Electronic Supplementary Information

Enantioselective deprotometalation of *N*,*N*-dialkyl ferrocenecarboxamides using metal amides

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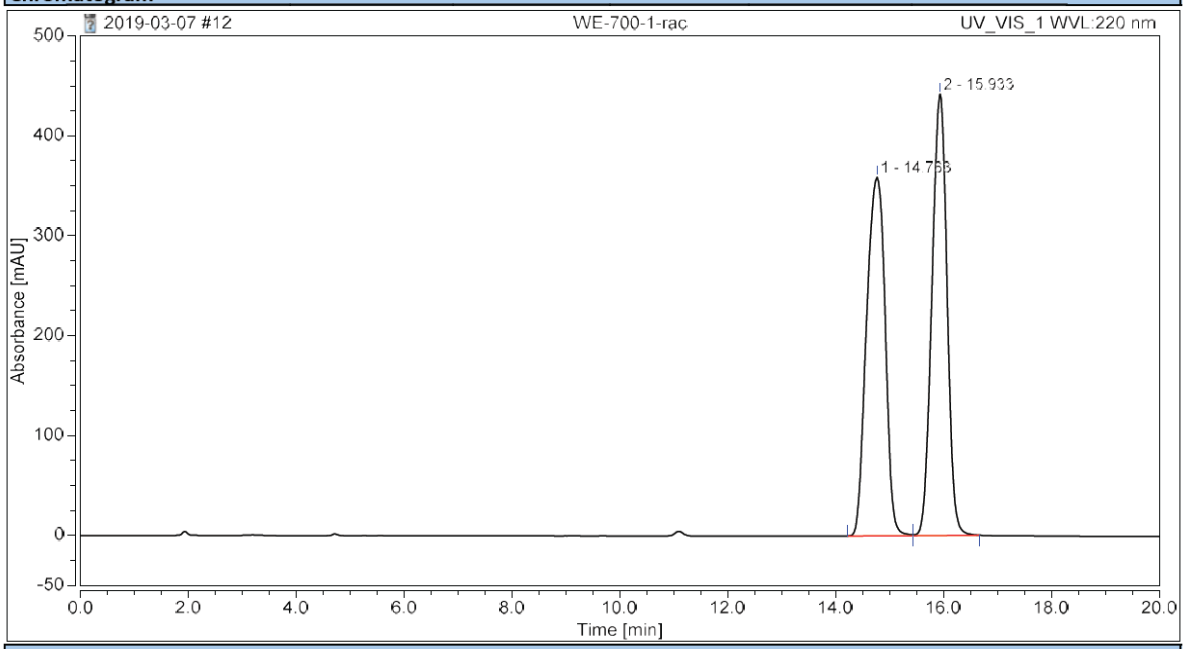
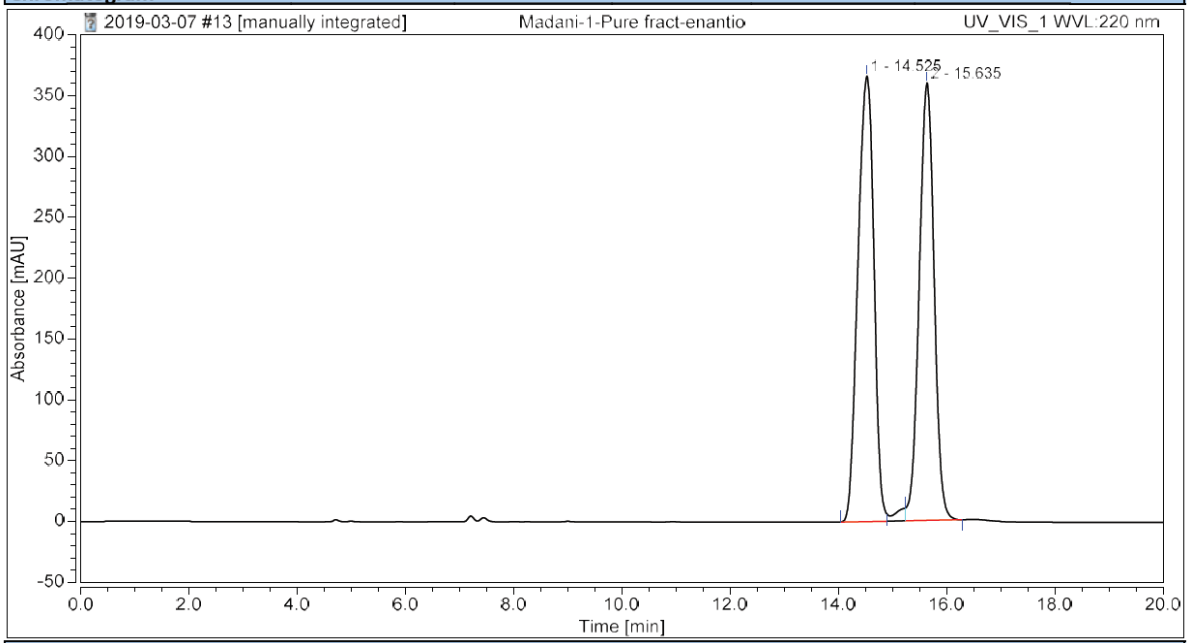
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		14.763	143.660	358.990	50.03	44.83	n.a.
2		15.933	143.462	441.858	49.97	55.17	n.a.
Total:			**287.122**	**800.847**	**100.00**	**100.00**	

Chromatogram

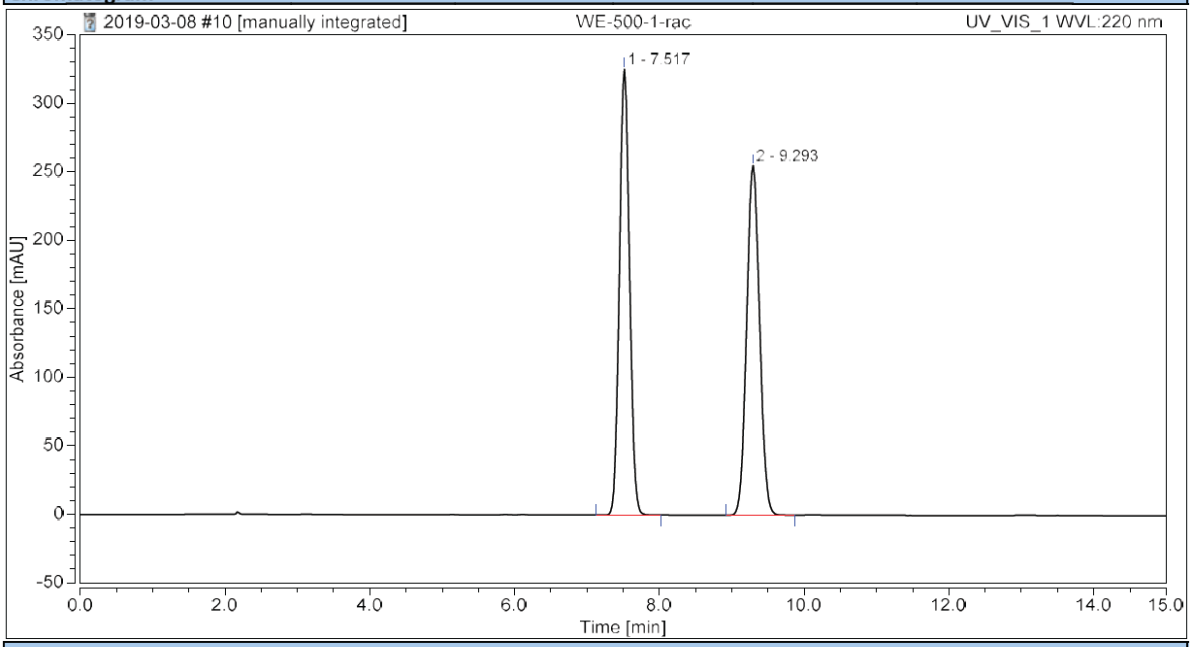


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		14.525	125.520	366.358	52.22	50.46	n.a.
2		15.635	114.849	359.669	47.78	49.54	n.a.
Total:			**240.369**	**726.027**	**100.00**	**100.00**	

Compounds (±)- and enantioenriched (R_p)-1-I

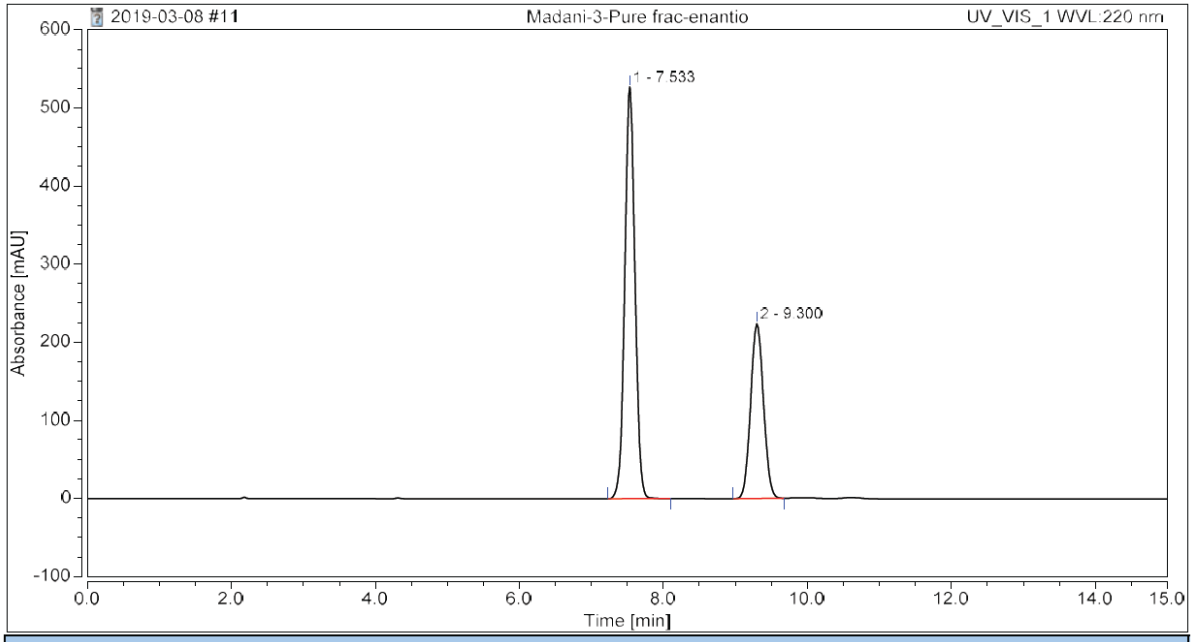
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		7.517	52.969	325.532	50.00	56.05	n.a.
2		9.293	52.976	255.275	50.00	43.95	n.a.
Total:			**105.945**	**580.807**	**100.00**	**100.00**	

Chromatogram

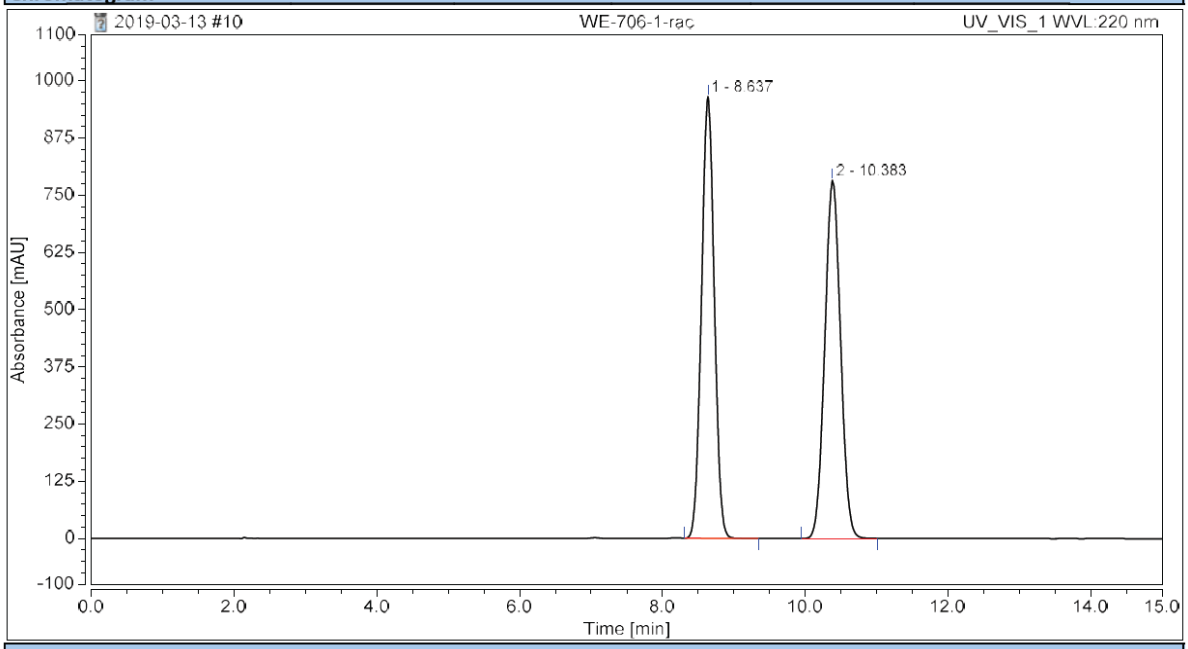


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		7.533	86.386	527.156	65.07	70.17	n.a.
2		9.300	46.382	224.131	34.93	29.83	n.a.
Total:			**132.767**	**751.287**	**100.00**	**100.00**	

Compounds (±)- and enantioenriched (R_p)-2-I

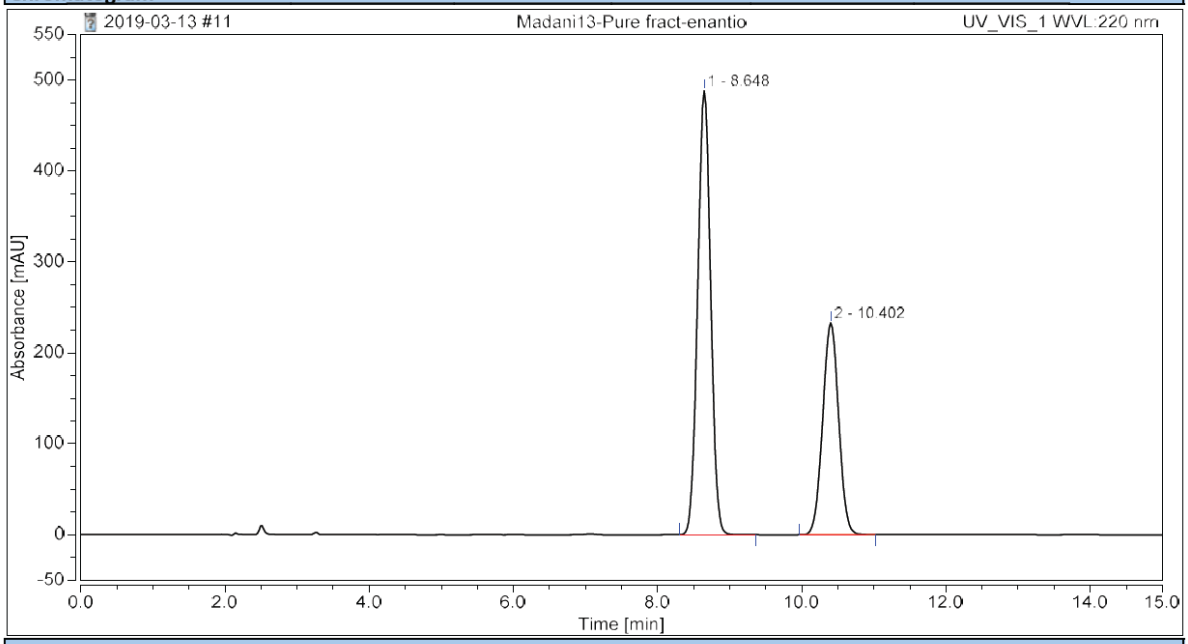
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		8.637	200.474	965.265	49.99	55.22	n.a.
2		10.383	200.592	782.891	50.01	44.78	n.a.
Total:			**401.066**	**1748.156**	**100.00**	**100.00**	

Chromatogram

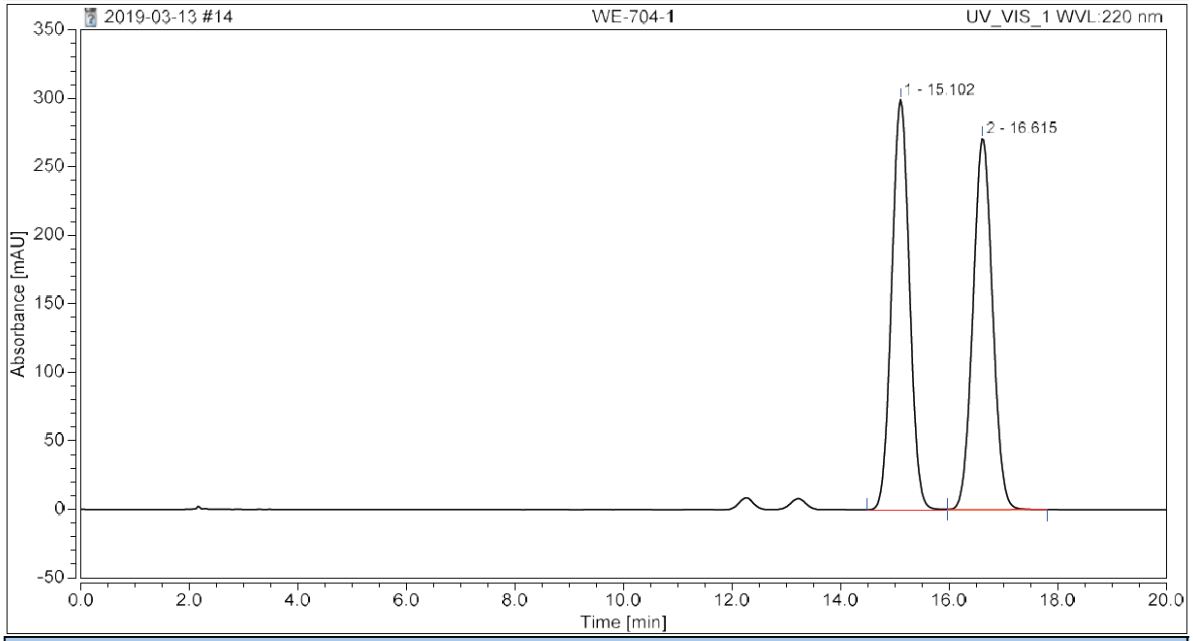


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		8.648	101.883	488.607	63.00	67.69	n.a.
2		10.402	59.845	233.176	37.00	32.31	n.a.
Total:			**161.728**	**721.783**	**100.00**	**100.00**	

Compounds (±)- and enantioenriched (R_p)-3-I

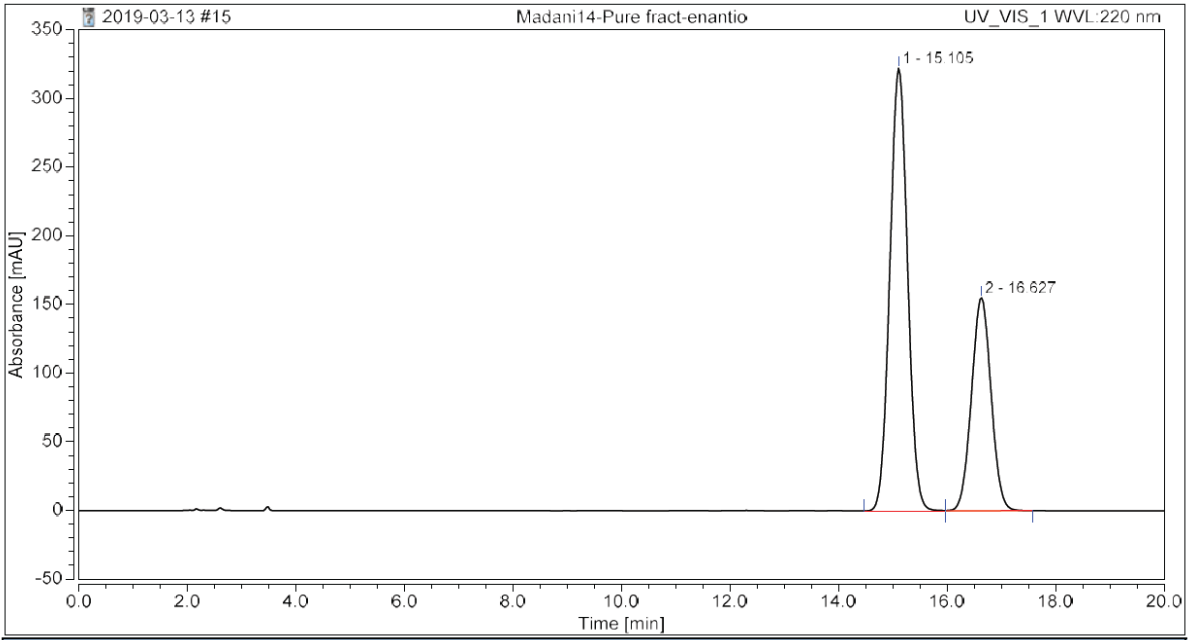
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		15.102	113.321	299.482	50.01	52.47	n.a.
2		16.615	113.262	271.317	49.99	47.53	n.a.
Total:			**226.583**	**570.799**	**100.00**	**100.00**	

Chromatogram

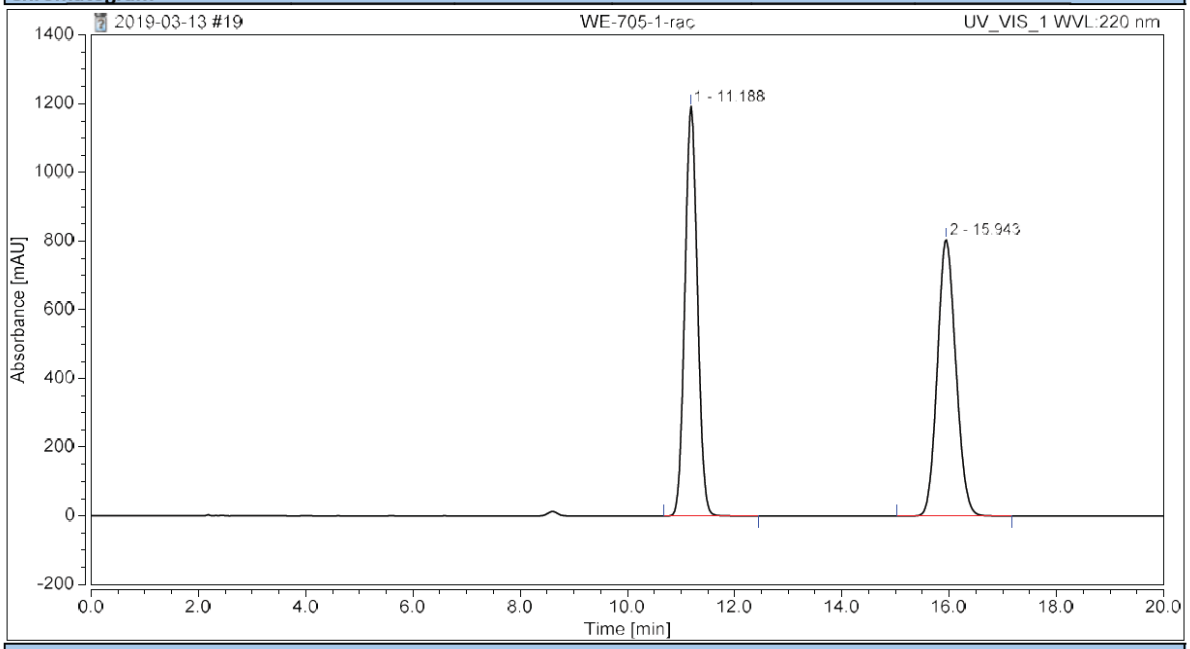


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		15.105	121.977	322.419	65.29	67.51	n.a.
2		16.627	64.836	155.203	34.71	32.49	n.a.
Total:			**186.812**	**477.622**	**100.00**	**100.00**	

Compounds (±)- and enantioenriched (R_p)-4-I

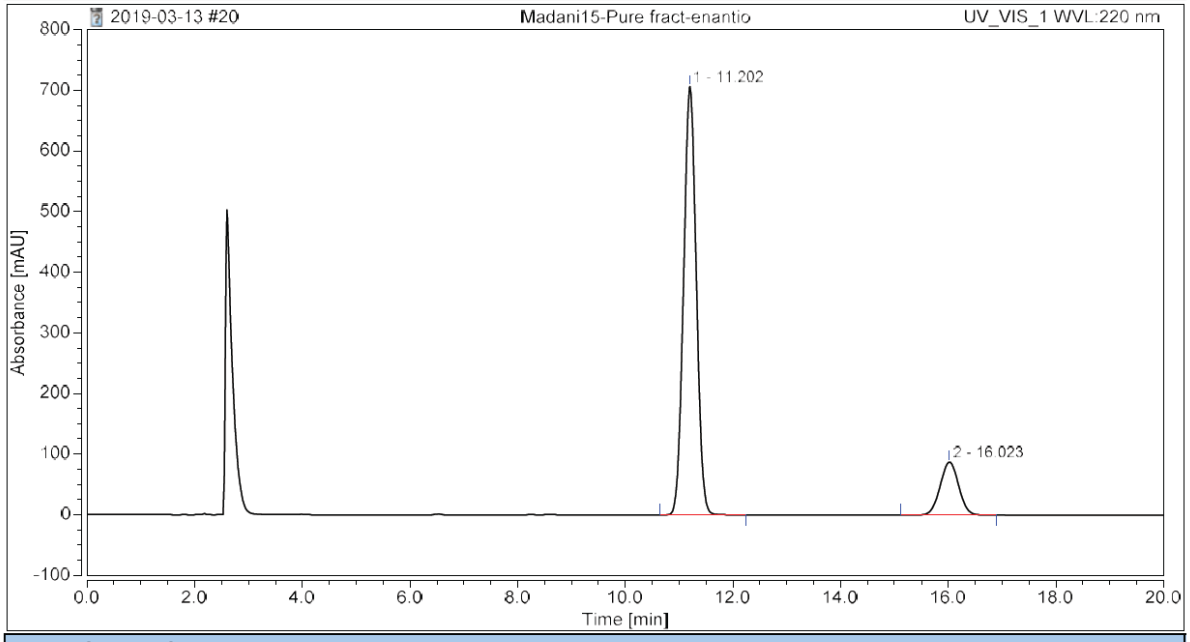
Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		11.188	323.840	1193.026	50.15	59.70	n.a.
2		15.943	321.907	805.339	49.85	40.30	n.a.
Total:			**645.747**	**1998.364**	**100.00**	**100.00**	

Chromatogram

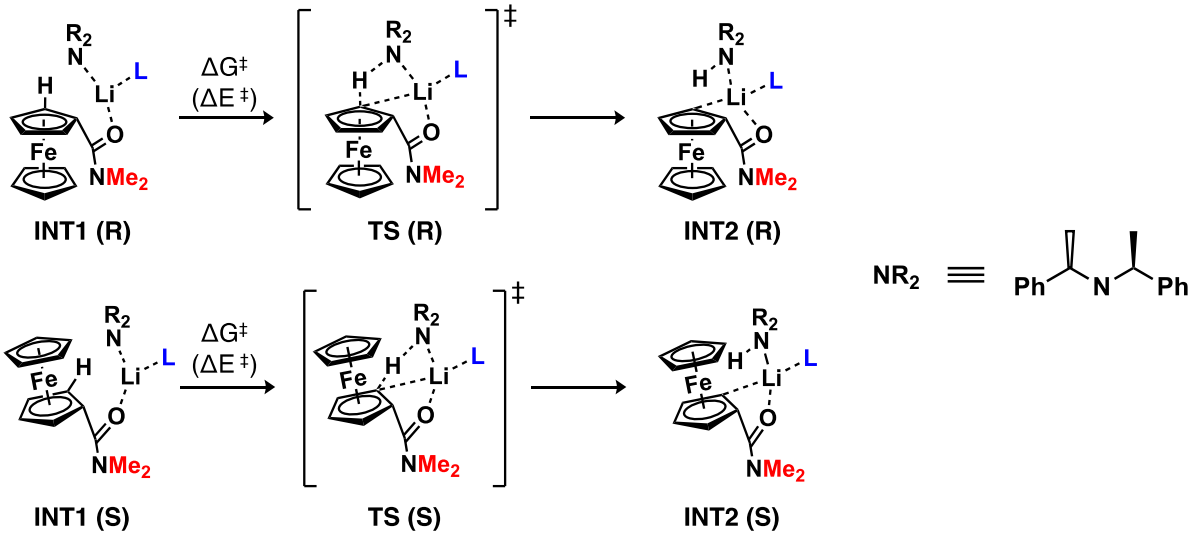


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		11.202	193.029	706.529	84.78	89.00	n.a.
2		16.023	34.641	87.340	15.22	11.00	n.a.
Total:			**227.671**	**793.869**	**100.00**	**100.00**	

Computational Details

All calculations were carried with the Gaussian 16 (revision A.03) program package.[1] The molecular structures and harmonic vibrational frequencies were obtained using the hybrid density functional method based on the unrestricted B3LYP[2] method. We used LanL2DZ basis set[3] for a Fe atom and 6–31+G** basis set for all other atoms. Geometry optimization and vibrational analysis were performed at the same level. All stationary points were optimized without any symmetry assumptions, and characterized by normal coordinate analysis at the same level of theory (number of imaginary frequencies, NIMAG, 0 for minima and 1 for TSs). The intrinsic reaction coordinate (IRC) method was used to track minimum energy paths from transition structures to the corresponding local minima.[4]



L	ΔG (INT1) kcal/mol		ΔG‡ (ΔE‡) kcal/mol		ΔG (INT2) kcal/mol	
	R	S	R	S	R	S
none	0	0	22.0 (20.7)	22.1 (20.0)	8.9 (5.0)	7.5 (3.1)
Me_2O	0	0	18.0 (18.2)	15.7 (16.1)	9.6 (8.3)	7.5 (7.6)

B3LYP/LanI2DZ for Fe and 6-31+G** for Others

Figure S1. Energy profile for the enantioselective deprotolithiation of *N*,*N*-dialkyl ferrocenecarboxamides using (*S*,*S*)-lithium bis(1-phenylethyl)amide

• **INT1 (R)**

Energy (RB3LYP): -1440.773126 A.U
Gibbs Free Energy: -1440.293651 A.U

Fe	3.08524900	-0.22498600	-0.79358100
C	1.42017000	-1.34374300	-0.25030900
C	2.36319100	-2.16962000	-0.96821700
C	2.54067500	-1.61096000	-2.26510000
C	1.72298200	-0.44375100	-2.36550800
H	1.66719900	0.22250900	-3.21522500
C	1.03130600	-0.27782600	-1.13631700
C	3.99809700	0.60879900	0.88816500
H	3.67417200	0.45113800	1.90818400
C	4.93938800	-0.19076500	0.16665600
H	5.46552200	-1.05792000	0.54279600
C	5.05387100	0.34952400	-1.15186600
H	5.66622600	-0.04708000	-1.95020500
C	4.18559600	1.48087600	-1.24121600
H	4.02035500	2.08544100	-2.12254900
C	3.53066300	1.64109200	0.01887100
H	2.77977400	2.38119200	0.25987600
H	3.20567000	-1.99231100	-3.02800900
C	0.75843000	-1.54217400	1.06536700
O	-0.36435600	-1.02334200	1.25687900
N	1.30926200	-2.31248900	2.04004000
N	-2.99836500	1.01038700	-0.24972900
C	-4.11612400	0.36701200	-0.92887500
H	-5.09586300	0.67721200	-0.51065400
C	-3.02519900	2.46293100	-0.27932600
H	-3.02248100	2.86026500	-1.31553400
C	-4.01028600	-1.12970100	-0.64068300
C	-3.06614400	-1.93978800	-1.29492000
C	-4.81694700	-1.72580200	0.34236700
C	-2.93962600	-3.29940000	-0.98357300
H	-2.43295100	-1.50690400	-2.06412200
C	-4.69897000	-3.08339600	0.65533700
H	-5.54729400	-1.11146400	0.86392600
C	-3.75712700	-3.87725000	-0.00843100
H	-2.20814500	-3.90704100	-1.51080000
H	-5.34202100	-3.52116200	1.41476100
H	-3.66616900	-4.93417200	0.22806100
C	-1.74724300	2.99191100	0.36465000
C	-1.45787500	2.73434400	1.71597800
C	-0.83089700	3.76275700	-0.36547000
C	-0.29722400	3.23163800	2.31528100
H	-2.15968700	2.14757100	2.30286100
C	0.33007400	4.27085600	0.22904700
H	-1.03706200	3.97386500	-1.41257400
C	0.60194800	4.00767000	1.57487900
H	-0.10053300	3.02580500	3.36479700
H	1.01605100	4.87785000	-0.35729200
H	1.49608700	4.40990500	2.04451500
C	-4.20826000	0.64827200	-2.45148900
H	-5.02257300	0.07661600	-2.91462600
H	-4.40344500	1.71041900	-2.63369800
H	-3.26911400	0.39600000	-2.95740400
C	-4.26317200	3.10624800	0.40742700
H	-4.19630000	4.20140700	0.39883200
H	-5.18654300	2.82603800	-0.11076000
H	-4.34759200	2.76943900	1.44722500
Li	-1.81313200	-0.13722200	0.54398500
H	0.34796400	0.52505000	-0.89624300
C	0.51799400	-2.61152000	3.23420100
H	0.76596000	-1.92388500	4.05293300
H	-0.54178600	-2.51604300	3.00589200
H	0.73604000	-3.63487400	3.55465700
C	2.69160900	-2.77692900	2.07509300
H	2.76237500	-3.84591300	1.83601900
H	3.30548400	-2.20599900	1.38212900
H	3.08616100	-2.62810600	3.08610700
H	2.84061900	-3.06992000	-0.61205800

• **TS (R)**

Energy (RB3LYP): -1440.740187 A.U
Gibbs Free Energy: -1440.258605 A.U

Fe	2.23092300	-0.65817100	-1.03175800
C	0.71414000	-1.60902900	0.01451600
C	1.42453400	-2.54869900	-0.83510600
C	1.27092700	-2.10543300	-2.17504600
C	0.48249200	-0.90974500	-2.14460600
H	0.24576200	-0.31821200	-3.02194800
C	0.09456700	-0.57697300	-0.80934000
C	3.66182000	0.16908500	0.25037500
H	3.66118800	0.06817400	1.32752000
C	4.29054900	-0.71505200	-0.68148500
H	4.85633700	-1.60519700	-0.44010900
C	4.02387800	-0.22551000	-1.99853100
H	4.33756600	-0.68879300	-2.92416300
C	3.23377500	0.95886300	-1.87591400
H	2.83693600	1.54292300	-2.69512200
C	3.00899300	1.20357000	-0.48645500
H	2.41478000	2.00219600	-0.06780100
H	1.71167300	-2.57221100	-3.04726800
C	0.48348100	-1.69173000	1.47799000
O	-0.50977500	-1.09766300	1.98024200
N	1.26484800	-2.43837100	2.30726400
N	-1.95416200	1.24790500	-0.46090500
C	-3.11308000	0.74694600	-1.22730500
H	-3.97742100	1.39844000	-1.03216600
C	-1.63441900	2.66696600	-0.65797300
H	-1.17011500	2.83729500	-1.64811300
C	-3.51458900	-0.61525700	-0.64772900

C	-3.17966500	-1.84266400	-1.23822600
C	-4.23459500	-0.64213100	0.56195800
C	-3.55353100	-3.05307300	-0.64353400
H	-2.61582000	-1.86217300	-2.16428100
C	-4.60900800	-1.84790200	1.16071600
H	-4.51764500	0.30084000	1.02607300
C	-4.26791800	-3.06224400	0.55643800
H	-3.27938400	-3.99038200	-1.12014000
H	-5.17226300	-1.83870000	2.09005500
H	-4.55745700	-4.00335200	1.01545000
C	-0.61706800	3.14108600	0.37858400
C	-0.78982100	2.88136600	1.74681200
C	0.47087300	3.93715100	-0.00690000
C	0.10193500	3.38585100	2.69684400
H	-1.64419900	2.29363400	2.07282800
C	1.36248000	4.45425100	0.93840800
H	0.62193300	4.15345200	-1.06231700
C	1.18437500	4.17565200	2.29627900
H	-0.05203100	3.16732600	3.75038100
H	2.19987800	5.06583500	0.61278100
H	1.87858800	4.56998000	3.03313500
C	-2.91649100	0.73051000	-2.75642200
H	-3.81200400	0.35752800	-3.26763600
H	-2.72339000	1.74463200	-3.12144500
H	-2.06609600	0.10922400	-3.05104800
C	-2.86002700	3.61190600	-0.58819200
H	-2.52860900	4.65455200	-0.63276900
H	-3.55364500	3.45094600	-1.41956300
H	-3.40654500	3.46908800	0.35137000
Li	-1.54244100	-0.01870600	0.94568600
H	-0.90222500	0.48012500	-0.67695600
C	0.85022400	-2.61571200	3.69787400
H	1.35875100	-1.89957400	4.35726100
H	-0.22413900	-2.46445000	3.78290800
H	1.10886400	-3.63048800	4.01757900
C	2.58655300	-2.96526200	1.98784700
H	2.55758000	-4.04913600	1.81462800
H	2.99546200	-2.46682400	1.11234600
H	3.25366700	-2.77490900	2.83628400
H	1.95842800	-3.43937400	-0.53681800

- **INT2 (R)**

Energy (RB3LYP): -1440.765198 A.U
Gibbs Free Energy: -1440.279540 A.U

Fe	2.79883300	-0.45543500	-0.82374300
C	1.67901400	-1.08429300	0.79899800
C	2.85438200	-1.92300900	0.62039600
C	2.72793600	-2.52332600	-0.66211600
C	1.50484400	-2.04673900	-1.24724900
H	1.18256600	-2.30806500	-2.24967200
C	0.80101100	-1.16951400	-0.36559200
C	3.38866600	1.53920500	-0.62098500
H	3.15922300	2.16428400	0.23228500
C	4.53998000	0.70129900	-0.76157500
H	5.34252000	0.59037600	-0.04446400
C	4.43895000	0.02500800	-2.01798100
H	5.13858100	-0.70290600	-2.40597100
C	3.22770600	0.44527400	-2.64903700
H	2.84645700	0.08401300	-3.59439800
C	2.57798900	1.38282400	-1.78766900
H	1.61957200	1.84934900	-1.96533000
H	3.45541000	-3.18499800	-1.11805600
C	1.22564700	-0.27887200	1.95423400
O	0.02172700	0.11176300	1.98808900
N	2.03276000	0.03016800	3.01146000
N	-2.88756000	0.35338200	0.09356000
C	-3.76327500	-0.76584300	0.56619100
H	-3.58375300	-0.85856100	1.64208600
C	-3.23177100	1.71474100	0.61264000
H	-4.28272200	1.94388600	0.38510300
C	-3.28801300	-2.06105100	-0.08027100
C	-3.51626700	-2.32561700	-1.43992600
C	-2.59570800	-3.01405400	0.67880000
C	-3.06120000	-3.50954500	-2.02374800
H	-4.05565800	-1.60851300	-2.05417900
C	-2.14145900	-4.20179000	0.09914200
H	-2.40152300	-2.82190100	1.73142000
C	-2.37299000	-4.45252500	-1.25447300
H	-3.24307300	-3.69491800	-3.07869800
H	-1.59750000	-4.92237100	0.70278400
H	-2.01465900	-5.37142700	-1.70935300
C	-2.39451300	2.74736700	-0.13093300
C	-1.02334100	2.91006300	0.12509200
C	-2.99561100	3.55649700	-1.10584200
C	-0.27835000	3.85868200	-0.57976000
H	-0.53294900	2.29940100	0.87876300
C	-2.25195800	4.50731200	-1.81190600
H	-4.05854800	3.44638600	-1.31066800
C	-0.88898900	4.66135000	-1.54857200
H	0.78161500	3.97216900	-0.37107100
H	-2.73753200	5.12605400	-2.56144800
H	-0.30588400	5.39836400	-2.09338400
C	-5.27123500	-0.53148700	0.35401200
H	-5.83144900	-1.41751700	0.66838800
H	-5.63715500	0.31796500	0.93844500
H	-5.50658700	-0.34355100	-0.69964900
C	-3.05344400	1.78241900	2.13631300
H	-3.21198200	2.80950400	2.47867400
H	-3.78169300	1.14730700	2.65109800
H	-2.05121900	1.46260600	2.43502700
Li	-0.85751800	-0.22189600	0.31660700
H	-2.96426000	0.39306000	-0.92422600
C	1.45606400	0.65938500	4.19527200

H	1.64363500	1.74223400	4.20362100
H	0.38071600	0.49200400	4.20879900
H	1.90979300	0.22254200	5.09196300
C	3.48604400	-0.08654400	3.01259800
H	3.82501700	-0.99451000	3.52920100
H	3.86779100	-0.08441400	1.99324300
H	3.90495500	0.77916600	3.53740200
H	3.67232200	-2.10229000	1.30360700

- **INT1 (S)**

Energy (RB3LYP): -1440.771820 A.U
Gibbs Free Energy: -1440.293648 A.U

Fe	-2.92786000	-0.53062600	-0.85245100
C	-1.58085500	-1.22957800	0.56754800
C	-0.95273200	-1.18237000	-0.72664700
C	-1.67753600	-2.02866000	-1.60636200
C	-2.75500900	-2.61665700	-0.87572200
H	-3.50168500	-3.29184300	-1.27108500
C	-2.70518500	-2.13031100	0.46061700
C	-3.57505500	1.39623600	-0.37395200
H	-3.26886000	1.95040200	0.50310900
C	-2.90338800	1.40019900	-1.63414800
H	-1.99862500	1.94394700	-1.86685400
C	-3.61018600	0.52113900	-2.51173600
H	-3.33261400	0.28241300	-3.52931000
C	-4.71636800	-0.02818100	-1.79347000
H	-5.42551500	-0.75079100	-2.17363200
C	-4.69613400	0.51335500	-0.47061400
H	-5.40159000	0.28506600	0.31706000
H	-1.46913800	-2.17220000	-2.65754300
C	-0.97961300	-0.55606400	1.74790700
O	0.23042600	-0.23923200	1.70798500
N	-1.68679000	-0.32808900	2.88577900
N	2.93572500	0.56971200	-0.57566900
C	3.05214900	1.90076800	-1.15303400
H	4.07190400	2.31970600	-1.01360000
C	3.89098900	-0.40716700	-1.08221600
H	3.78800300	-0.57118100	-2.17538500
C	2.13560000	2.82730300	-0.35213200
C	0.88164200	3.26086100	-0.80494600
C	2.54963700	3.24545500	0.92508700
C	0.06911600	4.08502500	-0.01438100
H	0.53705300	2.96905900	-1.79224100
C	1.74607600	4.06579700	1.72006500
H	3.52168700	2.92005700	1.28794600
C	0.49660100	4.49035100	1.25159900
H	-0.89292000	4.41944400	-0.39595500
H	2.09781400	4.38393000	2.69851000
H	-0.12764200	5.13858500	1.86123700
C	3.55040000	-1.74637000	-0.43283200
C	3.75815900	-1.95806000	0.94183200
C	2.97728900	-2.78829000	-1.17685500
C	3.40606800	-3.16868600	1.54908200
H	4.21538300	-1.17154600	1.53688500
C	2.62646400	-4.00239700	-0.57746300
H	2.80608200	-2.64144900	-2.24097700
C	2.83812200	-4.19709600	0.79077500
H	3.58375300	-3.31134200	2.61227600
H	2.18610400	-4.79447800	-1.17797700
H	2.56804900	-5.13965200	1.25943000
C	2.78886500	1.96863800	-2.67587800
H	2.83432100	2.99884700	-3.05169700
H	3.54441100	1.38834600	-3.21520400
H	1.81106900	1.54037400	-2.92757300
C	5.38394600	-0.04770300	-0.85631500
H	6.04035800	-0.86015600	-1.19224800
H	5.65721700	0.85229900	-1.41739900
H	5.58584800	0.14874800	0.20311000
Li	1.75250400	0.07332800	0.73129600
H	-3.38528500	-2.41785600	1.24781900
C	-0.98028100	0.18226800	4.06165800
H	-1.04630100	1.27619200	4.11713700
H	-1.43534800	-0.24734500	4.95914000
H	0.06957600	-0.10018800	4.01048600
C	-3.13872300	-0.39686400	3.01070500
H	-3.48232200	0.47279300	3.58095500
H	-3.60959600	-0.36811400	2.03062400
H	-3.45475400	-1.30187000	3.54545400
H	-0.08588100	-0.58905900	-0.98633100

- **TS (S)**

Energy (RB3LYP): -1440.739910 A.U
Gibbs Free Energy: -1440.258361 A.U

Fe	-2.30830100	-0.53071600	-1.00160200
C	-0.89200600	-1.52216800	0.14140300
C	-0.17929700	-0.61308400	-0.74703600
C	-0.57147000	-1.01491400	-2.06098600
C	-1.45851500	-2.13813100	-2.01520300
H	-1.92473200	-2.63404400	-2.85760400
C	-1.66756300	-2.46216100	-0.64874200
C	-3.68552400	0.48532000	0.19911900
H	-3.70976400	0.44898700	1.28009100
C	-2.93842800	1.41738200	-0.58394500
H	-2.28611800	2.18661800	-0.19737200
C	-3.16142700	1.10938400	-1.96134300
H	-2.70893500	1.61063000	-2.80618900
C	-4.04457600	-0.01180200	-2.02985400
H	-4.38199700	-0.50170300	-2.93311500
C	-4.37090400	-0.39812500	-0.69215400
H	-5.01127100	-1.22339900	-0.41030500
H	-0.26587000	-0.51788100	-2.97502000
C	-0.69397800	-1.48659000	1.61161200

O	0.31158400	-0.88876000	2.08387000
N	-1.52307200	-2.12445900	2.48459500
N	2.01773400	1.03901500	-0.57521200
C	1.80755900	2.45889100	-0.89317500
H	2.78443500	2.96681700	-0.93091700
C	3.03534900	0.33855500	-1.38054800
H	2.66082000	0.11815300	-2.39818000
C	1.06896700	3.13355000	0.26941100
C	-0.11084200	3.87371200	0.11387700
C	1.62139700	3.05178800	1.56118800
C	-0.72651700	4.49608200	1.20746100
H	-0.56158400	3.97625700	-0.86745700
C	1.01398900	3.66973300	2.65536500
H	2.55350400	2.50836100	1.69795200
C	-0.17109300	4.39403300	2.48352000
H	-1.64275200	5.06109300	1.05634200
H	1.46774700	3.59234100	3.64005900
H	-0.64869900	4.87648600	3.33168500
C	3.32208300	-1.01515300	-0.72769100
C	3.84717900	-1.08666900	0.57483200
C	3.08730200	-2.21645900	-1.41008200
C	4.12749600	-2.31784100	1.17487000
H	4.06007100	-0.16654500	1.11542000
C	3.36746600	-3.45085700	-0.81621500
H	2.66802000	-2.18365900	-2.41219100
C	3.88722800	-3.50697000	0.47972000
H	4.53635700	-2.34773400	2.18144600
H	3.17029800	-4.36877200	-1.36351400
H	4.10170700	-4.46560600	0.94375500
C	1.14477900	2.68558000	-2.26704300
H	1.06490700	3.75084400	-2.51369400
H	1.74694700	2.21435400	-3.05057300
H	0.14538200	2.23929900	-2.30443200
C	4.36012800	1.11118200	-1.56561700
H	5.09848000	0.46953800	-2.05820900
H	4.22907100	2.00138100	-2.18872700
H	4.77414000	1.42822200	-0.60163600
Li	1.40958700	0.08282600	1.00427600
H	-2.28081500	-3.27908300	-0.29765100
C	-1.14357300	-2.19499000	3.89474800
H	-1.63208300	-1.40215800	4.47699900
H	-1.45246200	-3.16568000	4.29616800
H	-0.06544600	-2.08226300	3.99074600
C	-2.86064700	-2.62008700	2.18101700
H	-3.52759200	-2.35293900	3.00827900
H	-3.24242600	-2.15952400	1.27289400
H	-2.87345500	-3.71268500	2.07313800
H	0.89852100	0.35749300	-0.69704200

- **INT2 (S)**

Energy (RB3LYP): -1440.766823 A.U

Gibbs Free Energy: -1440.281750 A.U

Fe	-2.74165800	-1.04920800	-0.76228000
C	-1.68737600	-1.09983100	1.01388900
C	-0.71189900	-1.30950800	-0.05424800
C	-1.20262100	-2.46894600	-0.73116300
C	-2.38734900	-2.98853000	-0.10682400
H	-2.96991400	-3.84578300	-0.42350300
C	-2.70534400	-2.13838000	0.98687400
C	-3.69019900	0.79478300	-1.02537600
H	-3.67235800	1.60367400	-0.30672900
C	-2.73589600	0.58182800	-2.06784300
H	-1.86477700	1.19014800	-2.26667700
C	-3.10692400	-0.61030900	-2.76360600
H	-2.56250800	-1.06205900	-3.58162500
C	-4.29023900	-1.13167000	-2.15503100
H	-4.80190100	-2.04204900	-2.43648900
C	-4.65182200	-0.26294900	-1.07751100
H	-5.49714500	-0.39276200	-0.41476700
H	-0.76654700	-2.89518400	-1.62893100
C	-1.46635300	0.03158300	1.94397600
O	-0.36399000	0.64950400	1.89737500
N	-2.38291600	0.41615700	2.88131100
N	2.67257700	0.70188000	0.23869900
C	2.63819000	2.14433500	0.64155700
H	2.13020900	2.18218500	1.61107800
C	3.57671100	-0.19114400	1.02785000
H	4.53565700	0.31399300	1.20312300
C	1.75918600	2.88617200	-0.36132700
C	2.21427400	3.16292200	-1.66130000
C	0.46556600	3.29294000	-0.00442300
C	1.39845500	3.82800000	-2.57916100
H	3.21511600	2.86574200	-1.96496800
C	-0.35175800	3.96303500	-0.92083700
H	0.09085800	3.06499500	0.98967600
C	0.11176800	4.23329000	-2.21012700
H	1.76788000	4.03175500	-3.58032700
H	-1.35143700	4.26987100	-0.62622900
H	-0.52319400	4.75155700	-2.92295100
C	3.89405100	-1.44523600	0.22376700
C	2.88244200	-2.29272300	-0.25748700
C	5.23166000	-1.78002300	-0.03462500
C	3.20950200	-3.44411800	-0.97852800
H	1.83355700	-2.05927200	-0.08516800
C	5.55958800	-2.93546600	-0.75043700
H	6.02590300	-1.13214000	0.33030100
C	4.54636700	-3.77188900	-1.22521200
H	2.41377000	-4.08718600	-1.34389900
H	6.60214700	-3.17799200	-0.93733600
H	4.79540300	-4.67019900	-1.78333600
C	4.01743800	2.81353600	0.80160500
H	3.88604700	3.88167800	1.00083500

H	4.58087600	2.38936600	1.63757400
H	4.62703000	2.71261600	-0.10329600
C	2.95929500	-0.51431600	2.39726200
H	3.64533300	-1.14355700	2.97271500
H	2.76811500	0.39579400	2.97527500
H	2.01123400	-1.04979500	2.29117000
Li	0.64149400	0.14436700	0.34527000
H	-3.54384500	-2.28731300	1.65133800
C	-2.00883700	1.40661900	3.88586400
H	-2.41264600	2.39844400	3.63847300
H	-2.41048600	1.10284300	4.85912600
H	-0.92408900	1.47493300	3.94175500
C	-3.78419600	0.01302200	2.89310500
H	-4.38671500	0.86273000	3.23123800
H	-4.11105100	-0.25671700	1.89020900
H	-3.96681400	-0.82709300	3.57636700
H	2.97711300	0.65864200	-0.73370600

- **INT1 (R) with Me_2O**

Energy (RB3LYP): -1595.822362 A.U
Gibbs Free Energy: -1595.267571 A.U

Fe	-3.11032900	-1.27203400	0.31337400
C	-1.62123700	-1.00365600	-1.12699700
C	-2.57654100	-1.99251700	-1.56595800
C	-2.57063300	-3.05794400	-0.62040900
C	-1.63014500	-2.73733300	0.40761500
H	-1.42741300	-3.32968300	1.28936100
C	-1.04315800	-1.47986200	0.09917800
C	-4.03881200	0.53416400	0.80193000
H	-3.77665900	1.49368000	0.37722800
C	-5.00360100	-0.38816800	0.28689800
H	-5.61977200	-0.24790500	-0.59112400
C	-5.00658800	-1.54024900	1.13298900
H	-5.60625100	-2.42949900	0.99384800
C	-4.04646700	-1.32842700	2.16932000
H	-3.78749900	-2.03197900	2.94870500
C	-3.44746100	-0.04748900	1.96389800
H	-2.65693000	0.38767500	2.55819500
H	-3.19659800	-3.93904300	-0.66162600
C	-1.07155500	0.18945400	-1.82872200
O	0.12910000	0.48306300	-1.65016800
N	-1.82607300	0.91831600	-2.69682900
N	2.04046600	0.40709600	1.32061600
C	2.80087000	-0.66502600	1.95029400
H	3.63199000	-0.27488400	2.57106200
C	1.54954600	1.39589000	2.27082500
H	0.83656700	0.96358100	3.00732000
C	3.47563900	-1.52670500	0.88570100
C	2.72820400	-2.22554200	-0.07781200
C	4.87165700	-1.66371000	0.85028400
C	3.35192800	-3.01925200	-1.04518500
H	1.64469200	-2.15665900	-0.06593400
C	5.50413000	-2.46126100	-0.10986200
H	5.47125600	-1.13613500	1.58898800
C	4.74546300	-3.14217100	-1.06643900
H	2.74779400	-3.55175900	-1.77601600
H	6.58772700	-2.55178600	-0.10861700
H	5.23128400	-3.76626300	-1.81194600
C	0.76027000	2.47539300	1.53250300
C	1.35586900	3.24393900	0.51793500
C	-0.56912000	2.76557500	1.87204800
C	0.64800400	4.25528500	-0.13751400
H	2.39065600	3.05102300	0.24999300
C	-1.28488200	3.77877100	1.22490300
H	-1.04386700	2.19516200	2.66710800
C	-0.67853700	4.52874000	0.21281200
H	1.13633000	4.83864400	-0.91456600
H	-2.31094600	3.98829900	1.51844200
H	-1.22685100	5.32368400	-0.28635400
C	1.97694000	-1.57740600	2.90708200
H	2.60626700	-2.35852100	3.35295000
H	1.54282700	-0.99131700	3.72464800
H	1.15533600	-2.06505800	2.36972700
C	2.64340700	2.09294400	3.13512200
H	2.20443900	2.87968100	3.76109700
H	3.13981100	1.37966400	3.80121000
H	3.40975100	2.54638900	2.49473800
Li	1.68681300	0.56219700	-0.53223400
H	-0.29777400	-0.94490600	0.67883800
C	-1.20460300	2.01125600	-3.44202800
H	-1.49521300	2.98021200	-3.01750100
H	-0.12226600	1.91916500	-3.38838900
H	-1.53268800	1.96901200	-4.48652600
C	-3.26639000	0.79352100	-2.87969700
H	-3.50541800	0.32802900	-3.84514400
H	-3.70599800	0.20947500	-2.07533400
H	-3.71404200	1.79389800	-2.86526500
H	-3.17817500	-1.95891100	-2.46261900
O	3.12184400	0.97126800	-1.86371800
C	4.43732000	1.26642200	-1.39436800
H	4.34951100	1.46071000	-0.32439800
H	5.10398100	0.40937000	-1.55096300
H	4.83876800	2.14804000	-1.91422600
C	3.08864200	0.59862400	-3.23517800
H	3.70122800	-0.29655000	-3.40924200
H	2.04808900	0.38182700	-3.48141100
H	3.45693100	1.41784600	-3.86969800

- **TS (R) with Me_2O**

Energy (RB3LYP): -1595.793637 A.U
Gibbs Free Energy: -1595.238574 A.U

Fe	-2.80510300	-1.38901600	-0.05418400

C	-1.34822500	-0.57154200	-1.32183100
C	-2.19985800	-1.51354400	-2.02555900
C	-2.03876500	-2.77271400	-1.38657700
C	-1.12338600	-2.58570700	-0.29674500
H	-0.85876200	-3.37195200	0.40172700
C	-0.65322200	-1.23363500	-0.23481800
C	-3.99048900	0.05116300	0.90340900
H	-3.87083200	1.12058200	0.79379200
C	-4.80892600	-0.79350100	0.08851600
H	-5.43428300	-0.47862000	-0.73623700
C	-4.65428200	-2.13642300	0.55318900
H	-5.11746800	-3.01452800	0.12397300
C	-3.74389400	-2.12054800	1.65339200
H	-3.39202000	-2.98523500	2.19927100
C	-3.33536400	-0.76894800	1.87146200
H	-2.62479000	-0.43864200	2.61534300
H	-2.55371100	-3.68710100	-1.65546600
C	-0.99425600	0.80315200	-1.75359700
O	0.17503800	1.22726200	-1.56340600
N	-1.86897500	1.60256600	-2.42872600
N	1.40807200	-0.15265100	1.27192700
C	2.32147400	-1.23378200	1.69540800
H	3.00155500	-0.84730400	2.46522900
C	0.75344200	0.57974100	2.38238400
H	-0.17562600	0.05811100	2.67709700
C	3.22504900	-1.68637600	0.55097100
C	2.72247000	-1.97769700	-0.72821000
C	4.59823200	-1.87119900	0.77665900
C	3.56864400	-2.42758700	-1.74658100
H	1.65922900	-1.86915400	-0.92439800
C	5.44788100	-2.32698200	-0.23643000
H	5.00824000	-1.65818600	1.76196700
C	4.93527700	-2.60461200	-1.50696500
H	3.15474400	-2.65050000	-2.72678200
H	6.50682300	-2.46454400	-0.03276100
H	5.59009200	-2.96115000	-2.29751700
C	0.33379900	1.97728200	1.91835900
C	1.28491600	2.89174400	1.43650600
C	-0.99484800	2.40970200	2.02467000
C	0.92212800	4.18927300	1.06802600
H	2.32575200	2.58683500	1.36075800
C	-1.36607200	3.70822500	1.66079500
H	-1.74790900	1.72125400	2.39634800
C	-0.40868400	4.60449100	1.17849700
H	1.67880400	4.87729000	0.69975800
H	-2.40341900	4.01914000	1.75658300
H	-0.69373300	5.61447100	0.89663900
C	1.60892600	-2.46701400	2.31085300
H	2.34167900	-3.18499500	2.69783700
H	0.95499700	-2.16965600	3.13783500
H	0.99682900	-2.97672000	1.56318700
C	1.58910600	0.74164100	3.67309900
H	1.03913000	1.36773600	4.38337500
H	1.78749000	-0.21626100	4.16260500
H	2.54905500	1.23128300	3.47253100
Li	1.59892600	0.86512800	-0.42917400
H	0.44423200	-0.66234900	0.63062400
C	-1.41301800	2.88711600	-2.95125100
H	-1.69404700	3.70716900	-2.27718700
H	-0.32986200	2.87945500	-3.05201300
H	-1.87625800	3.06112000	-3.92857700
C	-3.30199800	1.37044200	-2.55074500
H	-3.57660600	1.12446100	-3.58523600
H	-3.61325800	0.56471900	-1.89134600
H	-3.83787600	2.28403200	-2.26501000
H	-2.82092400	-1.32524800	-2.89131700
O	3.20542800	1.59470700	-1.31459200
C	4.52988500	1.54190400	-0.78841900
H	4.44696800	1.32875600	0.27788000
H	5.10606000	0.74143000	-1.26848700
H	5.03802100	2.50478700	-0.93661700
C	3.17434500	1.86405700	-2.71511800
H	3.71763000	1.08631600	-3.26845700
H	2.12545800	1.86501300	-3.01241500
H	3.62537900	2.84332100	-2.92674800

- **INT2 (R) with Me_2O**

Energy (RB3LYP): -1595.809101 A.U
Gibbs Free Energy: -1595.252340 A.U

Fe	-2.28890700	-0.45877800	1.55797900
C	-2.21124100	-1.62163000	-0.15142400
C	-2.93915800	-2.30213100	0.90676600
C	-2.02602400	-2.47404100	1.98086200
C	-0.77203800	-1.90150900	1.57811900
H	0.09172600	-1.85901000	2.23358100
C	-0.82375900	-1.38329000	0.24538100
C	-3.27904000	1.35062200	1.21153400
H	-3.74070900	1.63410400	0.27493100
C	-3.90893100	0.64296000	2.28320700
H	-4.93410100	0.29777500	2.30803000
C	-2.93662600	0.45321000	3.31520100
H	-3.09267800	-0.07373800	4.24676700
C	-1.71103100	1.04463700	2.87859100
H	-0.77652100	1.03833700	3.42302100
C	-1.92146000	1.60072300	1.57893400
H	-1.18019300	2.09341400	0.96663100
H	-2.25974200	-2.92240300	2.93923500
C	-2.63287100	-1.26472800	-1.52583200
O	-1.74124000	-1.01469900	-2.38634000
N	-3.93876500	-1.23852700	-1.92190800
N	2.62909400	1.03420200	0.33173200
C	3.51123300	0.39171100	1.33425100
H	4.44469100	0.96455900	1.34187300

C	2.73754500	2.50878400	0.28428300
H	2.83736000	2.92923100	1.30022600
C	3.87478300	-1.03386500	0.93468600
C	2.88525000	-1.97807000	0.61919700
C	5.21653300	-1.43836900	0.91100300
C	3.23323900	-3.29038000	0.28973500
H	1.83536500	-1.69497200	0.61127900
C	5.56891400	-2.75191500	0.58224800
H	5.99705000	-0.71892200	1.15052500
C	4.57579500	-3.68395400	0.27106500
H	2.45043500	-4.00532200	0.05049700
H	6.61582500	-3.04337100	0.56882400
H	4.84392000	-4.70594300	0.01738000
C	1.48503700	3.12341200	-0.32346500
C	0.94366700	2.63975700	-1.52548100
C	0.86877100	4.22250000	0.29098200
C	-0.18669000	3.23534400	-2.09070000
H	1.40687800	1.79107000	-2.01903800
C	-0.25700400	4.82742700	-0.27646700
H	1.27014900	4.60612400	1.22619200
C	-0.78965800	4.33401200	-1.46993100
H	-0.59756600	2.83898200	-3.01519800
H	-0.72193300	5.67460200	0.22003400
H	-1.66891400	4.79655200	-1.90943400
C	2.92015600	0.43061300	2.76031600
H	3.61934900	0.00472000	3.48798500
H	2.69642100	1.45930600	3.06472200
H	1.99256800	-0.15050200	2.80549200
C	3.98661200	2.92846300	-0.51561800
H	4.08807100	4.01880000	-0.52023700
H	4.89991100	2.50718100	-0.08282400
H	3.90888300	2.58211300	-1.55086300
Li	-0.04045200	-0.83706900	-1.56945300
H	1.66212800	0.77325900	0.52416200
C	-4.25421000	-1.05449100	-3.33511000
H	-4.53976400	-0.01471800	-3.54669000
H	-3.38414600	-1.30584300	-3.93842700
H	-5.09243300	-1.70674800	-3.60413200
C	-5.08755600	-1.23038800	-1.02425800
H	-5.56255300	-2.21844200	-0.95896300
H	-4.79121700	-0.90265000	-0.02995500
H	-5.82867300	-0.52257200	-1.41202800
H	-3.96356200	-2.64591200	0.90955100
O	1.30655600	-0.83151100	-2.98421400
C	2.72981700	-0.73837700	-2.85599200
H	2.93930200	-0.30111500	-1.87822400
H	3.18601100	-1.73403900	-2.92543200
H	3.13570600	-0.09537200	-3.64893600
C	0.89194300	-1.32242500	-4.26067900
H	1.29961200	-2.32722800	-4.43634000
H	-0.19774600	-1.36067400	-4.24938300
H	1.23721800	-0.64888800	-5.05670100

- **INT1 (S) with Me_2O**

Energy (RB3LYP): -1595.821958 A.U
Gibbs Free Energy: -1595.265863 A.U

Fe	-3.13930500	0.34016700	-0.63389900
C	-1.88924200	-1.05590500	0.27279200
C	-1.29187900	-0.59542600	-0.95232400
C	-2.17726800	-0.90046400	-2.01873000
C	-3.32351000	-1.56181900	-1.47979100
H	-4.18766600	-1.90064900	-2.03527700
C	-3.15695700	-1.66109800	-0.07041500
C	-3.45624500	1.98910400	0.60872100
H	-3.03810800	2.10749600	1.59949700
C	-2.84179900	2.40705300	-0.61130400
H	-1.87831500	2.88797100	-0.70738000
C	-3.70949400	2.04198100	-1.68629900
H	-3.51085900	2.19134600	-2.73872000
C	-4.85927300	1.40041200	-1.13176000
H	-5.68583000	0.98298600	-1.69050300
C	-4.70402300	1.36728100	0.28904700
H	-5.40409100	0.93715100	0.99271600
H	-2.02063300	-0.64592200	-3.05803600
C	-1.15801300	-0.98003800	1.56389600
O	0.06984500	-0.74604700	1.56740900
N	-1.78835400	-1.22465100	2.75067900
N	2.14603100	0.04980300	-1.18576400
C	2.35882100	1.35073300	-1.80277000
H	3.36720800	1.43982900	-2.25683800
C	2.32166100	-1.06979700	-2.10283000
H	1.56986200	-1.07162500	-2.92319200
C	2.29994500	2.44735200	-0.74219300
C	1.18035500	2.59558000	0.09429100
C	3.35408700	3.35946500	-0.58515800
C	1.12138300	3.60844000	1.05567800
H	0.34644200	1.90787900	-0.01163600
C	3.30140300	4.37983100	0.37119900
H	4.23058400	3.26632900	-1.22282800
C	2.18299500	4.50846900	1.19941600
H	0.24329000	3.70038100	1.69092900
H	4.13345400	5.07300800	0.46829100
H	2.13617100	5.30017500	1.94246800
C	2.09070300	-2.37576900	-1.34245500
C	2.93159300	-2.75327200	-0.28118400
C	1.04110400	-3.24175200	-1.68194300
C	2.72783700	-3.94712500	0.41738100
H	3.76049100	-2.10704300	-0.00789500
C	0.83182300	-4.43968100	-0.99033300
H	0.37707100	-2.97039000	-2.49882000
C	1.67456800	-4.79758500	0.06557500
H	3.39654800	-4.21735600	1.23121500
H	0.00946700	-5.09111000	-1.27587500

H	1.51650900	-5.72838400	0.60410700
C	1.36694200	1.70583400	-2.95185800
H	1.58009000	2.69909400	-3.36730200
H	1.44083500	0.97972200	-3.76903300
H	0.33265300	1.70114800	-2.58810700
C	3.69944800	-1.13410600	-2.82321300
H	3.78135400	-2.04593700	-3.42751400
H	3.83757500	-0.27921000	-3.49363700
H	4.52097400	-1.12601100	-2.09664500
Li	1.69364300	-0.30361100	0.62272300
H	-3.86152400	-2.13018700	0.59850700
C	-0.97336400	-1.37332000	3.95395900
H	0.00681300	-1.76558300	3.68639900
H	-0.84125000	-0.41416000	4.47304000
H	-1.47235900	-2.07240600	4.63175700
C	-3.22927700	-1.17372900	2.97400600
H	-3.41973300	-0.63385000	3.90808800
H	-3.72323600	-0.63555100	2.16771600
H	-3.66380400	-2.17769900	3.06677900
H	-0.30997700	-0.13781400	-1.04120300
O	3.04707300	0.06849200	2.04321400
C	4.35850000	0.45624000	1.63277600
H	5.11482200	-0.16512900	2.13336100
H	4.39613000	0.31271400	0.55177200
H	4.53710100	1.51358900	1.86655300
C	2.80722400	0.28106700	3.42678300
H	2.93741400	1.34109300	3.68586100
H	1.77622000	-0.01686900	3.62031100
H	3.48993200	-0.32588700	4.03914300

- **TS (S) with Me_2O**

Energy (RB3LYP): -1595.796333 A.U
Gibbs Free Energy: -1595.240849 A.U

Fe	-2.96501900	0.13490500	-0.57736700
C	-1.53930500	-1.09728000	0.31973800
C	-0.91977000	-0.51259300	-0.85606300
C	-1.77108000	-0.90758700	-1.93549000
C	-2.85086900	-1.73197800	-1.47361800
H	-3.64973900	-2.15650500	-2.06986200
C	-2.72237000	-1.85006400	-0.06421900
C	-3.57973300	1.70518200	0.66741600
H	-3.22140700	1.87949500	1.67351500
C	-3.00109100	2.23026600	-0.52849100
H	-2.12468400	2.85942000	-0.58916100
C	-3.76330400	1.74291200	-1.63432100
H	-3.55676700	1.93184200	-2.67892700
C	-4.81416400	0.92129800	-1.12333100
H	-5.54469300	0.38363700	-1.71239100
C	-4.70226000	0.89734500	0.30206600
H	-5.35128200	0.35745700	0.97868800
H	-1.64210800	-0.60529400	-2.96940700
C	-0.90379400	-1.01103500	1.65390700
O	0.31439200	-0.71139800	1.76031900
N	-1.58035500	-1.31866100	2.80221600
N	1.71053400	0.14565800	-1.26242300
C	1.89055100	1.49159300	-1.84232200
H	2.90747100	1.58270700	-2.24893200
C	2.08751400	-0.96606300	-2.16522600
H	1.33816100	-1.08215100	-2.96893900
C	1.78425500	2.56207700	-0.76094300
C	0.74189500	2.55601400	0.18062100
C	2.72092100	3.60564200	-0.70427100
C	0.64945400	3.55736000	1.15241600
H	-0.00678300	1.76863800	0.14124500
C	2.62864500	4.61240600	0.26222600
H	3.53356900	3.63127200	-1.42755100
C	1.59112400	4.59024600	1.19890800
H	-0.16489100	3.53284900	1.87228300
H	3.36570500	5.41119600	0.28309700
H	1.51451800	5.37006400	1.95178000
C	2.07203800	-2.27799200	-1.37953500
C	2.99095600	-2.51339900	-0.34320500
C	1.15485600	-3.29184700	-1.68777100
C	2.99294300	-3.71976900	0.36229400
H	3.72319700	-1.75084900	-0.09061400
C	1.15294400	-4.50231400	-0.98803100
H	0.42326700	-3.12350900	-2.47293200
C	2.07211400	-4.72179300	0.04121300
H	3.71586700	-3.87840500	1.15849300
H	0.42700300	-5.26984200	-1.24304400
H	2.07104900	-5.66108400	0.58751600
C	0.91175700	1.80865200	-3.00307100
H	1.09614300	2.81098800	-3.40664900
H	1.03209400	1.08987200	-3.82156700
H	-0.12459200	1.75881500	-2.65657400
C	3.45264700	-0.79773800	-2.86702200
H	3.70612200	-1.71478600	-3.40931700
H	3.44107400	0.02111700	-3.59289300
H	4.25340500	-0.60013000	-2.14476000
Li	1.74298200	-0.18395800	0.69588600
H	-3.38402600	-2.42405800	0.56883800
C	-0.82865800	-1.43551400	4.04795100
H	0.17819000	-1.79577700	3.83982500
H	-0.75568900	-0.47128200	4.57071100
H	-1.34123000	-2.14790200	4.70170900
C	-3.03092000	-1.34264800	2.95120500
H	-3.30290600	-0.77884800	3.85161800
H	-3.50841300	-0.87097000	2.09571200
H	-3.40969800	-2.36714800	3.06387900
H	0.47632200	-0.04219600	-1.06069300
O	3.22603700	0.32196200	1.89426100
C	4.43872900	0.92878200	1.45418200
H	5.30228400	0.46174400	1.94770700

H	4.50201600	0.77610400	0.37594600
H	4.43129700	2.00552600	1.66527800
C	3.00434900	0.46673100	3.29584000
H	2.97167800	1.52913700	3.57216100
H	2.04210000	0.00159200	3.51065800
H	3.80099100	-0.03321900	3.86392400

- **INT2 (S) with Me_2O**

Energy (RB3LYP): -1595.809828 A.U
Gibbs Free Energy: -1595.253886 A.U

Fe	-2.33325100	1.45474100	-0.86081900
C	-2.15545800	-0.56700400	-0.47739000
C	-0.79157400	-0.04677000	-0.58297100
C	-0.76431300	0.53036300	-1.89200700
C	-2.00629700	0.34644600	-2.58833600
H	-2.25467500	0.69694800	-3.58315200
C	-2.88792700	-0.33961300	-1.71218200
C	-3.40083900	2.40948600	0.65976600
H	-3.85489400	1.90497800	1.50247100
C	-2.06431700	2.91338400	0.60935700
H	-1.33123800	2.84388100	1.40069800
C	-1.85557800	3.47605100	-0.68806100
H	-0.93417200	3.91005200	-1.05187900
C	-3.06174300	3.32156800	-1.43843300
H	-3.21371500	3.62165900	-2.46632300
C	-4.01905200	2.66238300	-0.60463100
H	-5.02679700	2.39059900	-0.88947400
H	0.07177500	1.07337500	-2.32028300
C	-2.55922900	-1.26486500	0.76635400
O	-1.67128000	-1.55604100	1.61481400
N	-3.84484100	-1.65064000	1.02254200
N	2.81563200	-0.49184200	-0.74957400
C	3.61526100	0.68808100	-1.14228700
H	4.66549500	0.38086500	-1.10391600
C	2.98206700	-1.70536500	-1.57656100
H	2.70560200	-1.51940100	-2.62834000
C	3.45599600	1.80397400	-0.11578100
C	2.19461600	2.31990100	0.22468800
C	4.59020100	2.36642000	0.48693100
C	2.07929500	3.36852800	1.14142800
H	1.28996100	1.89601000	-0.20434800
C	4.47809800	3.41779100	1.40267300
H	5.57498200	1.97721000	0.23734200
C	3.21866400	3.92435000	1.73242800
H	1.09505600	3.75445400	1.39258100
H	5.37230100	3.83796300	1.85541000
H	3.12455500	4.74286900	2.44079100
C	2.04742200	-2.79593000	-1.06673700
C	2.08029000	-3.20916700	0.27468500
C	1.16076900	-3.43668500	-1.94104500
C	1.24955700	-4.23721200	0.72630200
H	2.75881200	-2.71729600	0.96487800
C	0.32964900	-4.46865400	-1.49408500
H	1.11049200	-3.11697700	-2.97908700
C	0.37168600	-4.87282300	-0.15803400
H	1.28483900	-4.54080600	1.76920600
H	-0.35657800	-4.94687000	-2.18772100
H	-0.27736900	-5.66970300	0.19424900
C	3.33683800	1.21795700	-2.56806500
H	3.98520600	2.07211500	-2.79172600
H	3.52180200	0.44875900	-3.32531800
H	2.29812100	1.55026900	-2.66643000
C	4.44094300	-2.19907000	-1.56825900
H	4.50912700	-3.16087500	-2.08553600
H	5.11304500	-1.50129200	-2.07805300
H	4.79770300	-2.33422800	-0.54154400
Li	-0.00329100	-0.78051800	1.17839400
H	-3.89701700	-0.62921000	-1.96528600
C	-4.11152600	-2.50604000	2.17541000
H	-3.19810000	-3.02289700	2.46397100
H	-4.47070000	-1.92089200	3.03368900
H	-4.88144100	-3.23786600	1.90759100
C	-5.02665800	-1.15280100	0.32854700
H	-5.83344800	-1.03243200	1.05940500
H	-4.82633700	-0.18005700	-0.11708100
H	-5.37270000	-1.84759500	-0.44838600
H	1.82128400	-0.25089400	-0.74614300
O	1.05582600	-0.66979000	2.80833600
C	2.42827300	-0.29336600	2.94148200
H	2.96791600	-1.04076800	3.53957600
H	2.84793500	-0.24700500	1.93557100
H	2.51241100	0.68891400	3.42384200
C	0.38890500	-0.82762800	4.05980700
H	0.39216500	0.11773100	4.61974300
H	-0.63613400	-1.12796000	3.83852200
H	0.88310900	-1.60346900	4.66067600

References

1 Gaussian 16, Revision A.03, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

2 (a) A. D. Beche, *Phys. Rev.* 1988, **A38**, 3098-3100. (b) A. D. Beche, *J. Chem. Phys.* 1993, **98**. 1372-1377. (c) A. D. Beche, *J. Chem. Phys.* 1993, **98**, 5648-5652. (d) C. Lee, W. Yang, R. G. Parr, *Phys. Rev.* 1988, **B37**, 785-788.

3 (a) P. J. Hay, W. R. Wadt, *J. Chem. Phys.* 1985, **82**, 270. (b) W. R. Wadt, R .J. Hay, *J. Chem. Phys.* 1985, **82**, 284. (c) P. J. Hay, W. R. Wadt, *J. Chem. Phys.* 1985, **82**, 299.

4 (a) K. Fukui, *Acc. Chem. Res.* 1981, **14**, 363. (b) K. Ishida, K. Morokuma, A. Komornicki, *J. Chem. Phys.* 1977, **66**, 2153. (c) C. Gonzalez, H. B. Schlegel, *J. Chem. Phys.* 1989, **90**, 2154. (d) H. B. Schlegel, C. J. Gonzalez, *Phys. Chem.* 1990, **94**, 5523.