	0.331434	0.82404	-2.271817
H	0.741014	-0.909204	-2.109976
H	1.987205	0.335051	-1.838467
H	2.078649	3.538651	1.124035
H	2.96826	2.336398	0.207906
H	2.786715	2.135792	1.957812
H	-1.324233	1.4481	2.413125
H	-1.813928	2.137761	0.841169
H	-0.865493	3.105455	1.958198
H	1.908014	2.649854	-1.823738
H	1.411441	4.181488	-1.083914
H	0.484746	3.505964	-2.439887

Table 19: Standard orientation of **bIM$_{eq}$** [B3LYP/6-31+G(d)].

Atomic Symbol	x	y	z
C	-0.055389	-2.99829	-0.234798
Li	1.260413	-1.440844	0.312687
C	1.103105	0.112876	2.131299
Li	-1.040889	-1.067027	-0.235658
O	0.561814	0.178424	-0.399938
O	3.112339	-1.737076	-0.139558
O	-2.369607	-1.205603	1.236254
O	-2.246617	-0.42321	-1.646976
C	-2.520417	0.934713	-2.010167
C	-3.059039	-1.371101	-2.330393
C	-3.565892	-0.44431	1.363127
C	-2.104097	-2.011181	2.384231
C	3.549838	-2.978921	-0.690085
C	4.069543	-0.68739	-0.268785
Si	0.545351	1.53706	0.81597
C	0.878876	0.336381	-1.784113
C	2.158277	2.555731	1.044463
C	-1.05495	1.95478	1.791952
O	-0.106392	2.615306	-0.507897
C	0.557537	3.558	-1.298017
H	0.388616	-3.709061	0.491692

H	0.347686	-3.315939	-1.217528
H	-1.118549	-3.309865	-0.265322
H	0.388137	-0.721549	2.233664
H	1.147281	0.578135	3.126438
H	2.108423	-0.315458	1.968525
H	-1.846368	1.575591	-1.433467
H	-3.569029	1.182609	-1.786877
H	-2.341406	1.079661	-3.085261
H	-4.122317	-1.212911	-2.096142
H	-2.75426	-2.364448	-1.992289
H	-2.913153	-1.293868	-3.417366
H	-3.673445	0.139386	0.448402
H	-3.506071	0.236577	2.221986
H	-4.433299	-1.110782	1.480348
H	-1.924889	-1.377513	3.263868
H	-1.213379	-2.598625	2.159008
H	-2.950773	-2.684215	2.582469
H	2.735737	-3.693372	-0.556089
H	4.450107	-3.332885	-0.168484
H	3.767833	-2.869223	-1.761978
H	4.998275	-0.946782	0.25809
H	3.632989	0.20699	0.177864
H	4.291254	-0.497829	-1.328615
H	0.210027	1.047527	-2.27226
H	0.78928	-0.644009	-2.268251
H	1.911223	0.692921	-1.905299
H	1.934555	3.617713	1.206853
H	2.782392	2.51116	0.140409
H	2.762947	2.201055	1.886497
H	-1.249668	1.291641	2.643333
H	-1.924974	1.953777	1.126317
H	-0.966164	2.983214	2.1692
H	1.479057	3.171062	-1.772349
H	0.843413	4.459498	-0.728266
H	-0.111635	3.884124	-2.11115

Table 20: Standard orientation of **bIM$_{eq}$** [B3LYP/6-31+G(d) pcm].

Atomic Symbol	x	y	z
C	-0.168266	-3.009318	-0.223668
Li	1.218016	-1.495829	0.325301
C	1.153532	0.129048	2.156821
Li	-1.103836	-1.028267	-0.218503
O	0.589562	0.171982	-0.376924
O	3.066454	-1.838778	-0.130809
O	-2.461435	-1.155415	1.235408
O	-2.271702	-0.374832	-1.660535
C	-2.506418	0.99238	-2.01548
C	-3.125062	-1.290556	-2.343698
C	-3.646469	-0.369936	1.340323
C	-2.184159	-1.897665	2.423018
C	3.473692	-3.104319	-0.655801
C	4.039806	-0.810539	-0.319814
Si	0.61486	1.536045	0.819688
C	0.894054	0.299543	-1.768804
C	2.239756	2.538959	1.061189
C	-0.998924	1.972252	1.766656
O	0.004303	2.652129	-0.506768
C	0.732559	3.49807	-1.351291
H	0.247075	-3.709502	0.529868
H	0.245116	-3.353845	-1.192565
H	-1.242776	-3.275776	-0.262544
H	0.430296	-0.695351	2.278838
H	1.209968	0.613997	3.142825
H	2.151671	-0.309953	1.984984
H	-1.811072	1.606687	-1.437249
H	-3.54467	1.272754	-1.785515
H	-2.326767	1.139105	-3.08976
H	-4.178523	-1.097074	-2.095969
H	-2.851633	-2.295891	-2.015554
H	-2.986721	-1.209343	-3.430654
H	-3.765087	0.158883	0.394164

H	-3.559793	0.358119	2.157294
H	-4.519142	-1.015274	1.514193
H	-1.983725	-1.218458	3.263112
H	-1.302063	-2.505292	2.216843
H	-3.032665	-2.549393	2.67437
H	2.65706	-3.805045	-0.473245
H	4.384982	-3.45225	-0.151113
H	3.658892	-3.030661	-1.736203
H	4.97808	-1.072672	0.187024
H	3.633117	0.104308	0.113391
H	4.232795	-0.656373	-1.39021
H	0.233117	1.014551	-2.261951
H	0.774971	-0.68608	-2.234137
H	1.932763	0.627215	-1.907886
H	2.029452	3.609599	1.181246
H	2.886203	2.449796	0.176574
H	2.816376	2.199172	1.928689
H	-1.209977	1.306393	2.611712
H	-1.856479	1.962158	1.0848
H	-0.918765	3.00066	2.146978
H	1.641318	3.033323	-1.774278
H	1.055048	4.423446	-0.841086
H	0.098912	3.797513	-2.202696

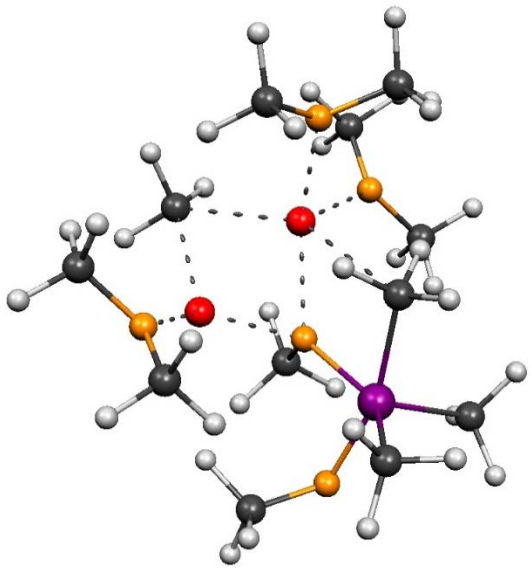


Figure 31: Molekel plot of **BPR** [M062X/6-31+G(d)].

Table 21: Standard orientation of **BPR** [M062X/6-31+G(d)].

Atomic Symbol	x	y	z
C	1.360698	1.657706	-1.972225
Li	-0.534375	1.191221	-1.250635
C	-0.114673	-0.507792	1.786745
Li	1.372851	0.169011	-0.359036
O	-0.420718	-0.630209	-0.715205
O	-1.483474	2.652686	-0.510377
O	2.562767	1.141358	0.948775
O	2.626946	-1.276127	-0.553071
C	2.27086	-2.644713	-0.616479
C	3.888735	-0.993565	-1.127888
C	3.212374	0.464836	2.008648
C	2.169554	2.448595	1.322353
C	-0.930867	3.94608	-0.696367
C	-2.540103	2.638603	0.435391
Si	-1.512913	-1.326173	0.659984
C	-0.406358	-1.264535	-1.990315
C	-2.884352	-0.753274	1.912476
C	-1.146358	-3.172358	0.886328
O	-2.695102	-1.612571	-0.635548

C	-3.43157	-0.572546	-1.176579
H	1.936207	2.55366	-1.684071
H	0.84786	1.957876	-2.910285
H	2.127999	0.950248	-2.34428
H	0.885118	-0.925991	1.590174
H	-0.32634	-0.676198	2.851097
H	-0.052411	0.587027	1.652255
H	1.28758	-2.743251	-0.153344
H	3.003395	-3.252107	-0.068556
H	2.224123	-2.982688	-1.660178
H	4.675074	-1.569654	-0.621338
H	4.067739	0.075715	-0.997239
H	3.887754	-1.240023	-2.197588
H	3.452798	-0.538826	1.653299
H	2.549601	0.392242	2.881148
H	4.13266	0.995349	2.28774
H	1.492577	2.410658	2.187668
H	1.655491	2.881159	0.463177
H	3.050376	3.052529	1.577834
H	-0.107952	3.848517	-1.406026
H	-0.553587	4.336034	0.257969
H	-1.694295	4.627964	-1.091118
H	-2.170286	2.95488	1.419183
H	-2.912857	1.616285	0.499367
H	-3.346598	3.308311	0.111234
H	-0.513582	-2.348922	-1.889728
H	0.547426	-1.032065	-2.48326
H	-1.228658	-0.919888	-2.631686
H	-3.915866	-0.898375	1.574366
H	-2.770002	0.274183	2.281521
H	-2.736512	-1.396191	2.792804
H	-0.38249	-3.370961	1.646829
H	-0.835126	-3.642575	-0.054874
H	-2.071638	-3.678199	1.184619
H	-2.797425	0.259038	-1.557425
H	-4.134841	-0.126255	-0.452007
H	-4.018951	-0.937097	-2.029175

Table 22: Standard orientation of **BPR** [M062X/6-31+G(d) pcm].

Atomic Symbol	x	y	z
C	1.362587	1.626824	-2.090089
Li	-0.580128	1.15755	-1.404297
C	-0.38764	0.112731	1.701919
Li	1.385016	0.183087	-0.437465
O	-0.429856	-0.661074	-0.700611
O	-1.588957	2.618428	-0.634691
O	2.696272	1.105858	0.799677
O	2.632838	-1.298412	-0.601363
C	2.35922	-2.663588	-0.34515
C	3.948647	-1.08251	-1.079622
C	3.233088	0.456603	1.937582
C	2.527004	2.495749	1.011375
C	-0.88295	3.75481	-0.158934
C	-2.926566	2.59542	-0.16162
Si	-1.544495	-1.153011	0.728927
C	-0.321592	-1.482115	-1.859524
C	-3.091036	-0.593099	1.77426
C	-0.950888	-2.834908	1.382387
O	-2.599718	-1.871337	-0.520635
C	-3.467223	-1.065428	-1.248954
H	1.329701	2.729086	-2.157077
H	1.186834	1.278972	-3.1271
H	2.432195	1.40502	-1.914818
H	0.667027	-0.197681	1.680115
H	-0.675743	0.169835	2.759975
H	-0.439191	1.141357	1.305106
H	1.355424	-2.719165	0.076803
H	3.083438	-3.065847	0.375489
H	2.406651	-3.247744	-1.27331

H	4.68232	-1.475074	-0.363118
H	4.082832	-0.005573	-1.186296
H	4.087722	-1.575451	-2.04983
H	3.267813	-0.611961	1.716436
H	2.597755	0.628922	2.816544
H	4.24553	0.827602	2.143012
H	1.775261	2.673802	1.792986
H	2.189304	2.92073	0.065622
H	3.478351	2.954614	1.310072
H	0.109684	3.727728	-0.606881
H	-0.801787	3.717955	0.935205
H	-1.404037	4.673011	-0.456301
H	-2.939468	2.613131	0.934972
H	-3.390227	1.67417	-0.516421
H	-3.477207	3.46177	-0.548279
H	-0.3351	-2.543623	-1.594996
H	0.625637	-1.248607	-2.362986
H	-1.14673	-1.308381	-2.560849
H	-4.003112	-1.156319	1.544986
H	-3.321783	0.476982	1.695687
H	-2.838179	-0.770713	2.828675
H	-0.08137	-2.764346	2.045956
H	-0.708577	-3.516689	0.557824
H	-1.767912	-3.306689	1.942103
H	-2.940443	-0.270993	-1.8146
H	-4.216021	-0.566491	-0.610205
H	-4.008873	-1.673735	-1.984981

Table 23: Standard orientation of **BPR** [B3LYP/6-31+G(d)].

Atomic Symbol	x	y	z
C	1.077087	2.07797	-1.828199
Li	-0.676573	1.174391	-1.163574
C	-0.309016	0.235329	1.773947
Li	1.466851	0.41413	-0.456052
O	-0.311123	-0.61452	-0.642227
O	-2.209229	2.263529	-0.733629
O	2.763927	1.340614	0.866814
O	2.839449	-0.969744	-0.86825
C	2.773198	-2.350784	-0.521415
C	3.936678	-0.649156	-1.718237
C	3.522801	0.621234	1.832487
C	2.380154	2.636749	1.324831
C	-1.916352	3.414477	0.061909
C	-3.611162	2.033118	-0.881864
Si	-1.318976	-1.219469	0.876419
C	-0.161215	-1.425539	-1.815606
C	-2.929723	-0.727084	1.85659
C	-0.432051	-2.737789	1.604874
O	-2.245707	-2.197428	-0.299738
C	-3.312939	-1.729645	-1.063139
H	0.844122	3.148843	-1.668539
H	0.857735	1.913048	-2.903543
H	2.182837	2.048249	-1.781014
H	0.779153	0.137401	1.671111
H	-0.52051	0.19652	2.851335
H	-0.584228	1.250491	1.446243
H	1.913923	-2.477451	0.137499
H	3.690652	-2.659131	0.001276
H	2.640941	-2.97083	-1.418733
H	4.889734	-0.902361	-1.231151
H	3.896112	0.425182	-1.905698
H	3.859192	-1.192731	-2.670629
H	3.76943	-0.344251	1.387487
H	2.940758	0.46452	2.752353
H	4.448416	1.162516	2.076853
H	1.731755	2.555433	2.20863
H	1.833775	3.106897	0.506502
H	3.269773	3.233614	1.57225
H	-0.830278	3.520649	0.079816

H	-2.295191	3.27818	1.083712
H	-2.365518	4.312034	-0.384841
H	-4.082114	1.881091	0.097754
H	-3.731267	1.129495	-1.480408
H	-4.083063	2.883795	-1.392614
H	0.015524	-2.47219	-1.551599
H	0.694876	-1.04768	-2.390811
H	-1.04993	-1.397423	-2.456021
H	-3.759585	-1.431527	1.726719
H	-3.293432	0.276509	1.589722
H	-2.686554	-0.684687	2.926974
H	0.474265	-2.480098	2.167912
H	-0.172795	-3.447558	0.809462
H	-1.110928	-3.270306	2.283467
H	-3.00953	-0.95705	-1.800833
H	-4.124183	-1.291114	-0.455419
H	-3.742338	-2.563959	-1.637044

Table 24: Standard orientation of **BPR** [B3LYP/6-31+G(d) pcm].

Atomic Symbol	x	y	z
C	1.171827	1.925185	-1.974105
Li	-0.679567	1.146682	-1.260315
C	-0.523573	0.173356	1.767288
Li	1.462056	0.351189	-0.464313
O	-0.308175	-0.656478	-0.650825
O	-2.039443	2.433828	-0.701644
O	2.5934	1.319523	0.934213
O	2.899515	-0.999879	-0.781179
C	2.848457	-2.380985	-0.427044
C	4.126707	-0.626759	-1.405412
C	3.292533	0.637501	1.973232
C	2.207709	2.642694	1.305593
C	-1.580125	3.633624	-0.07141
C	-3.446718	2.236918	-0.540957
Si	-1.412124	-1.293941	0.792821
C	-0.085034	-1.454071	-1.822718
C	-3.072557	-0.978852	1.78303
C	-0.525121	-2.836386	1.468723
O	-2.314966	-2.168759	-0.490663
C	-3.278544	-1.532795	-1.279734
H	0.886062	2.995008	-1.985952
H	1.09057	1.599209	-3.031616
H	2.261644	1.947981	-1.778646
H	0.569878	0.111107	1.726744
H	-0.809604	0.127011	2.827229
H	-0.808988	1.174581	1.410309
H	1.900071	-2.548244	0.083166
H	3.678831	-2.636135	0.246679
H	2.901797	-3.01309	-1.323925
H	4.973576	-0.804654	-0.727627
H	4.062247	0.437741	-1.636201
H	4.276735	-1.196952	-2.332586
H	3.537374	-0.355337	1.593301
H	2.665916	0.544667	2.871518
H	4.217012	1.173356	2.229671
H	1.48592	2.615937	2.133782
H	1.745333	3.091346	0.425509
H	3.087863	3.229049	1.603885
H	-0.510523	3.707723	-0.269298
H	-1.756684	3.588251	1.011747
H	-2.095769	4.507291	-0.491553
H	-3.705622	2.171103	0.523674
H	-3.704245	1.299658	-1.034829
H	-4.001387	3.064205	-1.00334
H	0.065966	-2.506186	-1.563323
H	0.812719	-1.082403	-2.332865
H	-0.926927	-1.404775	-2.52312
H	-3.853695	-1.720086	1.571975
H	-3.493627	0.017719	1.583876

H	-2.851812	-1.009384	2.859465
H	0.371653	-2.581459	2.047614
H	-0.23478	-3.510315	0.653263
H	-1.199572	-3.403532	2.123956
H	-2.860486	-0.683833	-1.856722
H	-4.125691	-1.139726	-0.689859
H	-3.68551	-2.247726	-2.009632

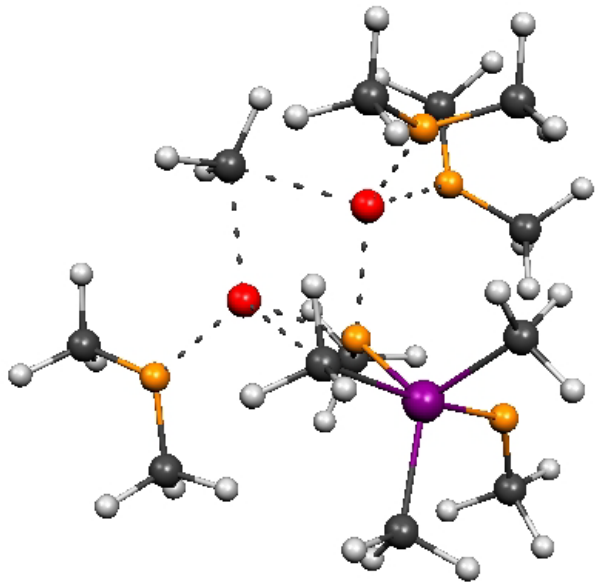


Figure 32: Molekel plot of **bBPR** [M062X/6-31+G(d)].

Table 25: Standard orientation of **bBPR** [M062X/6-31+G(d)].

Atomic Symbol	x	y	z
C	-0.982883	2.88213	0.550186
Li	0.719396	1.770792	0.087628
C	0.784526	0.379717	-1.881934
Li	-1.367873	0.744426	0.280597
O	0.426578	-0.010398	0.60354
O	2.511269	2.219294	0.49772
O	-2.724311	0.747301	-1.166077
O	-2.447931	-0.37942	1.43043
C	-2.201433	-1.707589	1.855506
C	-3.649767	0.157414	1.94635
C	-3.615717	-0.293532	-1.510767
C	-2.66028	1.75157	-2.165861
C	2.982499	3.550722	0.401624
C	3.542086	1.249661	0.393323
Si	1.045738	-1.201021	-0.710361
C	0.625053	-0.067371	2.00839
C	2.536047	-1.78161	-1.821383
C	-0.480952	-2.222193	-1.20844
O	1.661264	-2.044975	0.704416
C	2.25283	-3.309699	0.661126
H	-0.835703	3.726905	-0.149256
H	-0.639097	3.268962	1.528074
H	-2.084057	2.833489	0.658789
H	-0.100109	1.008692	-1.690638
H	0.679031	0.025062	-2.914389
H	1.669434	1.040646	-1.892871
H	-1.258632	-2.026231	1.40782
H	-3.013458	-2.367652	1.51855
H	-2.128362	-1.750585	2.950187
H	-4.506265	-0.468276	1.658613
H	-3.768183	1.156255	1.52176
H	-3.601415	0.223611	3.040762
H	-3.616235	-1.010693	-0.687877

H	-3.288143	-0.796208	-2.430464
H	-4.628363	0.107301	-1.654742
H	-2.277249	1.329391	-3.104186
H	-1.983373	2.523626	-1.798326
H	-3.657658	2.17833	-2.334725
H	2.116432	4.207928	0.5014
H	3.466948	3.718397	-0.569019
H	3.697578	3.758681	1.207143
H	4.004272	1.28759	-0.60188
H	3.09163	0.266804	0.55337
H	4.304745	1.429916	1.161221
H	0.390875	-1.052718	2.415112
H	-0.016614	0.694543	2.47355
H	1.668696	0.152024	2.266772
H	2.609624	-2.873378	-1.892635
H	3.49536	-1.43456	-1.408412
H	2.4642	-1.390444	-2.841985
H	-0.489251	-2.379049	-2.294387
H	-1.406889	-1.692153	-0.950804
H	-0.513747	-3.20749	-0.7266
H	3.295453	-3.270548	0.314148
H	1.708868	-4.007131	0.003097
H	2.247744	-3.732113	1.67428

Table 26: Standard orientation of **bBPR** [M062X/6-31+G(d) pcm].

Atomic Symbol	x	y	z
C	1.040173	2.877203	-0.703541
Li	-0.739309	1.839593	-0.244209
C	-0.838381	0.460224	1.839435
Li	1.386154	0.744947	-0.293973
O	-0.422758	-0.000538	-0.619104
O	-2.595495	2.159036	-0.590203
O	2.691927	0.807741	1.177707
O	2.483046	-0.414892	-1.395616
C	2.260615	-1.76426	-1.767988
C	3.706393	0.09801	-1.893091
C	3.617251	-0.196642	1.551685
C	2.617529	1.847101	2.141121
C	-3.137515	3.449649	-0.357034
C	-3.566542	1.130154	-0.468556
Si	-1.043701	-1.15618	0.717441
C	-0.573044	-0.115889	-2.026266
C	-2.547842	-1.737882	1.819293
C	0.482731	-2.143544	1.279027
O	-1.623558	-2.069454	-0.677903
C	-2.174916	-3.350531	-0.584252
H	0.899044	3.751261	-0.040386
H	0.742624	3.231303	-1.708658
H	2.140342	2.770008	-0.765362
H	0.04421	1.088484	1.639721
H	-0.759798	0.152573	2.889839
H	-1.731107	1.106811	1.784412
H	1.310558	-2.073482	-1.329441
H	3.069409	-2.400267	-1.382617
H	2.215392	-1.856093	-2.860736
H	4.548348	-0.520404	-1.55442
H	3.818627	1.110906	-1.501744
H	3.692324	0.122678	-2.989597
H	3.62236	-0.950064	0.762512
H	3.317936	-0.661753	2.499919
H	4.620811	0.234996	1.658309
H	2.251469	1.452766	3.097715
H	1.923008	2.593554	1.754099
H	3.607074	2.298592	2.285623
H	-2.327693	4.171185	-0.477639
H	-3.545422	3.51578	0.659305
H	-3.930048	3.66343	-1.083709
H	-3.969333	1.104422	0.552264
H	-3.076332	0.180175	-0.694415
H	-4.38248	1.30041	-1.181208
H	-0.291648	-1.105583	-2.389575

H	0.063094	0.645032	-2.500055
H	-1.613041	0.065346	-2.326483
H	-2.581027	-2.82729	1.944004
H	-3.505962	-1.448253	1.362338
H	-2.516303	-1.291766	2.819697
H	0.472409	-2.256242	2.370747
H	1.408255	-1.614647	1.018572
H	0.534747	-3.146286	0.836747
H	-3.224128	-3.33093	-0.255393
H	-1.620524	-3.999148	0.113473
H	-2.139931	-3.821302	-1.575532

Table 27: Standard orientation of **bBPR** [B3LYP/6-31+G(d)].

Atomic Symbol	x	y	z
C	-1.004385	2.893314	0.024217
Li	0.705873	1.70489	-0.279646
C	0.911192	0.023499	-2.005189
Li	-1.398041	0.74681	0.152891
O	0.427375	0.011873	0.51144
O	2.433481	2.467532	0.044145
O	-2.716731	0.436308	-1.339792
O	-2.513851	-0.067933	1.566297
C	-2.342343	-1.358269	2.149002
C	-3.605077	0.66555	2.11206
C	-3.594309	-0.676571	-1.46362
C	-2.631211	1.209217	-2.537339
C	2.565976	3.845627	0.389016
C	3.600842	1.692769	0.317022
Si	1.113133	-1.388249	-0.621663
C	0.672173	0.172827	1.910417
C	2.648148	-2.12585	-1.58366
C	-0.384143	-2.505806	-1.000943
O	1.669378	-1.99808	0.938657
C	2.307988	-3.226691	1.161692
H	-0.780245	3.624296	-0.779148
H	-0.715174	3.410715	0.961329
H	-2.112338	2.88608	0.053206
H	0.016025	0.66109	-1.931906
H	0.843984	-0.467861	-2.983793
H	1.793429	0.682986	-2.068575
H	-1.48134	-1.819898	1.664368
H	-3.23815	-1.975656	1.984982
H	-2.154378	-1.271754	3.228141
H	-4.554513	0.138585	1.935701
H	-3.624395	1.634663	1.609065
H	-3.468566	0.816448	3.192344
H	-3.620094	-1.174289	-0.492898
H	-3.230778	-1.380067	-2.225369
H	-4.607422	-0.340471	-1.729904
H	-2.207893	0.608275	-3.35421
H	-1.977533	2.054569	-2.320306
H	-3.62727	1.573861	-2.827041
H	1.611488	4.325115	0.162192
H	3.369161	4.312927	-0.197791
H	2.78427	3.954736	1.460778
H	4.449322	2.055298	-0.279528
H	3.377296	0.659389	0.047596
H	3.853979	1.741722	1.385017
H	0.319621	-0.684156	2.490454
H	0.152469	1.082463	2.246748
H	1.744043	0.279739	2.114617
H	2.764019	-3.207615	-1.440593
H	3.58535	-1.665315	-1.232086
H	2.588257	-1.943057	-2.663585
H	-0.469917	-2.680378	-2.081684
H	-1.327753	-2.060414	-0.666721
H	-0.286256	-3.482952	-0.510232
H	3.36869	-3.210479	0.864333
H	1.825243	-4.064025	0.627832
H	2.263686	-3.449482	2.238192

Table 28: Standard orientation of **bBPR** [B3LYP/6-31+G(d) pcm].

Atomic Symbol	x	y	z
C	1.081213	2.868414	-0.403874
Li	-0.696035	1.758989	-0.146362
C	-0.902393	0.309014	1.873433
Li	1.456274	0.70117	-0.210699
O	-0.411318	-0.06053	-0.61154
O	-2.493101	2.362473	-0.507463
O	2.69989	0.594855	1.375541
O	2.651163	-0.214547	-1.493697
C	2.593307	-1.591982	-1.861951
C	3.73737	0.485013	-2.098752
C	3.571358	-0.496278	1.660191
C	2.595524	1.515221	2.462643
C	-2.88457	3.712104	-0.248254
C	-3.599292	1.459379	-0.590399
Si	-1.15508	-1.248059	0.664413
C	-0.490764	-0.16318	-2.037485
C	-2.79309	-1.731668	1.623761
C	0.258242	-2.380827	1.268095
O	-1.68867	-2.097376	-0.808413
C	-2.31926	-3.35019	-0.832843
H	0.819463	3.65442	0.333672
H	0.850931	3.315219	-1.392109
H	2.187253	2.830189	-0.365759
H	0.007264	0.911126	1.733838
H	-0.862285	-0.067912	2.903945
H	-1.768177	0.990744	1.837008
H	1.753559	-2.034949	-1.324838
H	3.524054	-2.105149	-1.580929
H	2.434595	-1.695693	-2.94382
H	4.697875	0.052058	-1.785707
H	3.677619	1.523015	-1.766175
H	3.659088	0.445242	-3.193873
H	3.613129	-1.117012	0.764264
H	3.190816	-1.090306	2.502492
H	4.580149	-0.130716	1.898818
H	2.156822	1.024756	3.342536
H	1.947939	2.326785	2.129191
H	3.586323	1.913939	2.721627
H	-1.971495	4.310733	-0.214101
H	-3.410718	3.783946	0.713551
H	-3.536364	4.082529	-1.05059
H	-4.134101	1.416861	0.367871
H	-3.197143	0.473268	-0.827528
H	-4.289269	1.775966	-1.383516
H	-0.114917	-1.123833	-2.397416
H	0.11147	0.647618	-2.47099
H	-1.525211	-0.061917	-2.385385
H	-2.936501	-2.818027	1.690854
H	-3.675061	-1.332335	1.09994
H	-2.812519	-1.331941	2.645382
H	0.20723	-2.499373	2.359072
H	1.241285	-1.952999	1.038938
H	0.21544	-3.381059	0.817898
H	-3.392578	-3.28784	-0.589057
H	-1.863943	-4.075262	-0.135384
H	-2.231195	-3.768871	-1.847145

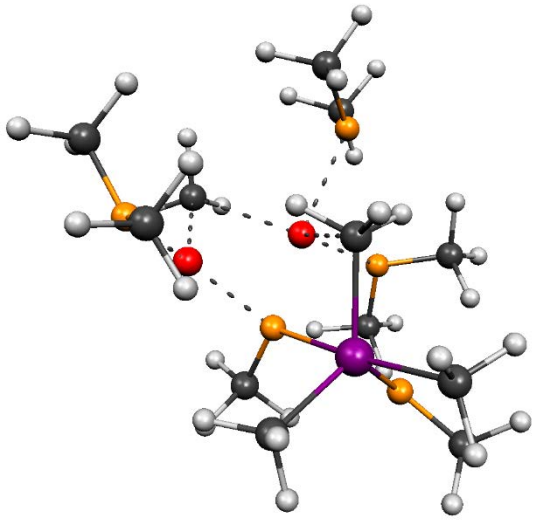


Figure 33: Molekel plot of **IM$_{ax}$** [M062X/6-31+G(d)].

Table 29: Standard orientation of **IM$_{ax}$** [M062X/6-31+G(d)].

Atomic Symbol	x	y	z
C	-2.410572	-1.001695	1.62572
Li	-1.508563	0.842649	1.245609
Li	-0.567907	-1.163717	0.44325
O	0.307863	0.542678	1.029661
O	-2.606093	2.207417	0.494289
O	-1.486465	-2.282554	-1.078986
O	0.854722	-2.519387	0.475202
C	1.566066	-2.773763	-0.727028
C	1.704144	-2.569341	1.608944
C	-1.866793	-3.549118	-0.563439
C	-2.518979	-1.722568	-1.868242
C	-3.97486	1.849633	0.381851
C	-2.208709	3.149862	-0.48871
Si	1.418492	1.312577	-0.415958
C	0.804593	0.56069	2.348968
C	1.361887	3.00728	0.468918
H	-3.297714	-1.269227	1.025247
H	-2.828874	-0.594519	2.567844
H	-1.992066	-1.975657	1.953035
H	0.835385	-2.765698	-1.538246
H	2.047644	-3.759788	-0.672714
H	2.318558	-1.992794	-0.886153
H	2.134498	-3.574967	1.708871
H	1.090724	-2.347785	2.484939
H	2.497449	-1.820522	1.512466
H	-1.041981	-3.907123	0.054093
H	-2.049526	-4.250747	-1.388672
H	-2.772723	-3.456211	0.048984
H	-2.794215	-2.414475	-2.675752
H	-2.140698	-0.795354	-2.299923
H	-3.401143	-1.511637	-1.249505
H	-4.192806	1.131098	1.17297
H	-4.163394	1.382649	-0.593681
H	-4.606585	2.740037	0.492588
H	-2.416022	2.760293	-1.493912

H	-1.135304	3.308472	-0.378014
H	-2.745804	4.095095	-0.341569
H	1.821509	0.156233	2.394744
H	0.153905	-0.043411	3.002021
H	0.833599	1.584412	2.754379
H	1.312764	3.824959	-0.260104
H	2.312024	3.135847	1.007868
H	0.557616	3.138248	1.201627
C	-0.025803	0.695985	-1.524102
H	0.216358	-0.333296	-1.834633
H	-0.116245	1.281774	-2.445761
H	-1.013934	0.6676	-1.044644
C	3.9259	0.177897	-0.125525
H	4.405371	-0.63346	0.437911
H	4.135251	0.026138	-1.192532
H	4.393891	1.123653	0.181373
O	2.552133	0.151632	0.160197
C	2.477682	1.943655	-1.93555
H	3.435078	2.410333	-1.666196
H	2.696284	1.149151	-2.664637
H	1.897016	2.708428	-2.471203

Table 30: Standard orientation of **IM_{ax}** [M062X/6-31+G(d) pcm].

Atomic Symbol	x	y	z
C	2.374962	1.079053	1.655948
Li	1.523104	-0.832926	1.327514
Li	0.533977	1.166834	0.463162
O	-0.314586	-0.552905	1.052154
O	2.66935	-2.139067	0.491021
O	1.444674	2.285788	-1.066488
O	-0.928064	2.485782	0.462136
C	-1.628111	2.742755	-0.745662
C	-1.784544	2.552379	1.589873
C	1.750279	3.591059	-0.598613
C	2.512501	1.76049	-1.83534
C	4.030494	-1.748033	0.378781
C	2.293953	-3.07246	-0.510545
Si	-1.37382	-1.34407	-0.398245
C	-0.840992	-0.568288	2.360204
C	-1.292766	-3.042287	0.482813
H	3.236019	1.347572	1.020252
H	2.816647	0.688585	2.593681
H	1.930014	2.047702	1.962646
H	-0.892969	2.724525	-1.552503
H	-2.10228	3.732239	-0.699198
H	-2.387332	1.968503	-0.907622
H	-2.207723	3.56156	1.679201
H	-1.180202	2.331758	2.472228
H	-2.585372	1.810778	1.494367
H	0.901364	3.928665	-0.002722
H	1.905022	4.26887	-1.448332
H	2.65404	3.571614	0.023841
H	2.747891	2.44004	-2.664661
H	2.194526	0.797117	-2.235724
H	3.404416	1.625139	-1.209855
H	4.244062	-1.060214	1.197818
H	4.19981	-1.239026	-0.578657
H	4.681564	-2.627901	0.447646
H	2.488107	-2.658297	-1.508125
H	1.225364	-3.261857	-0.399627
H	2.855894	-4.005703	-0.384248
H	-1.851809	-0.148355	2.385746
H	-0.197039	0.026535	3.027779

H	-0.889035	-1.592595	2.761954
H	-1.203522	-3.855399	-0.247554
H	-2.248325	-3.196915	1.005168
H	-0.494133	-3.148281	1.225785
C	0.06096	-0.696297	-1.496245
H	-0.200333	0.325701	-1.814206
H	0.179884	-1.285745	-2.412245
H	1.041448	-0.643329	-1.004327
C	-3.921812	-0.271798	-0.189671
H	-4.436695	0.520292	0.369103
H	-4.093703	-0.102651	-1.261066
H	-4.383981	-1.231915	0.080163
O	-2.56079	-0.226349	0.147544
C	-2.393922	-2.019286	-1.93983
H	-3.340328	-2.51474	-1.681483
H	-2.625589	-1.233323	-2.674727
H	-1.774143	-2.765422	-2.458308

Table 31: Standard orientation of **IM_{ax}** [B3LYP/6-31+G(d)].

Atomic Symbol	x	y	z
C	0.83958	-2.839553	0.58331
Li	1.696279	-1.099757	-0.20078
Li	-0.640347	-1.235989	0.081948
O	0.46216	0.085171	-0.904694
O	3.601532	-0.924546	-0.180865
O	-1.585231	-0.925968	1.819431
O	-2.058775	-1.965175	-1.085361
C	-2.266685	-3.354571	-1.312707
C	-2.953758	-1.128289	-1.811867
C	-1.00705	-1.236653	3.083853
C	-2.743627	-0.107103	1.92707
C	4.411355	-2.008363	0.275134
C	4.295174	0.320664	-0.245887
C	0.241096	-0.045068	-2.295717
H	1.522338	-2.97852	1.445981
H	1.185259	-3.57771	-0.169573
H	-0.119187	-3.256486	0.946782
H	-1.511249	-3.892851	-0.738126
H	-2.152299	-3.591444	-2.380893
H	-3.271831	-3.655044	-0.98145
H	-2.864249	-1.313132	-2.892368
H	-2.66385	-0.100627	-1.591403
H	-3.992854	-1.311423	-1.499003
H	-0.118107	-1.837347	2.889752
H	-1.716845	-1.809222	3.699006
H	-0.723537	-0.317411	3.615207
H	-3.507217	-0.601004	2.546559
H	-3.123463	0.048855	0.918254
H	-2.490207	0.868913	2.363937
H	3.772862	-2.893309	0.306765
H	4.799862	-1.801039	1.282144
H	5.250742	-2.17504	-0.414317
H	4.679702	0.599307	0.745317
H	3.578214	1.070944	-0.58209
H	5.129719	0.25827	-0.958087
H	-0.578819	0.605735	-2.632258
H	-0.029009	-1.082106	-2.552546
H	1.137395	0.220521	-2.880797
Si	0.161288	1.957889	-0.029652
C	1.273217	2.711288	-1.392681
C	1.005522	1.168765	1.503326
C	-2.543828	2.46401	-0.460661
O	-1.471665	1.543475	-0.442105
C	-0.20507	3.658019	0.872374
H	1.857157	3.541493	-0.974872
H	0.638251	3.142319	-2.180385
H	1.958779	2.011821	-1.881048
H	0.494245	1.496524	2.416282
H	2.030068	1.564809	1.565343

H	1.065875	0.075926	1.541952
H	-3.425197	1.950186	-0.870368
H	-2.802735	2.830867	0.542573
H	-2.338117	3.335419	-1.098592
H	-0.589805	4.447565	0.211124
H	-0.90714	3.56505	1.714564
H	0.739705	4.033453	1.293739

Table 32: Standard orientation of **IM_{ax}** [B3LYP/6-31+G(d) pcm].

Atomic Symbol	x	y	z
C	1.029165	-2.753726	0.633511
Li	1.826449	-0.96967	-0.180328
Li	-0.542605	-1.242761	0.070577
O	0.49793	0.16236	-0.855886
O	3.744243	-0.748288	-0.14289
O	-1.613255	-1.038284	1.761702
O	-1.836884	-2.105335	-1.158838
C	-2.039194	-3.512925	-1.247539
C	-2.818952	-1.348929	-1.864487
C	-1.073684	-1.282007	3.059137
C	-2.830642	-0.298898	1.803107
C	4.585932	-1.834446	0.251956
C	4.415532	0.512921	-0.148941
C	0.35497	0.023152	-2.257454
H	1.710621	-2.807375	1.50661
H	1.433795	-3.487088	-0.094137
H	0.089225	-3.21131	0.995556
H	-1.21878	-3.991388	-0.710569
H	-2.029708	-3.836847	-2.298021
H	-2.99797	-3.796282	-0.789705
H	-2.809097	-1.607388	-2.932955
H	-2.555138	-0.299464	-1.732984
H	-3.821905	-1.542106	-1.456036
H	-0.135725	-1.820663	2.919974
H	-1.768585	-1.891212	3.654679
H	-0.880332	-0.335067	3.58151
H	-3.584559	-0.834488	2.398018
H	-3.174973	-0.186036	0.776011
H	-2.663206	0.697935	2.233332
H	3.970643	-2.736025	0.24257
H	4.977618	-1.668243	1.26468
H	5.422644	-1.944605	-0.450945
H	4.804276	0.746872	0.851508
H	3.68282	1.267161	-0.440428
H	5.243576	0.503375	-0.870419
H	-0.525362	0.569785	-2.625465
H	0.224906	-1.035582	-2.533684
H	1.236107	0.405914	-2.799002
Si	-0.000857	2.002407	-0.007824
C	1.132819	2.82082	-1.316632
C	0.812461	1.288354	1.574239
C	-2.720861	2.281972	-0.564932
O	-1.568585	1.465215	-0.508197
C	-0.552162	3.67927	0.854803
H	1.509893	3.783551	-0.949515
H	0.553739	3.02819	-2.227955
H	1.984364	2.199696	-1.613146
H	0.273841	1.631114	2.465831
H	1.831559	1.697873	1.642465
H	0.887939	0.198313	1.634311
H	-3.53153	1.692209	-1.014315
H	-3.054022	2.610793	0.429537
H	-2.570738	3.176051	-1.187032
H	-0.966598	4.427503	0.163364
H	-1.287538	3.528838	1.659403
H	0.338776	4.130909	1.318007

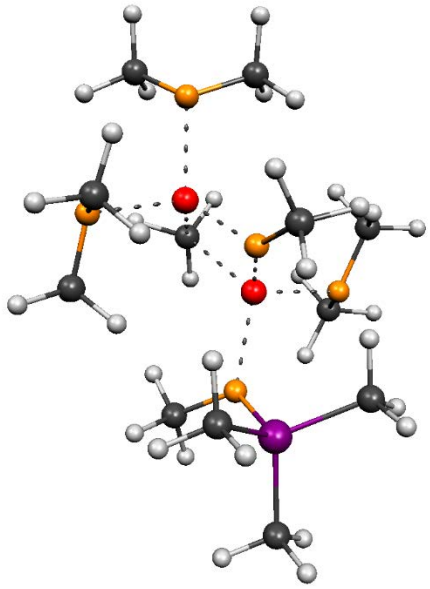


Figure 34: Molekel plot of **Pr** [M062X/6-31+G(d)].

Table 33: Standard orientation of **Pr** [M062X/6-31+G(d)].

Atomic Symbol	x	y	z
Si	-2.866858	-0.544761	-0.391345
C	-4.631313	-0.758073	0.224968
C	-2.022657	-0.696563	2.180097
O	-1.927115	-0.037712	0.926551
C	0.617471	-0.178471	-2.426984
C	-2.758149	0.808805	-1.667891
O	0.526629	-0.076322	-1.058199
Li	-0.221497	0.741628	0.382392
Li	1.809119	-0.285141	0.209092
C	1.303937	0.858331	1.93821
O	2.053558	-2.209324	0.604389
O	3.62356	0.089697	-0.352488
C	3.664197	1.369197	-0.955179
C	4.53046	-0.034167	0.729155
C	2.147068	-2.841624	-0.660857
C	0.880948	-2.59231	1.30048
O	-0.744419	2.604676	0.068872
C	0.283466	3.216084	-0.685211
C	-1.048114	3.316115	1.252148
C	-2.20474	-2.180395	-1.022874
H	-5.292639	-1.034193	-0.604729
H	-4.711991	-1.546055	0.98266
H	-5.014853	0.171843	0.660177
H	-2.06034	-1.788146	2.058829
H	-1.135945	-0.439851	2.764672
H	-2.92309	-0.370752	2.714516
H	1.572584	-0.631798	-2.761778
H	-0.189622	-0.798734	-2.869782
H	0.551053	0.804185	-2.941986
H	-3.151393	1.751218	-1.27298
H	-3.333755	0.537846	-2.560832
H	-1.717016	0.97428	-1.961609

H	0.496915	1.139034	2.641819
H	1.909485	1.784117	1.847906
H	1.94061	0.175974	2.535751
H	2.886162	1.385694	-1.721593
H	4.64742	1.54492	-1.41192
H	3.460052	2.149395	-0.209043
H	5.563499	0.077701	0.373513
H	4.385096	-1.030206	1.151643
H	4.317913	0.722051	1.496455
H	2.260562	-3.926994	-0.535575
H	3.027008	-2.428662	-1.1591
H	1.254263	-2.623686	-1.26115
H	-0.008169	-2.2837	0.732917
H	0.895222	-2.076913	2.262432
H	0.866147	-3.680655	1.453404
H	-0.034898	4.209138	-1.031118
H	0.481379	2.563942	-1.538433
H	1.196123	3.308895	-0.080517
H	-1.813508	2.743454	1.780611
H	-1.435852	4. 314858	1.008285
H	-0.157163	3.408768	1.886744
H	-1.151278	-2.053331	-1.295581
H	-2.280498	-2.974931	-0.270718
H	-2.759489	-2.511197	-1.908882

Table 34: Standard orientation of **Pr** [M062X/6-31+G(d) pcm].

Atomic Symbol	x	y	z
Si	-2.868228	-0.548856	-0.405546
C	-4.636634	-0.7595	0.194837
C	-2.060587	-0.68599	2.17473
O	-1.936284	-0.035421	0.917036
C	0.622545	-0.175147	-2.416036
C	-2.747755	0.804161	-1.683707
O	0.536894	-0.079233	-1.047272
Li	-0.222674	0.742238	0.384724
Li	1.82485	-0.291274	0.21507
C	1.315339	0.866856	1.943328
O	2.039778	-2.216746	0.638063
O	3.634738	0.08587	-0.364187
C	3.683599	1.367029	-0.967536
C	4.570446	-0.052844	0.69201
C	2.148783	-2.865473	-0.61914
C	0.844624	-2.576954	1.311863
O	-0.737148	2.609475	0.084903
C	0.280696	3.24129	-0.668174
C	-1.0622	3.321186	1.263532
C	-2.199721	-2.18453	-1.02975
H	-5.288104	-1.033721	-0.643273
H	-4.722859	-1.5484	0.950809
H	-5.021385	0.171143	0.627485
H	-2.091905	-1.777992	2.060962
H	-1.189133	-0.423159	2.778844
H	-2.973246	-0.357722	2.685338
H	1.575196	-0.629938	-2.756543
H	-0.188191	-0.79185	-2.85808
H	0.557563	0.8102	-2.926079
H	-3.169334	1.739037	-1.299682
H	-3.296799	0.520329	-2.589258
H	-1.701952	0.987124	-1.949504
H	0.491398	1.127041	2.634953
H	1.906329	1.800611	1.849357
H	1.958261	0.181725	2.530867

H	2.89221	1.397069	-1.719497
H	4.660432	1.528339	-1.441203
H	3.505993	2.14955	-0.217534
H	5.593954	0.052109	0.310069
H	4.429063	-1.049642	1.113866
H	4.387118	0.702638	1.46742
H	2.220706	-3.952233	-0.481214
H	3.056864	-2.489809	-1.095483
H	1.280725	-2.623116	-1.245669
H	-0.026397	-2.253329	0.725777
H	0.847694	-2.060765	2.273466
H	0.80679	-3.663849	1.466467
H	-0.057161	4.225588	-1.018664
H	0.496279	2.590955	-1.518583
H	1.188877	3.357563	-0.061031
H	-1.815498	2.734842	1.794345
H	-1.470663	4.309315	1.013301
H	-0.174939	3.439567	1.899107
H	-1.145525	-2.058805	-1.30037
H	-2.277086	-2.973683	-0.272144
H	-2.755248	-2.51771	-1.914445

Table 35: Standard orientation of **Pr** [B3LYP/6-31+G(d)].

Atomic Symbol	x	y	z
Si	-2.930794	-0.625111	-0.390112
C	-4.679104	-0.994535	0.221062
C	-1.988075	-0.773823	2.169446
O	-2.01664	-0.056721	0.931599
C	0.611602	-0.004884	-2.464819
C	-2.926255	0.764338	-1.645854
O	0.551586	0.026694	-1.086825
Li	-0.260486	0.769026	0.372432
Li	1.791866	-0.266773	0.220219
C	1.226583	0.820661	1.98722
O	2.144822	-2.235238	0.486013
O	3.662996	0.204142	-0.296553
C	3.723004	1.474755	-0.936571
C	4.601497	0.062565	0.767267
C	2.278478	-2.844322	-0.796792
C	1.160041	-2.863467	1.300637
O	-0.780502	2.67774	0.086864
C	0.317184	3.378875	-0.488536
C	-1.372206	3.358531	1.186404
C	-2.11156	-2.187146	-1.043174
H	-5.312537	-1.332334	-0.60975
H	-4.689386	-1.785458	0.981716
H	-5.148514	-0.102693	0.655436
H	-1.801795	-1.844583	2.008235
H	-1.172262	-0.369795	2.772636
H	-2.938832	-0.6544	2.705232
H	1.550483	-0.460591	-2.847929
H	-0.216253	-0.586901	-2.924428
H	0.554477	1.006892	-2.927519
H	-3.364818	1.676941	-1.226033
H	-3.506817	0.481039	-2.533431
H	-1.904748	0.996913	-1.960226
H	0.405976	1.266578	2.584786
H	1.960324	1.649733	1.892844
H	1.704751	0.108962	2.690493
H	2.948098	1.474846	-1.70531
H	4.709932	1.628722	-1.397527
H	3.524358	2.282883	-0.217699
H	5.629881	0.16788	0.390988
H	4.457827	-0.939149	1.178115
H	4.416433	0.809368	1.552086
H	2.58948	-3.894762	-0.694907
H	3.045374	-2.28073	-1.332545
H	1.333145	-2.786706	-1.352527
H	0.180984	-2.855925	0.801953

H	1.09868	-2.284696	2.224072
H	1.448438	-3.901845	1.523552
H	-0.013073	4.3469	-0.894092
H	0.700948	2.746525	-1.290925
H	1.108711	3.540472	0.257202
H	-2.183085	2.722432	1.548902
H	-1.778482	4.330219	0.867462
H	-0.640381	3.512877	1.992154
H	-1.060125	-1.960455	-1.252579
H	-2.15678	-3.00831	-0.316305
H	-2.588665	-2.53828	-1.967048

Table 36: Standard orientation of **Pr** [B3LYP/6-31+G(d) pcm].

Atomic Symbol	x	y	z
Si	-2.89254	-0.7473	-0.418507
C	-4.619258	-1.239469	0.161808
C	-2.004571	-0.761284	2.168724
O	-2.047564	-0.084749	0.906333
C	0.648791	0.140652	-2.428129
C	-2.96693	0.623485	-1.694366
O	0.585649	0.121411	-1.051233
Li	-0.301494	0.801088	0.394102
Li	1.804143	-0.20323	0.267768
C	1.140214	0.805378	2.070648
O	2.220031	-2.176481	0.482709
O	3.662835	0.316129	-0.282273
C	3.720066	1.61802	-0.860848
C	4.702827	0.074829	0.662756
C	2.428107	-2.742718	-0.811396
C	1.307174	-2.930808	1.27645
O	-0.916253	2.681313	0.100713
C	0.164627	3.498005	-0.340807
C	-1.730654	3.30557	1.087301
C	-1.944149	-2.24668	-1.042614
H	-5.21198	-1.605134	-0.687058
H	-4.587211	-2.041441	0.909825
H	-5.153618	-0.386804	0.599769
H	-1.591267	-1.773137	2.063934
H	-1.351597	-0.191357	2.833051
H	-3.007803	-0.825504	2.608496
H	1.64467	-0.160194	-2.8217
H	-0.084912	-0.544504	-2.907073
H	0.442646	1.146917	-2.859025
H	-3.496177	1.498889	-1.299911
H	-3.495499	0.279197	-2.592691
H	-1.959362	0.93727	-1.983287
H	0.394128	1.530597	2.456052
H	2.101402	1.360157	2.108022
H	1.218208	0.033787	2.862836
H	2.873757	1.693295	-1.545543
H	4.662173	1.755034	-1.41071
H	3.634535	2.392979	-0.085402
H	5.688585	0.157222	0.18297
H	4.556449	-0.940297	1.037727
H	4.643186	0.787263	1.498014
H	2.847846	-3.755418	-0.72608
H	3.133552	-2.090537	-1.330122
H	1.485803	-2.778693	-1.374325
H	0.328519	-3.001394	0.782318
H	1.197342	-2.401465	2.224708
H	1.697328	-3.943126	1.456298
H	-0.212254	4.424105	-0.798502
H	0.712992	2.911663	-1.080345
H	0.832562	3.747931	0.496133
H	-2.505884	2.585098	1.35664
H	-2.194144	4.218583	0.68625
H	-1.14044	3.560181	1.979711
H	-0.910411	-1.942547	-1.242605
H	-1.936232	-3.059007	-0.304826

H	-2.384342	-2.64184	-1.967215

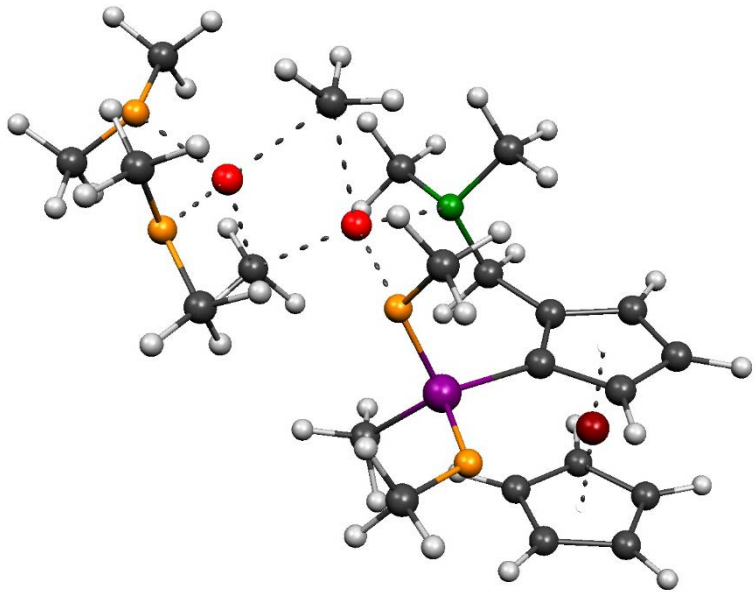


Figure 35: Molekel plot of **EdFc** [M062X/6-31+G(d)].

Table 37: Standard orientation of **EdFc** [M062X/6-31+G(d)].

Atomic Symbol	x	y	z
Fe	3.625735	-0.300636	0.108618
Si	0.584612	1.402579	-0.063942
N	-0.397775	-2.139057	-0.617279
C	1.818986	0.264528	-0.825008
C	1.886794	-1.165565	-0.719905
C	3.020731	-1.606496	-1.452911
C	3.666542	-0.470781	-2.011012
C	2.924963	0.675752	-1.633773
C	4.084384	0.939381	1.758393
C	3.610442	-0.317655	2.224887
C	4.493639	-1.323447	1.747704
C	5.513195	-0.689168	0.987545
C	5.260377	0.709552	0.995633
C	-1.005598	1.445934	-2.206596
C	0.932506	-2.069623	0.009581
C	-0.296921	-2.46544	-2.040777
C	-1.184795	-3.172765	0.062501
C	-2.544721	-0.638816	1.711008
Li	-3.989504	-0.290529	0.172372
Li	-1.826389	-0.568012	-0.352389
C	-3.443101	-0.95176	-1.792231
C	0.315588	1.258791	1.770219
O	-0.901847	1.176741	-0.807515
O	-4.6362	1.568601	0.246949
O	-5.684195	-1.062245	0.738682
C	-5.615452	1.852099	-0.733213
C	-3.605791	2.536813	0.281961
C	-5.716089	-2.461134	0.521325
C	-6.015125	-0.708937	2.070548
H	3.352921	-2.635239	-1.528696
H	4.583111	-0.477521	-2.586462
H	3.171404	1.70495	-1.863913
H	3.609825	1.899702	1.914743
H	2.714609	-0.483776	2.810148
H	4.384511	-2.389108	1.902592
H	6.317582	-1.187313	0.462503

H	5.834355	1.46357	0.473448
H	-0.565929	2.422325	-2.443054
H	-2.065136	1.433676	-2.468486
H	-0.489918	0.671084	-2.786414
H	1.3803	-3.080909	0.05306
H	0.785607	-1.738656	1.045415
H	0.236593	-1.673094	-2.572047
H	-1.30376	-2.553795	-2.455931
H	0.244187	-3.416636	-2.196972
H	-0.74119	-4.172325	-0.092296
H	-2.205456	-3.164285	-0.330617
H	-1.22813	-2.96002	1.133583
H	-1.514033	-0.883078	2.025236
H	-3.12267	-1.53408	2.021409
H	-2.858915	0.156651	2.414467
H	-4.433187	-0.540191	-2.077169
H	-2.807807	-0.718027	-2.665311
H	-3.586894	-2.048734	-1.852135
H	1.085834	1.833103	2.298626
H	-0.672365	1.632651	2.059313
H	0.368563	0.223422	2.116252
H	-6.346168	1.041544	-0.698796
H	-5.159497	1.88988	-1.73197
H	-6.107145	2.810673	-0.5174
H	-3.129452	2.625894	-0.703485
H	-2.864433	2.184814	1.000676
H	-4.011919	3.511602	0.586498
H	-5.457271	-2.628315	-0.525498
H	-6.720145	-2.855366	0.727697
H	-4.984598	-2.965323	1.168113
H	-7.047828	-1.007753	2.295043
H	-5.913174	0.37515	2.145688
H	-5.327427	-1.188067	2.779123
O	1.120388	2.926338	-0.461623
C	0.35332	4.05578	-0.086394
H	0.268304	4.134757	1.005383
H	0.854952	4.949154	-0.465484
H	-0.658196	4.008717	-0.513588

Table 38: Standard orientation of **EdFc** [B3LYP/6-31+G(d)].

Atomic Symbol	x	y	z
Fe	-3.633577	0.331117	0.133529
Si	-0.622573	-1.485298	-0.022377
N	0.368077	2.14174	-0.691219
C	-1.882392	-0.33187	-0.733978
C	-1.915316	1.11234	-0.673759
C	-3.053655	1.557099	-1.416996
C	-3.737092	0.416665	-1.930454
C	-3.018866	-0.741501	-1.515519
C	-3.816572	-0.558814	1.986701
C	-3.70083	0.858631	2.124646
C	-4.786921	1.459441	1.415906
C	-5.569877	0.41285	0.83795
C	-4.969193	-0.834902	1.190381
C	0.964321	-1.545321	-2.211077
C	-0.93676	2.033037	0.004349
C	0.20093	2.43289	-2.122271
C	1.162469	3.208455	-0.059228
C	2.544992	0.654829	1.685439
Li	4.006983	0.320201	0.145649
Li	1.828867	0.534766	-0.391085
C	3.431423	0.873691	-1.856302
C	-0.270346	-1.361913	1.808419
O	0.847108	-1.235228	-0.811305
O	4.736455	-1.560459	0.257336
O	5.728331	1.184644	0.711492
C	5.759891	-1.863047	-0.684946
C	3.740562	-2.574386	0.351452
C	5.803468	2.584309	0.455026
C	6.106077	0.838214	2.043157

H	-3.358325	2.590654	-1.528203
H	-4.65991	0.42689	-2.496601
H	-3.291616	-1.770091	-1.712772
H	-3.129953	-1.293824	2.383073
H	-2.911077	1.384922	2.645995
H	-4.964435	2.521672	1.305298
H	-6.442801	0.543992	0.211162
H	-5.303952	-1.815164	0.876294
H	0.577054	-2.550032	-2.417509
H	2.022569	-1.488282	-2.471111
H	0.410862	-0.818351	-2.818084
H	-1.407861	3.030817	0.082403
H	-0.729765	1.698028	1.02641
H	-0.328526	1.612681	-2.61302
H	1.186966	2.535645	-2.581269
H	-0.37157	3.364696	-2.287449
H	0.690116	4.199188	-0.196999
H	2.161609	3.222616	-0.502697
H	1.267066	3.010131	1.010145
H	1.500582	0.88656	1.966325
H	3.106832	1.555787	2.010822
H	2.844642	-0.135687	2.402438
H	4.32067	0.320098	-2.222704
H	2.692589	0.735941	-2.668124
H	3.722435	1.941326	-1.941543
H	-0.872376	-2.100927	2.351072
H	0.787064	-1.540442	2.023243
H	-0.513105	-0.373321	2.208719
H	6.449909	-1.01643	-0.683017
H	5.339195	-1.986693	-1.693015
H	6.293695	-2.780772	-0.395424
H	3.253019	-2.733388	-0.620292
H	2.997431	-2.214991	1.063614
H	4.18507	-3.518311	0.701247
H	5.503164	2.732383	-0.58387
H	6.83115	2.947982	0.601902
H	5.12229	3.138133	1.117586
H	7.150967	1.125515	2.231967
H	5.995591	-0.244668	2.127359
H	5.448919	1.327992	2.774711
O	-1.182703	-3.005378	-0.428006
C	-0.48596	-4.191443	-0.063943
H	-0.39126	-4.284666	1.027379
H	-1.056579	-5.046291	-0.439861
H	0.520955	-4.217431	-0.505076

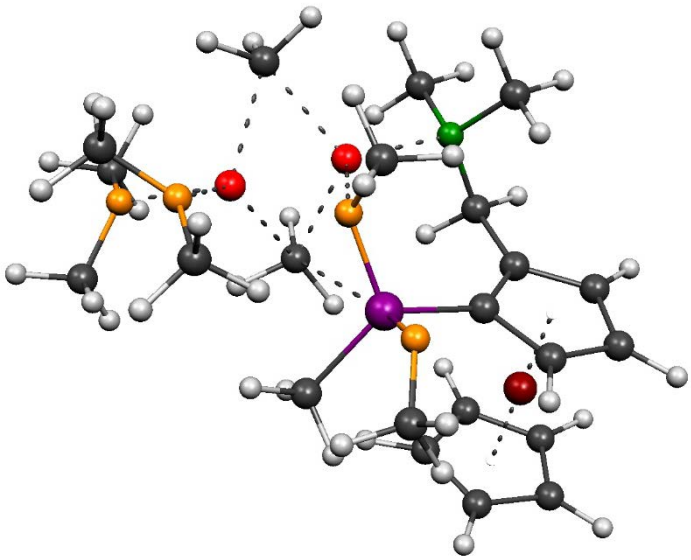


Figure 36: Molekel plot of **AtFc** [M062X/6-31+G(d)].

Table 39: Standard orientation of **AtFc** [M062X/6-31+G(d)].

Atomic Symbol	x	y	z
Fe	-3.150771	-0.253353	0.321676
Si	0.222116	-1.026781	-0.601234
N	-0.16553	2.879469	-0.812048
C	-1.409973	-0.164197	-0.898868
C	-1.959053	1.156608	-0.711365
C	-3.276367	1.167085	-1.246317
C	-3.578739	-0.12058	-1.754855
C	-2.434479	-0.92569	-1.557254
C	-2.69036	-0.912845	2.286279
C	-3.381656	0.325671	2.344487
C	-4.65938	0.143917	1.747388
C	-4.75459	-1.206841	1.317615
C	-3.536119	-1.860471	1.648889
C	1.859585	-0.010606	-2.522819
C	-1.355936	2.391986	-0.097795
C	-0.425139	3.088753	-2.233432
C	0.294583	4.126019	-0.198297
C	0.92995	0.849694	1.645383
Li	3.000905	0.387923	0.304866
Li	1.363363	1.688072	-0.25828
C	3.35232	2.400642	-0.479873
C	0.475159	-2.071871	0.931954
O	1.516136	-0.085638	-1.13768
O	4.13138	-1.08202	-0.549474
O	4.145323	0.254507	1.919584
C	5.533182	-0.905278	-0.462852
C	3.782839	-2.351284	-1.059506
C	4.168344	1.412132	2.740448
C	4.092213	-0.940549	2.667692
H	-3.94403	2.020335	-1.221679
H	-4.519504	-0.437848	-2.185629
H	-2.347267	-1.96615	-1.842192
H	-1.681196	-1.086345	2.634534
H	-2.98482	1.252195	2.739742
H	-5.409521	0.910537	1.603655
H	-5.591084	-1.649158	0.792491
H	-3.286221	-2.890018	1.426726
H	2.22916	-0.974347	-2.882365
H	2.635343	0.753431	-2.608646
H	0.984545	0.270869	-3.119921
H	-2.135201	3.178272	-0.097024
H	-1.060988	2.216317	0.939677
H	-0.749573	2.153553	-2.696289
H	0.496488	3.424494	-2.718468
H	-1.209897	3.849493	-2.395096
H	-0.467232	4.920791	-0.284685
H	1.21615	4.455703	-0.686428
H	0.508492	3.955836	0.861562
H	-0.11045	0.59276	1.911156
H	1.070335	1.888605	2.009203
H	1.550551	0.236915	2.322859
H	4.412474	2.077456	-0.51257
H	3.191401	2.835367	-1.487086
H	3.359021	3.276087	0.196747
H	-0.256613	-2.890325	0.934472
H	1.473416	-2.52996	0.896319
H	0.390667	-1.524072	1.867543
H	5.711451	0.104764	-0.09549
H	5.991998	-1.032607	-1.451993
H	5.971398	-1.63234	0.23633
H	4.25592	-2.51599	-2.037354
H	2.697831	-2.378568	-1.179303
H	4.104745	-3.146845	-0.370629
H	4.180926	2.272861	2.071128
H	5.067379	1.40451	3.371247
H	3.270378	1.449755	3.369725
H	4.988873	-1.042315	3.294737
H	4.048346	-1.767852	1.954101

H	3.198152	-0.961105	3.305841
O	0.242241	-2.195619	-1.825495
C	-0.063159	-3.560152	-1.692861
H	-1.042097	-3.726813	-1.21971
H	-0.087148	-4.00419	-2.692681
H	0.693736	-4.088925	-1.095999

Table 40: Standard orientation of **AtFc** [B3LYP/6-31+G(d)].

Atomic Symbol	x	y	z
Fe	-3.169319	-0.207862	0.383456
Si	0.196866	-1.131631	-0.492689
N	-0.211707	2.759836	-1.09662
C	-1.469832	-0.318674	-0.796721
C	-2.005462	1.031795	-0.76437
C	-3.339867	0.991874	-1.282148
C	-3.667212	-0.350352	-1.618311
C	-2.525104	-1.146301	-1.333126
C	-2.678042	-0.816039	2.296408
C	-3.140975	0.533729	2.307022
C	-4.472529	0.547223	1.788085
C	-4.830083	-0.795735	1.45379
C	-3.719071	-1.638949	1.767665
C	1.722201	-0.288791	-2.625231
C	-1.385839	2.326417	-0.304338
C	-0.499283	2.813341	-2.53418
C	0.245717	4.074513	-0.620818
C	0.960773	0.930971	1.516028
Li	3.061625	0.406325	0.268009
Li	1.363012	1.601545	-0.467504
C	3.366009	2.271699	-0.823693
C	0.553208	-2.053049	1.108597
O	1.451323	-0.237366	-1.21168
O	4.250391	-1.220229	-0.299696
O	4.194104	0.557598	1.966918
C	5.635738	-0.892264	-0.405895
C	3.906797	-2.371515	-1.062769
C	4.170481	1.838371	2.599931
C	4.236459	-0.521699	2.892053
H	-3.999543	1.848537	-1.352939
H	-4.620186	-0.705631	-1.989837
H	-2.458899	-2.214745	-1.484225
H	-1.694315	-1.145774	2.598076
H	-2.562878	1.395518	2.615068
H	-5.088494	1.424679	1.637391
H	-5.763603	-1.112658	1.006218
H	-3.664576	-2.707713	1.603696
H	1.945425	-1.310117	-2.942716
H	2.577384	0.367816	-2.800799
H	0.858635	0.07279	-3.195918
H	-2.171787	3.103759	-0.348274
H	-1.060323	2.251062	0.733574
H	-0.809792	1.827559	-2.888413
H	0.406588	3.111976	-3.071408
H	-1.302798	3.536184	-2.767453
H	-0.517382	4.857583	-0.785089
H	1.164	4.354894	-1.145162
H	0.465729	4.023019	0.450172
H	-0.068549	0.702664	1.835032
H	1.103748	2.007598	1.742593
H	1.605616	0.405895	2.239719
H	4.420393	1.930654	-0.884271
H	3.131803	2.555536	-1.871553
H	3.427032	3.239974	-0.288002
H	-0.146409	-2.894286	1.201381
H	1.565762	-2.475816	1.065226
H	0.484608	-1.441876	2.005524
H	5.80476	-0.019426	0.224815
H	5.896273	-0.654717	-1.446927
H	6.257166	-1.730362	-0.056298

H	4.167397	-2.229829	-2.121397
H	2.829885	-2.514779	-0.980626
H	4.432718	-3.258468	-0.678774
H	4.138205	2.57973	1.801213
H	5.074972	1.975736	3.210649
H	3.276103	1.939187	3.228743
H	5.144899	-0.467237	3.510518
H	4.247402	-1.442054	2.303768
H	3.352337	-0.512992	3.54571
O	0.156528	-2.415558	-1.615249
C	-0.068385	-3.787818	-1.385756
H	-1.034138	-3.980135	-0.891759
H	-0.075785	-4.299951	-2.35531
H	0.721887	-4.237048	-0.765002

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