

SUPPLEMENTARY MATERIAL for:

Computational study of diastereoselective *ortho*-lithiations of chiral ferrocenes

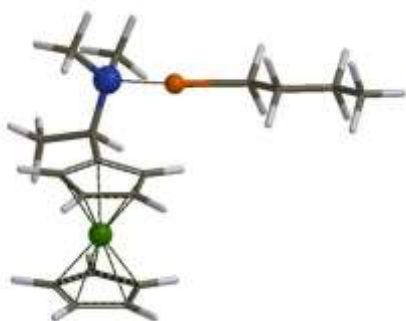
Andrea Škvorcová, Radovan Šebesta*

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1. THEORETICAL CALCULATION OF LITHIATION OF (R)-1.

1.1. The coordinates and energie of complexes C1-3.

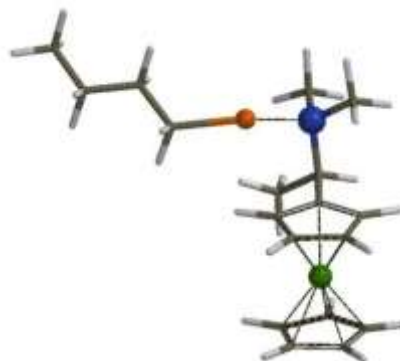
(R)-1...*n*-BuLi (C1a)
(RI-DFT: BP-86/def2-TZVP)



E = -2029.31625528445 au
Imaginary frequencies: 0

Fe	-5.13553117	0.00671471	-0.13992771
C	-1.36732276	-0.19960760	-0.95972063
C	-2.82378771	-1.21765739	-3.00317097
C	-4.30306872	-3.26967388	-2.03951301
C	-3.75778882	-3.53379691	0.59979064
C	-1.93420178	-1.63458953	1.29707057
C	-5.99611285	3.78265706	0.22395546
C	-6.56379922	2.46291622	2.51906706
C	-8.37328552	0.52684715	1.95197935
C	-8.92442387	0.65166380	-0.69681001
C	-7.45465582	2.66231975	-1.76400122
C	-0.63494215	-1.28145804	3.81485501
C	-2.16881095	-2.28817691	6.05936845
Li	3.46433156	-0.80395903	0.31415453
N	2.01543291	-2.32424795	3.63670239
H	-2.83405602	-0.51790061	-4.93269032
H	-5.63932989	-4.40227039	-3.11059491
H	-7.42338590	3.21740384	-3.74011188
H	-10.20645845	-0.58104235	-1.72215456
H	-4.66793356	5.33438198	0.01848828
H	-9.17451655	-0.81054017	3.28799279
H	-1.18503062	-1.96118644	7.85738196
H	-2.55197071	-4.32135130	5.89571665
H	-0.35172884	0.76459345	4.08814839
H	-4.61208548	-4.90998557	1.86151343
C	2.10317260	-5.10249222	3.50849307
H	0.85279378	-5.78097983	1.99851573
H	4.04464453	-5.70246098	3.07503431
H	1.54411298	-6.01803916	5.30241853
C	5.57127182	1.89379648	-1.44127012
C	5.78493824	1.79638054	-4.33956268

(R)-1...*n*-BuLi (C1b)
(RI-DFT: BP-86/def2-TZVP)



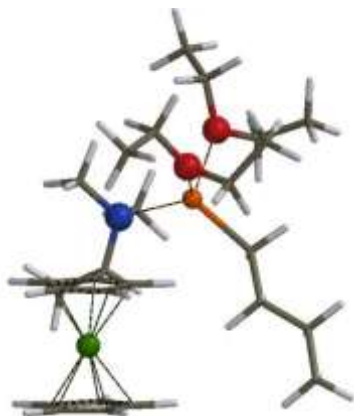
E = -2029.31529811354au
Imaginary frequencies: 0

Fe	2.40171813	4.50640245	2.71549774
C	3.69785263	4.30758165	-0.91149573
C	1.98354692	6.38586480	-0.63851094
C	-0.39990311	5.39577860	0.18232571
C	-0.16762154	2.70840760	0.41350171
C	2.37984227	2.01060491	-0.27167584
C	5.42199247	5.39370197	5.00248080
C	4.39885001	2.98496412	5.69695229
C	1.80093665	3.33785871	6.38054688
C	1.22022894	5.96931127	6.11084624
C	3.45780519	7.23945176	5.26185738
C	3.37590608	-0.65397039	-0.54737377
N	2.59299110	-1.68105889	-3.09924328
C	3.67571502	-0.16773739	-5.17477045
C	3.38925500	-4.33394944	-3.43280732
H	3.04963299	-0.95540862	-6.99045752
H	2.90681171	-4.94181934	-5.35728763
H	5.45465243	-4.56847519	-3.17391045
H	5.77025369	-0.18890197	-5.14386501
H	3.03992589	1.79865811	-5.04980797
H	-1.66297822	1.42462501	1.00719066
H	-2.08365565	6.49168956	0.60437050
H	2.42805497	8.36642062	-0.94799711
H	-0.60568003	6.84155357	6.45622135
H	3.62350082	9.24382756	4.84941860
H	7.34159201	5.75343065	4.36948996
H	5.42368054	1.20582292	5.70372111
H	0.49297882	1.87196431	6.97650604
H	5.66644921	4.43205517	-1.48770429
H	2.40033026	-5.57673939	-2.10636255
C	2.44276821	-2.39749617	1.57212921

C	7.41874226	3.86782802	-5.57625310
C	7.56998418	3.69199954	-8.46395266
H	6.66067507	5.73101446	-5.02105186
H	8.37694380	1.86840590	-9.06227157
H	8.75023230	5.19768496	-9.28174066
H	5.67966224	3.84081372	-9.32436974
H	9.33725460	3.77276328	-4.76204476
H	6.55282679	-0.05595825	-4.94411104
H	3.88281675	1.89279646	-5.21372352
H	4.87656745	3.80393673	-0.90508210
H	7.51442589	1.83366464	-0.64612202
C	3.64145981	-1.39735208	5.69652389
H	5.60068215	-1.98374529	5.33724567
H	3.08233427	-2.13472779	7.57209281
H	3.59335820	0.67678971	5.74721857
H	-3.99539305	-1.31142593	6.14850049
H	-5.75823695	2.86387424	4.36510177
H	-0.08269652	1.40904812	-1.09085821

H	5.47275912	-0.57948439	-0.49772262
H	0.41121015	-2.81148597	1.37159672
H	3.47440670	-4.19476916	1.61183352
C	-5.97599750	-4.86498310	-2.62046353
H	2.72356872	-1.45789653	3.39437407
C	-4.82218673	-2.38740925	-1.62263107
C	-8.65047669	-5.51126084	-1.66248071
C	-9.71610351	-7.99407678	-2.70740620
Li	-1.32894427	-1.43465585	-2.92594097
H	-9.92738000	-3.93469029	-2.14895380
H	-6.14945269	-0.82437692	-2.07904273
H	-6.04813517	-4.83537749	-4.71369608
H	-4.73206696	-6.48416772	-2.15167495
H	-8.50139850	-9.60576622	-2.19537990
H	-11.62539668	-8.39451797	-1.98438671
H	-9.83078990	-7.94453276	-4.78563251
H	-4.85448689	-2.46648988	0.47852705
H	-8.60845596	-5.58317790	0.42248145

(R)-1...n-BuLi...2Et₂O (C2a)
(RI-DFT: BP-86/def2-TZVP)



E = -2496.83984663150 au
Imaginary frequencies: 0

Fe	-6.36455327	0.93822936	-3.48681647
C	-2.60222814	0.30897456	-2.80268518
C	-3.21709373	-0.27278672	-5.37404950
C	-5.12424454	-2.20219124	-5.36747015
C	-5.68317822	-2.80916599	-2.78628259
C	-4.11809468	-1.26140149	-1.18100648
C	-6.94792184	4.74473962	-2.97709897
C	-8.46324091	3.32132817	-1.24243661
C	-10.09197265	1.69955972	-2.67910858
C	-9.58376927	2.12346818	-5.30611627
C	-7.64196068	4.00497858	-5.48893264
C	-3.97017738	-1.27604439	1.67002536
C	-6.43859190	-2.19470852	2.89988811

(R)-1...n-BuLi...2Et₂O (C2b)
(RI-DFT: BP-86/def2-TZVP)



E = -2496.83917280484 au
Imaginary frequencies: 0

Fe	7.89182816	2.50782361	-0.67869250
C	5.05875616	4.39907689	-2.48647692
C	5.90315715	5.79566264	-0.32238688
C	5.53818496	4.23223082	1.86270911
C	4.46035573	1.88622224	1.04795615
C	4.14105941	1.97253713	-1.65142942
C	11.62040978	3.57591571	-0.81519919
C	10.91130204	2.34253809	-3.12024564
C	10.06573303	-0.15547811	-2.50472021
C	10.24629104	-0.46657585	0.18077093
C	11.20816822	1.84077400	1.22442812
C	2.97206713	-0.06374322	-3.28429887
C	3.53989121	-2.71428993	-2.26215435

Li	1.94883641	-0.64631224	1.27473889	N	0.16015588	0.32311979	-3.53046954
N	-1.64740693	-2.67337153	2.54342315	C	-0.39514441	2.73093119	-4.79521428
H	-2.42563161	0.63241327	-7.03891354	H	-2.45078512	2.94263275	-4.98939876
H	-6.81245945	4.71781384	-7.22649780	H	0.33131535	4.32288491	-3.68854787
H	-6.02061665	-3.02608894	-7.02155613	H	0.44762658	2.82841240	-6.71655115
H	-10.48873544	1.16533517	-6.88055540	H	3.79940500	0.12321024	-5.20967527
H	-5.49375996	6.10348344	-2.47425399	H	6.03446395	4.72295859	3.79400814
H	-11.45900021	0.37111914	-1.91542800	H	6.72314067	7.67847516	-0.34207613
H	-6.37942295	-2.00840681	4.96493164	H	9.72466792	-2.14397652	1.24337057
H	-6.84999773	-4.17976670	2.44717482	H	11.53514217	2.21889599	3.21567277
H	-3.61550242	0.68475335	2.27350492	H	12.31297094	5.50091380	-0.64010665
H	-7.08066899	-4.17748427	-2.16059120	H	5.12575501	5.04341667	-4.43645497
C	-1.67273769	-5.36605313	1.88574765	H	3.22073457	-4.17621925	-3.69650546
H	-1.96222924	-5.59322761	-0.15541099	H	5.52269414	-2.82152580	-1.67727704
H	0.16029453	-6.20254828	2.39519832	H	9.39137584	-1.55955170	-3.84205716
H	-3.15431728	-6.45467377	2.89073174	H	3.96372175	0.30088876	2.25457536
C	2.05328825	3.31516314	2.00637596	C	-0.97479196	-1.73136744	-5.03101858
C	0.83828283	5.52301675	0.56704198	H	-0.04085048	-1.94983153	-6.89786881
C	1.38296100	8.20698740	1.56737953	H	-2.97710038	-1.29467672	-5.34771232
C	0.11491971	10.32741027	0.05414818	H	-0.87041490	-3.52489794	-4.00233406
H	0.77842092	8.30345385	3.56202062	Li	-2.10096408	-0.30119492	0.16124427
H	0.56425846	12.21168587	0.81317467	C	-1.38666136	-3.52298348	2.49889619
H	0.72101157	10.29420643	-1.93765786	C	-1.33408010	-6.32669739	1.74168235
H	-1.95763013	10.12758240	0.07221665	C	-0.80212745	-8.25934762	3.85913045
H	3.44936815	8.49593298	1.58959191	C	-0.78041618	-11.01803802	2.97333235
H	1.41844319	5.49023210	-1.45125177	H	1.02910135	-7.78624186	4.74045449
H	-1.24412847	5.28646278	0.51824288	H	0.67318720	-11.32545492	1.51464349
H	1.39173425	3.46023071	4.00510501	H	-2.61190793	-11.55214389	2.13884867
H	4.11447272	3.73686907	2.14933008	H	-0.39336565	-12.34164046	4.53134045
C	-1.27417186	-2.35789018	5.27908383	H	0.09261685	-6.64882070	0.23956753
H	0.58072611	-3.12918429	5.79944488	H	-3.15310293	-6.87788928	0.85137340
H	-2.72938667	-3.33020361	6.42737441	H	-2.23097057	-8.00989331	5.35930011
H	-1.28504387	-0.33440758	5.74285069	H	-2.79530984	-3.33493631	4.05793603
H	-8.02467212	-1.05533660	2.20496527	H	0.44248532	-3.11141847	3.46579358
H	-8.37594682	3.44655799	0.80533150	H	2.32399110	-3.12258957	-0.62302310
O	3.57777738	-1.91040993	-2.11323651	H	10.97938628	3.16510517	-5.00018979
C	4.74499959	0.19947238	-3.40372861	O	-2.48618951	3.07109303	2.30567977
H	4.14176803	1.83548119	-2.27147109	C	-1.38403714	5.54565702	2.07360004
O	4.86851348	-2.29612514	3.87778786	C	-3.68197230	2.60730881	4.71836530
C	6.39377999	-4.51797557	3.56470636	H	0.13796795	5.35900493	0.67531769
C	5.73587781	-0.52689936	5.77374421	O	-6.04208954	-0.39846547	-1.13029784
H	5.61431819	-5.45558428	1.88403396	C	-7.27224535	-2.74991846	-0.46549623
H	8.35738309	-3.98230290	3.10757690	C	-7.65186311	1.50919677	-2.19306085
H	5.76725432	-1.46117929	7.63949160	H	-6.35416496	3.02235934	-2.77875022
H	4.26713615	0.93703854	5.79835843	H	-5.79996244	-3.77243614	0.58189173
C	3.86300096	-4.33568335	-3.29943451	H	-8.85084879	-2.36776974	0.84228343
H	3.92758841	0.38608213	-5.31215146	H	-8.57933801	0.78564123	-3.91791784
H	5.88688686	-4.83599577	-3.41583350	H	-0.48313035	6.08573858	3.87371227
H	2.97202667	-5.66805858	-1.97692856	H	-4.96999823	1.01542256	4.38096039
C	6.34374220	-6.31523629	5.81924546	C	-9.61522653	2.56494177	-0.36552869
C	8.28502191	0.67155158	5.18610903	C	-8.17573156	-4.27254836	-2.73496941
H	9.85192536	-0.69215858	5.22241803	H	-11.04059734	1.15265549	0.16511232
H	8.23691400	1.60342313	3.33243652	H	-10.61660535	4.14822847	-1.26679516
H	8.69332101	2.12257554	6.61655913	H	-9.67810533	-3.31590535	-3.80565872
H	7.40311599	-8.04213792	5.35321399	H	-8.94717873	-6.08540946	-2.07331042

H	7.22291700	-5.48555184	7.50674553	H	-6.60236102	-4.68440332	-4.02527299
H	4.39769507	-6.86072460	6.29791443	H	-8.70747788	3.26822829	1.36303685
C	7.61609692	0.04612224	-3.52540642	C	-3.29116208	7.54331553	1.25280040
C	2.61975997	-4.55566084	-5.88889472	H	-4.12689817	7.05867850	-0.58515870
H	8.35645814	1.80627049	-4.34583242	H	-4.82895645	7.76047848	2.63203524
H	8.29310931	-1.52075249	-4.71034087	H	-2.34809480	9.38721758	1.06759765
H	8.42322195	-0.16442920	-1.62408644	H	-4.83272264	4.26763834	5.24578974
H	2.72679135	-6.52932993	-6.53329905	C	-1.80672950	1.93328341	6.79267311
H	3.56798865	-3.38621585	-7.31835312	H	-2.83257256	1.57608317	8.56589921
H	0.62218974	-3.99944828	-5.79927771	H	-0.76989556	0.21089776	6.28094522
H	-1.24996561	1.70867483	-2.13487915	H	-0.45307155	3.46814379	7.15200819

(R)-1...(n-BuLi)₂...3Et₂O (C3)
(RI-DFT: BP-86/def2-TZVP)



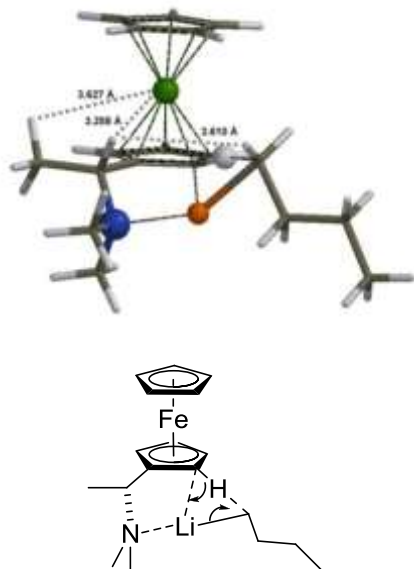
E = -2896.04334694625 au
Imaginary frequencies: 0

C	0.24409524	-1.85162147	-4.41172807	H	0.66201653	6.84195800	-0.13200797
C	-4.21504682	0.01208211	0.82372524	H	-1.34298340	4.40924920	1.04640108
Li	-2.47612767	1.00599841	-2.93910132	O	-2.50926076	-6.33644465	-0.57413982
Li	-1.05834475	-2.52749156	-0.45244638	C	-4.71934787	-6.95720218	0.89248623
H	-1.01594886	-3.06597523	-5.58466058	C	-1.89529967	-8.08121014	-2.57358018
H	1.54191986	-3.25928467	-3.52506455	H	-4.44089263	-8.79354236	1.84499341
H	-5.73034006	-1.38866525	0.40291060	H	-4.78779608	-5.49003502	2.35866812
H	-5.04035631	1.79943954	0.06104024	H	-3.51798805	-8.27024306	-3.86879787
C	4.27212401	-4.81006259	1.02158619	H	-0.38065632	-7.13645294	-3.63302418
C	1.29113949	-4.72119468	4.42787219	O	-5.36668750	1.44973530	-5.68840531
H	3.35101564	-6.54342851	0.34497765	C	-7.51743313	3.05993320	-5.23650393
H	5.01574103	-3.80596901	-0.63086721	C	-5.62151854	-0.20885736	-7.83454153
H	2.72487547	-5.38938544	5.79765244	H	-8.12313668	3.93947931	-7.02908491
H	-0.09903454	-3.55925640	5.44170789	H	-7.51252086	-1.08795197	-7.82330057
O	-1.61862292	4.90820114	-2.71374302	H	-4.22361904	-1.70875436	-7.51574076
C	-1.13608075	6.54296976	-4.83421746	H	-6.79573114	4.57224546	-4.01010817
C	-1.25164931	6.02304761	-0.25509995	C	-4.14414957	0.34801367	3.71031789
H	-2.28857787	8.27480315	-4.66810859	H	-2.66529096	1.73449076	4.24852950
H	-1.84469447	5.47907648	-6.46981445	H	-3.53671445	-1.43631849	4.62674549

C	1.88984857	-0.30510234	-6.24092549	H	-7.26885027	-8.49371186	-1.99691910
H	3.24008204	0.87413607	-5.15820698	H	-2.55478947	-11.71441269	-0.68227802
H	0.70654972	1.07328447	-7.28998747	H	-0.42834284	-11.81526182	-3.26634835
C	-6.62035323	1.17273947	5.00826848	H	0.56797336	-10.50186900	-0.33657502
C	-6.41981256	1.45589493	7.88408478	H	-10.49102831	0.18558593	-5.14640722
H	-8.10824278	-0.21177741	4.53662358	N	2.37984742	-3.26049432	2.33512042
H	-7.24220271	2.97677668	4.16409014	H	0.31443856	-6.37699985	3.64386190
H	-8.21947974	2.05128086	8.73994625	H	5.86804462	-5.36431687	2.25768773
H	-4.98273019	2.87062737	8.40085195	C	3.37783312	-0.74255218	3.19715186
H	-5.86657762	-0.34068872	8.77857606	Fe	7.37594189	1.77028797	7.19542136
C	3.42301941	-1.80050533	-8.21797542	C	8.15814284	-1.07304996	4.67263111
C	5.02737754	-0.15149831	-9.97796120	C	5.47760621	-0.96273889	5.13792320
H	2.10396751	-2.95999928	-9.34476561	C	5.13488891	-1.31771071	7.81718055
H	4.64900456	-3.15763776	-7.21335837	C	7.55994169	-1.66074130	8.97166442
H	3.83976047	1.18210044	-11.04819237	C	9.43338008	-1.50638235	7.02177659
H	6.09223032	-1.28548068	-11.35871153	C	8.46300138	5.14169817	5.60075992
H	6.40486134	0.97706335	-8.89995450	C	9.93263303	4.62166003	7.81702098
C	-7.17708807	-6.95292422	-0.60795083	C	8.23338764	4.39910257	9.91619686
C	-1.03838924	-10.66968810	-1.64275866	C	5.71294592	4.78068395	8.99878706
C	-9.71073874	1.70038512	-3.95856349	C	5.85612201	5.24292379	6.33378710
C	-5.12261207	1.11369009	-10.34441033	C	4.10033760	0.87492593	0.91365381
C	-3.24726972	7.98053839	0.43872763	H	9.07431324	-0.82972487	2.85168684
C	1.64363902	7.20254404	-5.19844456	H	11.46526569	-1.64892766	7.28344461
H	-11.24588962	3.05340122	-3.58767465	H	7.91839916	-1.94106245	10.97415107
H	-9.09926964	0.88795496	-2.14836096	H	1.74563494	0.15407835	4.13020518
H	-3.18791176	9.65308796	-0.79142114	H	2.58132861	0.83564887	-0.50600380
H	-3.20743223	1.91330336	-10.38263658	H	4.42358818	2.83310264	1.51103938
H	-6.48506578	2.63691314	-10.71733691	H	5.84270475	0.21429683	-0.00095726
H	-5.14922213	7.15315265	0.34873398	H	3.33084677	-1.28866036	8.79903961
H	-2.92448577	8.63220089	2.38581279	H	11.97275400	4.40164799	7.88763682
H	1.86597662	8.29610347	-6.95251509	H	8.76047075	3.97823410	11.85547849
H	2.39195880	8.36306195	-3.64774787	H	9.19499415	5.39040486	3.69877602
H	2.78865939	5.47943800	-5.35706857	H	3.99469915	4.70450532	10.11981856
H	-5.27766123	-0.25727089	-11.89963868	H	4.26057207	5.58990562	5.08968472
H	-8.77285826	-7.20088691	0.70039618				
H	-7.42379527	-5.14331375	-1.59346863				

1.2. The coordinates and energies of transition states TS1-3.

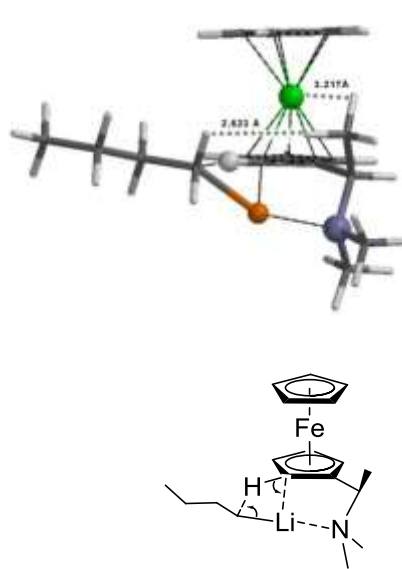
(*R,R*)-TS 1 (preferred)
(RI-DFT: BP86/def2-TZVP)



E = -2029.29366191565 au
Imaginary frequencies: 1 (-1210.77 cm⁻¹)

Fe	-4.81060897	0.29182314	-0.16234667
C	-1.18360950	-0.71308646	-1.31487368
C	-3.05379740	-1.44114469	-3.14857252
C	-4.87308542	-3.10416204	-2.00920000
C	-4.16555612	-3.44534066	0.58255204
C	-1.91647430	-1.96672544	1.02066387
C	-4.73664960	4.14295165	0.33907597
C	-5.52182306	2.90809651	2.61873928
C	-7.75898209	1.47615519	2.07517856
C	-8.35658470	1.82590211	-0.54397096
C	-6.48806115	3.47019148	-1.61669395
C	-0.37961018	-1.76746185	3.42886374
C	-1.59544016	-3.11015068	5.68888204
Li	2.70079314	-0.48380139	-0.41393266
N	2.31252198	-2.57333914	2.86954923
H	-3.12483745	-0.78948105	-5.09835662
H	-6.52520185	-3.92226341	-2.91935503
H	-6.39373197	4.07288793	-3.57701969
H	-9.92801529	0.96690648	-1.54827399
H	-3.07355351	5.32486719	0.11581847
H	-8.80686763	0.31598860	3.40680286
H	-0.47322180	-2.88283187	7.42063820
H	-1.85885979	-5.13977057	5.34129715
H	-0.18866838	0.25294958	3.90499151
H	-5.19179171	-4.57491870	1.95946255
C	2.52630475	-5.28917574	2.29947237
H	1.16337233	-5.79725492	0.82014721

(*R,S*)-TS1 (non-preferred)
(RI-DFT: BP86/def2-TZVP)



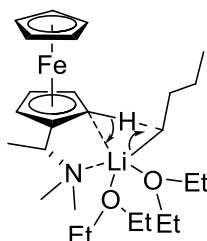
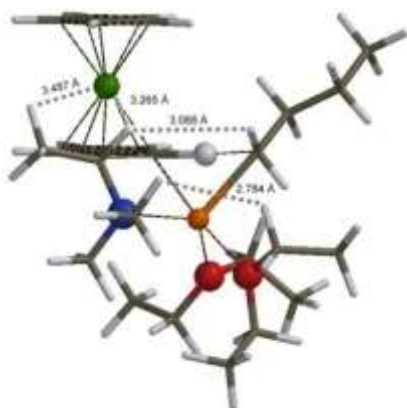
E = -2029.290104441au
Imaginary frequencies: 1 (-1289.10 cm⁻¹)

Fe	-2.44107122	1.74378342	3.23611271
C	-5.49172417	0.63665706	1.13096158
C	-5.12453564	-1.02744654	3.23481896
C	-2.64693259	-2.11605265	2.99131404
C	-1.41540028	-1.16435818	0.75980267
C	-3.22770868	0.55917805	-0.38369313
C	-3.36083866	5.02013786	5.12185129
C	-1.36990135	5.49472346	3.34868676
C	0.72265004	3.89290736	3.97918914
C	0.02435237	2.43253112	6.15057850
C	-2.49518064	3.13208416	6.85926320
C	-2.87471369	1.71022857	-2.98580477
C	-0.54457783	3.41819562	-3.16185555
N	-2.68070753	-0.45191224	-4.86183949
C	-5.05279297	-1.92233709	-4.88330169
H	-4.85372065	-3.53714400	-6.17412312
H	-5.47837135	-2.62159704	-2.98041151
H	-6.67188615	-0.76385122	-5.53250713
H	-4.57383934	2.83910547	-3.47540458
H	-1.80529216	-3.41465208	4.34688184
H	-6.46016025	-1.34737282	4.76495637
H	1.18553597	1.01044001	7.06896299
H	-3.57665394	2.33358901	8.41142734
H	-5.20673141	5.91950211	5.13496442
H	-7.17019207	1.76784943	0.75964678
H	-0.41024914	4.39314884	-4.98830590
H	-0.66709492	4.85297005	-1.67795146

H	4.44389782	-5.70119994	1.61218856
H	2.17959133	-6.49567767	3.97066614
H	0.45226281	1.36910545	-1.40237062
C	2.62339259	3.27264268	-1.66887250
C	4.81157436	2.11526278	-3.17849449
C	6.12149175	3.80853235	-5.15101625
C	8.23979889	2.49063487	-6.61672179
H	4.66785956	4.50268401	-6.47231553
H	9.10855176	3.75782284	-8.01632256
H	9.74966391	1.84031010	-5.34052814
H	7.52524991	0.82446217	-7.63835495
H	6.86468906	5.49366036	-4.17834241
H	6.31254115	1.41996293	-1.87933493
H	4.14346647	0.40273020	-4.23232050
H	1.48837001	4.49608629	-2.91666655
H	3.33212291	4.48373043	-0.12599003
C	4.06214498	-1.86685227	4.90825352
H	6.01519430	-2.23747673	4.30282180
H	3.73657920	-2.93441175	6.67669248
H	3.87612536	0.16017168	5.31880225
H	-3.46726225	-2.28789632	6.04372244
H	-4.58148660	3.03223513	4.44118530

H	2.50843255	3.77504323	2.97462200
H	1.12271671	-1.69118321	-0.02558445
C	-2.15775494	0.42093389	-7.45375120
H	-3.59007479	1.79463788	-8.12358352
H	-2.19013229	-1.21360509	-8.73346037
H	-0.28721615	1.29771659	-7.58070194
Li	0.03310385	-2.39171145	-2.80433482
C	3.66428780	-2.44496461	-1.10439943
C	4.66242025	-4.08827079	1.06322382
C	7.48528219	-4.76146194	0.95810326
H	3.56819989	-5.86914776	1.16111470
H	4.28506064	-3.12489029	2.88056425
H	7.87768733	-5.75202522	-0.83560278
H	4.78429605	-0.68431321	-1.22603193
H	4.06813950	-3.44794719	-2.91869800
H	1.20930868	2.34669989	-2.83769616
H	-1.43888870	6.85896809	1.81551977
C	8.38247256	-6.38225817	3.18320714
H	10.40903216	-6.82727264	3.05033329
H	7.34735841	-8.18588230	3.26465231
H	8.07091472	-5.40737839	4.99496226
H	8.59209351	-2.99529889	0.88298848

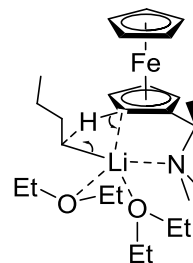
(*R,R*_p)- TS 2 (preferred)
(RI-DFT: BP86/def2-TZVP)



E = -2496.81617855802 au
Imaginary frequencies: 1 (-1284.16 cm⁻¹)

Fe	-5.80737590	-1.33446935	-0.68069624
C	-3.25467413	-0.66598536	-3.51562473

(*R,S*_p)- TS2 (non-preferred)
(RI-DFT: BP86/def2-TZVP)



E = -2496.81201735225 au
Imaginary frequencies: 1 (-1283.82 cm⁻¹)

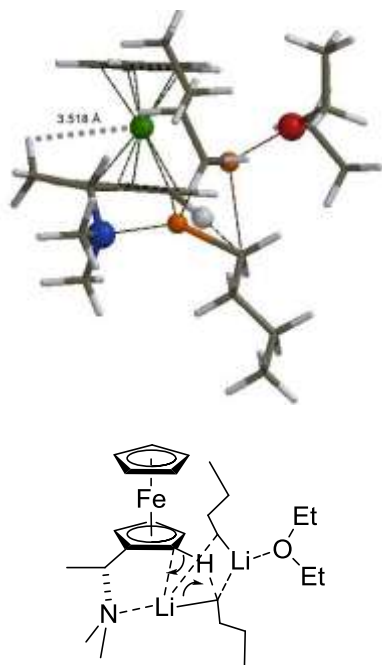
Fe	5.97887060	0.82430358	-0.33281631
C	4.33679800	3.69403179	-2.31747228

C	-1.95043377	-0.53388928	-1.13097062	C	2.07566687	1.01411261	0.46175163
C	-4.43528260	-3.09949363	-3.81943414	C	4.90080934	4.47332533	0.21690993
C	-3.88556098	-4.54749376	-1.59477255	C	3.52395318	2.82417477	1.88924661
C	-2.38240657	-2.96648821	0.04996567	C	2.61795898	1.58030818	-2.15659204
C	-7.24344679	1.47143665	1.59500592	C	9.57329165	0.29781877	-1.71403932
C	-7.73152279	-0.96484081	2.67416138	C	8.05150932	-1.88744012	-2.21306437
C	-9.19790931	-2.39467866	0.89727874	C	7.16396353	-2.85481325	0.15823938
C	-9.61243194	-0.84096485	-1.28297839	C	8.14009268	-1.26679964	2.12244926
C	-8.40018227	1.54531767	-0.85435961	C	9.63306010	0.67691533	0.96720787
C	-1.29266467	-3.62848888	2.60472334	C	1.24904671	0.32184184	-4.32741669
C	-2.40733089	-6.04601318	3.75501540	C	1.47666110	-2.56090020	-4.26474111
Li	2.35516672	-0.06452523	0.21852884	N	-1.48384503	1.12431823	-4.20682231
N	1.55652996	-3.60070513	2.43485271	C	-1.68335861	3.86236853	-4.64245122
H	-3.40468103	0.86957106	-4.87902084	H	-3.66399887	4.45616390	-4.44393775
H	-5.58835749	-3.72429312	-5.40449148	H	-0.52385654	4.89244758	-3.27137345
H	-8.33917376	3.12239106	-2.16762569	H	-1.03618181	4.39579365	-6.56659569
H	-10.63272370	-1.38911190	-2.97873482	H	2.05165415	1.01420681	-6.14327561
H	-6.14731670	2.97692718	2.45730012	H	3.62619110	2.90590799	3.94459037
H	-9.85960655	-4.32284547	1.14776821	H	6.19015397	5.98298097	0.75617867
H	-1.63044631	-6.43987889	5.64023021	H	7.77343424	-1.47491180	4.13175925
H	-2.07479374	-7.70920423	2.55705147	H	10.59817723	2.20072928	1.94910258
H	-1.71895735	-2.04407492	3.88715080	H	10.49918555	1.47226777	-3.12143815
H	-4.55199996	-6.45664402	-1.22025686	H	5.09383953	4.53072648	-4.03937844
C	2.55657752	-5.73229199	0.96637834	H	0.68542660	-3.45549053	-5.96193061
H	1.59361646	-5.82700896	-0.86898253	H	3.47858270	-3.06738541	-4.15049840
H	4.59229947	-5.45323105	0.64861852	H	5.93614482	-4.47832942	0.42378227
H	2.32128310	-7.57418810	1.93264211	H	0.49745102	-0.90185342	1.57507135
H	-0.61865959	1.53565673	0.04556094	C	-3.02568256	-0.15841197	-6.12610679
C	0.64125726	3.65799592	1.35275931	H	-2.26181821	0.11126524	-8.06262671
C	-0.94981856	5.85928687	0.35756062	H	-4.94724202	0.62434103	-6.08638949
C	-0.69136433	8.38613151	1.76780653	H	-3.15263199	-2.18752377	-5.74352775
C	-2.34580247	10.50359031	0.68757594	Li	-2.36420435	0.29009423	0.20080670
H	-1.16366026	8.08180854	3.77682586	C	-1.04047704	-2.76294589	2.98181400
H	-2.12070571	12.28114973	1.74296068	C	-0.36101076	-5.47016718	2.22371271
H	-1.86781120	10.88926338	-1.30111550	C	-0.76250186	-7.51687056	4.25116749
H	-4.36024026	9.98654722	0.74970682	C	-0.00408671	-10.17909263	3.40083345
H	1.30965603	8.97649115	1.74090019	H	0.32266024	-6.98538589	5.95091409
H	-0.49965783	6.19710184	-1.65977994	H	2.00621575	-10.25075858	2.86894755
H	-2.96680583	5.30842875	0.35785191	H	-1.10407672	-10.78120517	1.73931830
H	0.27761157	3.41729783	3.40402434	H	-0.30736605	-11.58986696	4.89806971
H	2.66958527	4.17166501	1.18534406	H	1.64682008	-5.53280998	1.63688156
C	2.72909089	-3.55270972	4.94772028	H	-1.43006995	-6.03875182	0.51401031
H	4.77037212	-3.23954832	4.74355237	H	-2.76545291	-7.50796590	4.83745111
H	2.44873162	-5.32917970	6.01993658	H	-3.09849481	-2.64084657	3.38909572
H	1.93422444	-1.98766805	6.05704439	H	-0.12756391	-2.33709556	4.81755480
H	-4.46026969	-5.82308820	3.95238370	H	0.54178480	-3.34636999	-2.58432805
H	-7.10167995	-1.61176943	4.51969036	H	7.66556793	-2.67560835	-4.06983918
O	3.91948842	-0.09085828	-3.41360592	O	-3.63165088	3.38526976	2.30876911
C	3.34823486	2.18535667	-4.81737753	C	-2.50653349	5.87089803	2.23734288
H	2.25287873	3.35254765	-3.49760491	C	-5.18289559	2.91985104	4.50773090
O	6.46177470	0.73547204	2.03195567	H	-0.84277973	5.68563200	1.01260699
C	8.82922648	0.14087436	0.84187167	O	-6.45539539	-1.13388414	-0.44452158
C	6.65088764	2.11362180	4.37659312	C	-7.22227684	-3.72834026	-0.09290575
H	8.29839347	-0.53606114	-1.04602308	C	-8.31241156	0.48790029	-1.59079938
H	9.95215081	1.87823187	0.57513867	H	-7.36768812	2.33270959	-1.71160748

H	7.72187544	0.99284869	5.77515574
H	4.69193368	2.25290537	5.04513113
C	4.71448607	-2.20587968	-4.93535449
H	2.09989380	1.72156233	-6.41737038
H	6.33109149	-1.63850645	-6.12691339
H	5.42036689	-3.60076047	-3.56729263
C	10.38295090	-1.84931552	2.23424349
C	7.77327884	4.75313072	4.11801966
H	9.77915845	4.72618491	3.58152035
H	6.71506697	5.86362127	2.71958150
H	7.63639918	5.72928028	5.94769865
H	12.08214000	-2.30326408	1.12593203
H	11.01816130	-1.19359064	4.09909466
H	9.29747900	-3.60116872	2.49316590
C	5.70123585	3.58662124	-5.70352009
C	2.62073173	-3.36432608	-6.53731945
H	5.13687160	5.34527219	-6.65698742
H	6.82256194	2.48087440	-7.05811794
H	6.91239590	4.08706464	-4.09396303
H	3.32398166	-5.11097408	-7.41944139
H	2.00976491	-2.10242070	-8.06749620
H	0.96042788	-3.82094376	-5.37964939

H	-8.70756739	-0.14845962	-3.53904427
H	-5.64346016	-4.58736511	0.94126069
H	-8.89408061	-3.80016765	1.15181393
H	-1.80086129	6.37136638	4.13117144
H	-6.24812097	1.20273005	4.03581566
C	-10.77504817	0.74057584	-0.11394674
C	-7.72300583	-5.16509079	-2.53706388
H	-11.87153335	-1.02173583	-0.08711523
H	-11.96021879	2.19135663	-1.01403119
H	-9.35763731	-4.42347558	-3.58203965
H	-8.12664007	-7.15294498	-2.08527384
H	-6.06527065	-5.11753123	-3.78517872
H	-10.42077867	1.32523689	1.84608190
C	-4.31470839	7.88469554	1.25552129
H	-4.96481226	7.42962615	-0.66304278
H	-5.98025104	8.10534203	2.47710276
H	-3.34343394	9.72134554	1.18634980
H	-6.55262832	4.47924769	4.72778877
C	-3.67629054	2.52080572	6.92748489
H	-4.98288396	2.04958605	8.47487347
H	-2.33925458	0.95193795	6.70005524
H	-2.62757227	4.21918463	7.49833586

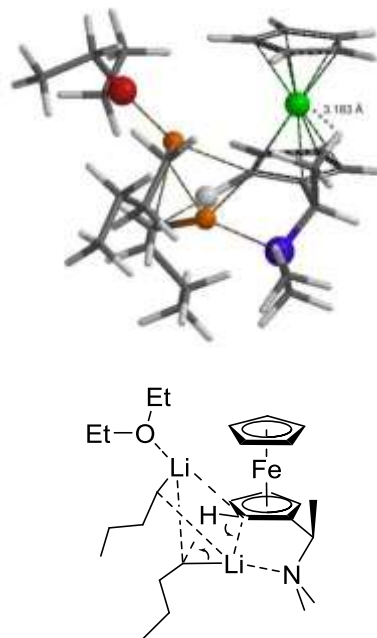
(*R,R*)- TS3 (preferred)
(RI-DFT: BP86/def2-TZVP)



E = -2428.49702474624au
Imaginary frequencies: 1 (-1007.47 cm⁻¹)

C	2.08569751	2.61484611	3.35334821
C	4.59971670	1.38852763	-2.64146630
Li	0.48628816	2.32924377	-0.40288814

(*R,S*)- TS3 (non-preferred)
(RI-DFT: BP86/def2-TZVP)



E = -2428.49017423087 au
Imaginary frequencies: 1 (-1081.50cm⁻¹)

C	2.82386896	1.42007997	3.80125505
C	4.35351408	0.60144022	-2.45773346
Li	1.15825467	2.16448308	-0.42230668

Li	3.76177217	-0.31444449	1.10361443	Li	3.28172452	-1.56027811	0.78484385
H	2.43911864	4.64090976	2.89053920	H	3.52219782	3.17663604	2.89506963
H	3.88424419	2.12253872	4.34747108	H	4.58534793	0.34942746	4.21493059
H	4.11950459	3.42063799	-2.80463909	H	4.45912751	2.62649186	-3.02155669
C	4.64346160	-4.10099814	4.80901627	H	3.93077251	-0.37286147	-4.26550110
C	4.91774562	-5.96323078	0.65218970	C	1.66797568	-6.06391216	3.73416555
H	6.64485766	-3.54299828	4.74776455	C	4.18390930	-7.08862392	0.13124753
H	3.61695988	-2.72937909	5.98253821	H	3.38098473	-5.84865189	4.88558475
H	4.76566754	-7.90809689	1.40789601	H	0.19439816	-4.83129429	4.50223367
H	4.13673825	-5.93061900	-1.26750284	H	3.50403940	-9.06827330	0.01582138
O	-1.15082592	5.36686708	-1.91417829	H	4.84275470	-6.50033697	-1.74071107
C	-2.25376434	5.33051678	-4.41413478	O	0.43666564	5.89565105	-0.80615992
C	-0.93808315	7.85231934	-0.79443680	C	1.40106655	7.33690784	-2.92092962
H	-3.93582229	6.56075696	-4.44168734	C	-0.61201154	7.41003968	1.21326560
H	-0.25983942	9.19914241	-2.23172596	H	0.01085984	8.79858468	-3.44568677
H	0.54489101	7.67191400	0.64725858	H	0.61077749	9.06370799	1.54193098
H	-2.90411179	3.37587495	-4.67897382	H	-0.49835703	6.21755459	2.90934452
C	-0.00928768	2.54479894	5.37285378	H	1.51178786	5.98388048	-4.49222180
H	-0.36092176	0.56955427	5.97546379	C	7.06022659	-0.14279840	-1.66359003
H	-1.83303290	3.15902894	4.54369793	H	7.13889548	-2.15557698	-1.04078367
C	0.44387329	4.12863106	7.77221307	H	7.63520816	0.95574766	0.02326409
C	-1.69740042	3.97620504	9.71564537	C	1.58456776	2.11217016	6.33492614
H	0.74896307	6.11527033	7.21213438	H	-0.23045351	3.09988587	5.99443309
H	2.23505427	3.51129752	8.64619421	H	2.74632879	3.47279954	7.42454634
H	-3.49709170	4.63839098	8.90643762	C	9.14791087	0.15899248	-3.67207806
H	-1.30511222	5.13176261	11.39933021	C	11.78408945	-0.62786457	-2.76982547
H	-1.99300764	2.01779321	10.35544794	H	9.17602918	2.15096778	-4.28832091
C	-0.39038314	6.06946911	-6.47884794	H	8.61334190	-0.94791912	-5.35637164
C	-3.39911155	8.75003850	0.39399297	H	13.21873327	-0.37721761	-4.25378970
H	-1.31406354	5.91080159	-8.33456985	H	11.81843846	-2.62953518	-2.19968569
H	1.26505388	4.81819194	-6.46250151	H	12.38161630	0.49512816	-1.12287818
H	-4.02067762	7.44248706	1.88064302	C	1.04083358	-0.15779426	8.04950193
H	-4.92348074	8.93401498	-1.00432340	C	-0.11644115	0.57120000	10.59879114
H	-3.11261600	10.61879193	1.25786697	H	2.82049391	-1.20096827	8.36609769
H	0.26625763	8.02892145	-6.27587826	H	-0.23570356	-1.47120236	7.05808673
N	3.60845325	-4.08871540	2.22993014	H	1.14372600	1.84165895	11.66020117
H	6.93538873	-5.47889351	0.55360502	H	-0.47653622	-1.09599698	11.78704950
H	4.53998919	-5.97639979	5.72909750	H	-1.92824451	1.56155252	10.34324166
C	0.76930071	-4.37937990	2.21352114	C	3.98694869	8.49059548	-2.41446009
Fe	-3.68457101	-2.69237157	-1.56980814	C	-3.32862842	8.21203712	0.71030379
C	-1.56073484	-5.89524446	-1.91690522	H	4.64545746	9.48499849	-4.11689432
C	-0.20892722	-4.03359220	-0.45541819	H	5.36772002	7.01335727	-1.94984289
C	0.14590030	-1.77349286	-1.98145693	H	-4.55036584	6.55403365	0.45799847
C	-1.02272488	-2.34162587	-4.38178286	H	-3.48912955	9.41221697	-0.97687056
C	-2.07384029	-4.83692022	-4.35154975	H	-4.04225639	9.30645856	2.32710764
C	-6.90580874	-3.78312179	0.31148545	H	3.94142295	9.87020007	-0.86338709
C	-7.51131138	-2.94465835	-2.19150057	N	2.21916038	-5.36515831	1.09197052
C	-6.68847471	-0.37494336	-2.43346192	H	5.80439603	-7.04324213	1.42799851
C	-5.58439282	0.37776936	-0.07440187	H	1.01761526	-8.05115517	3.87675574
C	-5.70713236	-1.73302938	1.61671206	C	-0.17114308	-5.49846676	-0.44144907
C	-0.19039539	-6.81445549	3.46495664	Fe	-4.53366614	-1.07552441	-1.27883771
H	-2.14918135	-7.75875662	-1.28340251	C	-1.55941560	-0.97659989	1.35946086
H	-3.10868865	-5.75356828	-5.87238288	C	-3.92338184	-0.09658677	2.41292343
H	-1.10641307	-1.06131513	-5.99124632	C	-4.30100449	1.92358748	-3.77597668
H	0.10694665	-2.76024612	3.34748142	C	-6.82925886	1.63422020	-2.84662134

H	0.40217779	-6.93751368	5.44962335	C	-2.05801493	-3.55665492	0.54669054
H	-2.26474552	-6.83577837	3.43119598	C	-4.65628630	-4.16756608	1.06615559
H	0.47497187	-8.51875217	2.48202880	C	-5.81795507	-2.02316021	2.22881476
H	2.15775499	-0.22760673	-2.04145855	C	-7.69035896	-0.84146113	-3.52794725
H	-8.40687724	-4.06825540	-3.65817459	C	-5.69117250	-2.08198290	-4.86854536
H	-6.88566154	0.79344699	-4.11052352	C	-3.59792187	-0.37153935	-5.02366031
H	-7.27150314	-5.65392185	1.07511034	C	0.35644124	-5.28770445	-3.27853060
H	-4.79954272	2.22577770	0.35709775	H	0.55693477	0.07594677	2.31660881
H	-5.01068811	-1.76379463	3.54823902	H	-4.24071086	1.77603951	3.20443244
H	4.66791054	0.65750080	-4.59595984	H	-7.78191680	-1.87724029	2.81677615
C	7.24620526	1.14631417	-1.46719266	H	-1.01983407	-7.39152698	-0.10149573
C	9.39701103	2.48178447	-2.90753345	H	1.46289433	-6.89516332	-3.98631542
C	11.99890745	2.17247285	-1.67779879	H	-1.45299284	-5.27761052	-4.28326928
H	13.48137319	3.15046742	-2.75776171	H	1.35634998	-3.52006878	-3.71395929
H	12.53781541	0.16653278	-1.55034919	H	-5.57857088	-5.95559030	0.63575782
H	12.01613214	2.94683720	0.25338061	H	-7.90090450	3.03149772	-1.78976421
H	9.44012970	1.74436770	-4.85629137	H	-9.52164013	-1.65046296	-3.07162834
H	7.77623635	-0.87472093	-1.29642724	H	-3.12370189	3.59100657	-3.55184979
H	7.26247423	1.91445079	0.48746704	H	-5.75987969	-3.98883436	-5.62817798
H	8.92547066	4.50547934	-3.06886146	H	-1.78665417	-0.74627072	-5.91138605

1.3. The coordinates and energies of intermediates Int1-2.

(R,R_p)-Int1 (preferred)
(RI-DFT: BP86/def2-TZVP)



E = -1870.81366236058
Imaginary frequencies: 0

Fe	3.26177242	0.55728823	-0.27474338
C	0.10036500	2.56020440	-1.69890693
C	2.08439451	4.21144551	-0.83917824
C	2.67607094	3.76793256	1.77811991
C	1.05341696	1.78224971	2.64642240
C	-0.50227938	1.04277433	0.52821931
C	6.40166224	0.08002807	-2.49134142
C	4.49383182	-1.72484674	-3.16531432
C	3.92807926	-3.20226291	-0.96353136
C	5.49711969	-2.32198730	1.06601829

(R,S_p)-Int1 (non-preferred)
(RI-DFT: BP86/def2-TZVP)



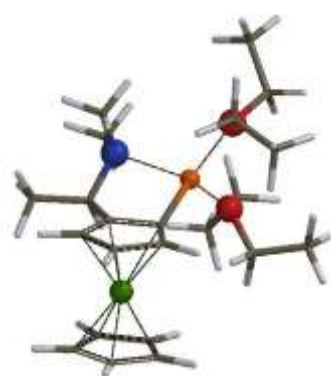
E = -1870.81247747716 au
Imaginary frequencies: 0

Fe	0.15488079	2.34239917	1.83612226
C	3.18047839	2.21509236	-0.55375621
C	2.46874645	4.77521956	-0.04404977
C	-0.09024002	5.08654740	-0.90690490
C	-1.04423729	2.79608332	-2.01278753
C	1.03849863	1.01353320	-1.74956579
C	1.37338362	1.18399580	5.34148357
H	3.64286578	6.18616234	0.88418906
H	-3.54777502	5.13378319	4.47176823
C	-0.55365649	-0.48876215	4.43182552

C	7.02716355	-0.29613545	0.11967091
C	-2.53273498	-0.99733545	0.52815616
N	-4.73284944	-0.14388181	-1.10755407
C	-6.12213827	1.99373449	0.01837127
C	-6.47419473	-2.22732543	-1.68868498
H	-7.17291173	1.44947537	1.74036248
H	-7.88517417	-1.58792034	-3.07566222
H	-5.41857885	-3.81996303	-2.50487319
H	-7.50161883	2.72634133	-1.35470508
H	-4.78139340	3.50314486	0.49451892
H	1.05378633	0.98774153	4.54321921
H	4.11563473	4.71816922	2.89846448
H	3.06679624	5.58716306	-2.01513215
H	5.50927302	-3.04782061	2.98727443
H	8.39183928	0.79234618	1.20129976
H	7.21017001	1.50079804	-3.73377210
H	3.61469268	-1.91074884	-5.01172782
H	2.56032800	-4.73321484	-0.85121116
H	-7.51441098	-2.92570558	-0.01483381
C	-3.28933470	-1.84986538	3.19315253
H	-1.81299857	-2.67360591	-0.48112894
H	-3.92475962	-0.25922489	4.36584566
H	-4.78260424	-3.29365826	3.16198876
H	-1.63933476	-2.69196199	4.12811273
Li	-2.59390852	1.41672713	-3.94928177

H	-3.51563218	-4.99482400	-5.94027835
H	-4.48849707	-4.47663927	-1.49243566
H	-1.46683591	-5.77527870	-0.79998553
H	-0.35084664	-6.00674691	-5.42347881
H	-0.96090748	-3.28335844	-7.32767674
H	-1.16478519	6.82972856	-0.68700184
C	-2.79764589	0.97523439	3.99188844
C	-2.24998986	3.55058028	4.62925328
C	0.32169824	3.67629320	5.47231827
C	1.11933754	-1.56255513	-3.01041307
N	-1.50559628	-2.64688580	-3.41972434
C	-1.57213939	-4.32118596	-5.63638409
C	-2.48732349	-3.99285990	-1.18630582
H	1.31509146	5.37552973	6.05761142
H	3.29630057	0.65683718	5.83323225
H	-0.35626688	-2.52011108	4.19650333
H	-4.60785847	0.26445122	3.32882220
H	5.00256185	1.37373960	-0.10357833
H	-2.32856507	-2.75496907	0.46734375
C	2.97654761	-3.42422425	-1.78890853
H	1.79182264	-1.21436547	-4.95900144
H	2.59270871	-3.66488746	0.23578114
H	2.93225433	-5.28712204	-2.71057304
H	4.91040707	-2.69778226	-1.97696515
Li	-3.62404880	0.57508685	-3.40545427

(R,R_p)-Int2 (preferred)
(RI-DFT: BP86/def2-TZVP)



E = -2338.35285956503 au
Imaginary frequencies: 0

Fe	4.36043122	-3.70452380	-1.28524915
C	1.26317727	-1.18635649	-1.89782365
C	1.91339073	-2.64754396	-4.11030996
C	4.50659702	-2.26156858	-4.84950454
C	5.58567599	-0.52383524	-3.07558328
C	3.62077354	0.09838983	-1.28105644
C	3.69530569	-7.45245242	-0.54872681
C	3.39359690	-5.98302689	1.71072004

(R,S_p)-Int2 (non-preferred)
(RI-DFT: BP86/def2-TZVP)



E = -2338.34777951698 au
Imaginary frequencies: 0

Fe	-5.95215633	0.55032119	0.48329589
C	-5.49195498	0.57839006	-3.35560842
C	-6.19657916	-1.88279407	-2.47651731
C	-4.24210407	-2.69770118	-0.76024276
C	-9.46298541	1.92154602	1.38087442
C	-1.50540461	3.49992388	-2.75693876
C	0.85625164	1.08304969	-5.86967620
C	-1.31868758	5.38728923	-0.57229671

C	5.73642399	-4.71002265	2.19924966	C	-2.26295330	-0.83244197	-0.52022442
C	7.49170156	-5.40660873	0.25198267	C	-3.12264885	1.20184779	-2.15750281
C	6.23042094	-7.10256939	-1.44342161	C	-7.57069434	3.77853289	1.94482512
C	3.82384222	1.90380900	0.93584241	C	-5.85332344	2.70246603	3.74545864
C	6.45772062	3.08005012	1.23906668	C	-6.68028807	0.18339007	4.28947479
N	1.69128758	3.79287687	0.77091130	C	-8.91426003	-0.29937962	2.83430084
H	0.64545745	-3.94578141	-5.08982111	N	1.07895681	2.57086251	-3.52997176
H	5.49691162	-3.15087184	-6.41902652	H	2.71745265	0.33036198	-6.40148944
H	7.03954055	-7.94235581	-3.13398827	H	-0.45480716	-0.49277549	-5.57574788
H	9.42862547	-4.74564124	0.07731518	H	0.14344828	2.24693363	-7.46316787
H	2.25183937	-8.61049007	-1.43939241	H	-2.34251494	4.50420442	-4.40429120
H	6.11963263	-3.44512772	3.77317141	H	-4.32089787	-4.48411195	0.26820030
H	-2.10096374	-3.59236113	1.24752500	H	-7.91887513	-2.89621618	-2.96911848
C	-6.51167813	3.63929803	-1.58892010	H	-5.75273226	-1.15027850	5.54605074
H	-4.42084752	3.80433841	-5.99995514	H	-9.97461780	-2.05812634	2.79966529
H	-8.01469299	2.76807967	-2.74183269	H	-11.02204166	2.14772565	0.06302958
H	-6.84383811	3.06932480	0.38160376	H	-6.56533658	1.75283232	-4.66337698
C	-2.68733446	-0.00956060	7.67586875	H	-0.34961896	7.14327967	-1.11415881
C	-6.16016718	-3.93449290	1.85407574	H	-3.23313065	5.87367905	0.04310954
H	-7.62052506	-3.48801085	3.26361739	H	-4.20625221	3.63135361	4.54428623
H	-6.65858073	-3.00400241	0.06679502	C	2.87322099	4.64178384	-3.96796541
H	-6.20471356	-5.98946565	1.54377263	H	2.17322937	6.02359752	-5.38501947
H	-3.53238126	0.88800377	9.34980454	H	4.65625032	3.85202775	-4.68616787
H	-2.52966123	-2.04128336	8.06868773	H	3.28176911	5.65571734	-2.20917474
H	-0.77396095	0.75377146	7.42264938	Li	1.61460139	-0.20901455	-0.37372208
C	-5.03171486	-0.27273059	-5.84466959	H	-0.32810823	4.54003768	1.04534963
C	-6.57220095	6.50890502	-1.83860147	H	-7.47894353	5.67363305	1.15672431
H	-4.66177023	-0.53553583	-7.87321574	O	3.82923253	-3.24624897	-1.50280760
H	-7.09287334	-0.22397966	-5.58530784	C	2.58375978	-5.62667847	-0.96787149
H	-4.25545554	-1.90614668	-4.82742931	C	5.89047184	-3.35632376	-3.26672385
H	-8.43403969	7.23248330	-1.26132145	H	1.18437772	-5.12957595	0.48218584
H	-6.23966945	7.11866428	-3.79548273	O	3.17778975	0.92784347	2.97759263
H	-5.13133112	7.38727448	-0.62930198	C	1.47311610	0.61038372	5.10019634
Li	-1.36208264	1.01350142	0.01155818	C	5.78971283	1.34150859	3.59189905
H	7.02494958	4.16138181	-0.44075972	H	6.70859026	1.68734450	1.76084457
H	3.39732960	0.84029679	2.67792627	H	-0.34659596	0.20091837	4.17745378
H	7.53528468	0.13258462	-3.08366036	H	2.03484826	-1.07472792	6.19298140
C	1.91594385	5.47035505	-1.42726992	H	5.98375571	3.08789924	4.71591713
H	2.23899502	4.32902904	-3.12861685	H	3.95955543	-6.95197726	-0.13137226
H	0.14892652	6.53740135	-1.66611039	H	6.41148819	-1.37019500	-3.58494951
H	3.48038286	6.85011710	-1.24303517	C	7.05300400	-0.87216131	4.93543705
C	1.41240018	5.27909483	3.08637274	C	1.29947094	2.92018697	6.80557119
H	-0.33768462	6.39910187	2.98695033	H	6.30023151	-1.16508846	6.84749194
H	2.98990079	6.61757154	3.41998050	H	9.08947221	-0.49879643	5.12057503
H	6.56769438	4.33441533	2.89152828	H	3.06025005	3.29711466	7.84264792
H	1.28949488	4.00781792	4.72528943	H	-0.19172221	2.60665166	8.21844077
H	7.85365688	1.56776609	1.50801683	H	0.80257638	4.61749854	5.71686254
H	1.68568400	-5.83900193	2.83915346	H	6.80265761	-2.62702675	3.85499438
O	-4.10476946	2.57306433	-2.25839621	C	1.25675834	-6.79376871	-3.23531795
C	-3.75408804	2.13771364	-4.93799646	H	-0.14006974	-5.47270786	-4.01545585
H	-1.70040890	1.97898814	-5.18478928	H	2.57443347	-7.36795222	-4.73494119
O	-3.27533336	-0.44676624	3.05119063	H	0.24390501	-8.50023139	-2.61758440
C	-4.31973600	0.52410711	5.36220859	H	5.22938265	-4.11995177	-5.09124065
C	-3.52438273	-3.15558729	2.70250182	C	8.17565325	-4.83740764	-2.32442173
H	-4.49024776	2.57459700	5.06607854	H	9.72496955	-4.66137809	-3.69877438

H -6.24819378 -0.22352676 5.63673910
H -2.98378239 -4.13184065 4.46245448

H 8.84208625 -4.10243104 -0.50043442
H 7.76708654 -6.86083207 -2.10790882

1.4. The coordinates and energies of starting materials and product of lithiation of (R)-1.

***n*-BuH**
(RI-DFT: BP-86/def2-TZVP)



E = -158.51212776257 au
Imaginary frequencies: 0

C	-0.011188	0.019288	1.122430
C	0.005879	-0.010064	-0.407835
C	0.715919	-1.239945	-0.984508
C	0.732839	-1.269381	-2.514773
H	-0.526696	0.912151	1.504345
H	-0.526166	-0.863318	1.531487
H	1.010612	0.024001	1.531588
H	-1.029002	0.021379	-0.789805
H	0.496217	0.901898	-0.789683
H	0.225658	-2.151906	-0.602558
H	1.750839	-1.271322	-0.602640
H	-0.288999	-1.274149	-2.923833
H	1.247750	-0.386781	-2.923928
H	1.248337	-2.162250	-2.896688

***n*-BuLi**
(RI-DFT: BP-86/def2-TZVP)



E = -165.38476010235 au
Imaginary frequencies: 0

C	-0.56102062	-0.00004588	3.77854581
C	0.91082702	0.00006470	1.28444322
C	-0.77827983	0.00005454	-1.08654600
C	0.63909988	-0.00005925	-3.62841266
Li	-1.43714511	0.00015896	-6.78159463
H	0.70319852	0.00011565	5.43005000
H	-1.78609139	-1.67645927	3.92709780
H	2.16698063	-1.66347433	1.20594889
H	1.92803742	-1.65328394	-3.66907010
H	-2.04723411	-1.65954159	-0.96218438
H	-2.04713172	1.65973640	-0.96228195
H	-1.78644992	1.67611249	3.92703728
H	2.16686486	1.66369472	1.20602108
H	1.92834436	1.65292680	-3.66905436

(R)-Ugi amine (1)
(RI-DFT: BP-86/def2-TZVP)



E = -1863.89967130283 au
Imaginary frequencies: 0

Fe	2.45321098	0.38233540	-0.05303421
C	-0.40688351	2.27375219	-1.82876184

***n*-BuLi...2Et₂O**
(RI-DFT: BP-86/def2-TZVP)

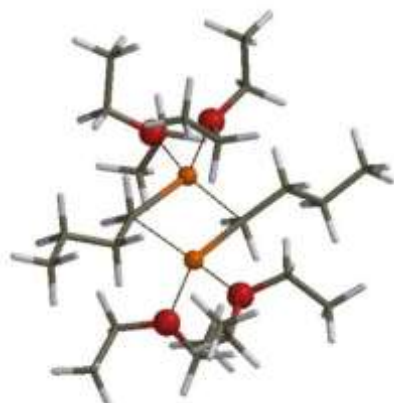


E = -632.94011664348
Imaginary frequencies: 0

Li...0.31587758	0.59553151	0.27834670	
C	-3.14426075	2.35326372	-0.21233705

C	1.34877706	4.02154083	-0.73479645	C	-5.52049754	0.76113432	-0.73408097
C	-0.28024433	1.52332006	2.47414614	C	-8.03275658	2.21457559	-1.00226734
C	1.43062296	3.54942370	1.93210772	C	-10.33194684	0.53068288	-1.52336069
C	-1.44331079	0.72397549	0.15288661	H	-8.34613637	3.31940828	0.73943564
C	4.45938852	-1.50402994	-2.79289649	H	-12.08812620	1.63158271	-1.70383788
C	3.38219351	-3.26635298	-1.04127638	H	-10.08662953	-0.54893906	-3.28704245
C	4.33196947	-2.68343336	1.42907423	H	-10.61385872	-0.84945294	0.01027146
C	6.00181376	-0.56194246	1.20153926	H	-7.82300408	3.61740911	-2.53225127
C	6.08141873	0.16538091	-1.40726397	H	-5.26972427	-0.36548491	-2.48535646
C	-3.52121214	-1.22279746	-0.13642767	H	-5.78524644	-0.66095821	0.78484235
N	-6.02721081	-0.04758985	0.34800549	H	-3.52769762	3.49433786	1.51451852
C	-6.51328315	2.14864613	-1.25115556	H	-3.01049847	3.79930132	-1.73520783
C	-8.09751201	-1.85359994	0.08089258	O	3.86519651	2.02472039	0.22082518
H	-8.37040081	2.93886267	-0.76184619	C	5.90865895	0.47503828	-0.70689846
H	-9.89606349	-0.86513793	0.39563627	H	6.36483171	1.04495991	-2.66339524
H	-8.17699174	-2.73520413	-1.83143623	C	4.18026951	4.68612084	-0.34425791
H	-6.53436534	1.68194180	-3.30549100	H	5.14380200	-1.45481226	-0.76480338
H	-5.08524489	3.61428468	-0.93470104	H	6.13947236	5.24390500	0.09345022
H	-0.63257242	0.71956758	4.32984239	H	3.87237305	4.96424154	-2.39101943
H	2.61466772	4.52693831	3.29582181	C	8.24922890	0.56558181	0.96795552
H	2.45684047	5.42055498	-1.75065199	C	2.31586674	6.21571427	1.19843963
H	7.00546181	0.35392428	2.74073151	H	9.69368239	-0.72725349	0.21750355
H	7.15211533	1.73255079	-2.19033971	H	7.79015464	-0.02714517	2.90353941
H	4.09059853	-1.43006748	-4.81121382	H	9.08990469	2.46186245	1.04603001
H	2.06923358	-4.77300242	-1.51158243	H	2.48209618	8.22384788	0.69117596
H	3.86063130	-3.66367151	3.17054384	H	2.70253602	6.02552498	3.22997370
H	-0.88294244	2.12755810	-3.82214667	H	0.36739889	5.59636517	0.82401930
H	-7.95915058	-3.36687423	1.48880045	C	-0.71892874	-4.53695852	-1.37152532
C	-3.12096687	-3.49393253	1.62454416	H	-2.76866992	-4.32663527	-1.04860380
H	-3.44963475	-1.91325943	-2.12999915	C	-0.05831637	-4.23232541	3.07568471
H	-3.56281036	-2.97363210	3.58722583	H	-0.24074753	-6.56842895	-1.28058614
H	-4.31534831	-5.10403165	1.09643407	H	-2.12192297	-4.04374642	3.33079064
H	-1.14627821	-4.10883798	1.53705273	H	0.41358283	-6.26680359	3.12837403
				C	0.02179208	-3.40687394	-3.89669439
				C	1.35568073	-2.80042007	5.11511919
				H	-0.96746625	-4.40825482	-5.42345023
				H	2.06407328	-3.57803969	-4.23442673
				H	-0.53436379	-1.40413105	-3.99429465
				H	0.87843772	-3.58668640	6.97699289
				H	0.83052524	-0.78980326	5.13200403
				H	3.40937014	-2.95519426	4.85505813
				O	0.62159845	-3.24741502	0.62962103

(*n*-BuLi...2Et₂O)₂
(RI-DFT: BP-86/def2-TZVP)



E = -1265.89848365089 au
Imaginary frequencies: 0

C	2.05009676	-1.09299221	-2.74491925
C	-3.04403782	0.12734039	2.07132200
Li	-0.84317336	1.60321771	-1.26737720
Li	0.31055710	-2.15765101	0.93157652
H	0.93745570	-2.25556939	-4.10647706
H	3.31733978	-2.52558401	-1.85386649
H	-4.51039958	-1.14218715	1.24895070
H	-3.78382291	2.04384553	1.59080944
C	2.95976097	-3.24279867	6.07249455
H	2.33817748	-1.59390078	7.19354207
O	0.09290916	5.35989297	-0.30721969
C	0.77447750	7.33868471	-2.04363413
C	0.30958150	5.97347649	2.33877571
H	-0.34708664	9.05168435	-1.64003960
H	0.17066337	6.62107909	-3.89559668
H	2.24208785	6.63982695	2.75333202
H	0.03765397	4.15139017	3.29549429
O	-0.70593653	-5.95172554	0.72213211
C	-3.22160429	-6.81153650	1.31203667
C	0.82432601	-7.76200134	-0.62284227
H	-3.13336995	-8.74952103	2.08191376
H	-3.87940577	-5.55664467	2.82940865
H	-0.34379166	-8.75310018	-2.03639953
H	2.22465121	-6.63363053	-1.66192912
O	-3.32413702	2.52668731	-4.23881884
C	-5.54156254	4.05356124	-3.82007140
C	-3.30572558	1.15032252	-6.59073842
H	-5.93748483	5.19506638	-5.52113211
H	-5.14664916	0.21230150	-6.87194237
H	-1.87720606	-0.33069244	-6.32231308
H	-4.99778992	5.36153078	-2.30142890
C	-3.23633554	-0.10668739	4.96320758
H	-1.83206844	1.14552700	5.88876515
H	-2.68238214	-2.03560672	5.57142186
C	3.78858974	0.63912285	-4.30138892

Et₂O
(RI-DFT: BP-86/def2-TZVP)



E = -233.75950742158 au
Imaginary frequencies: 0

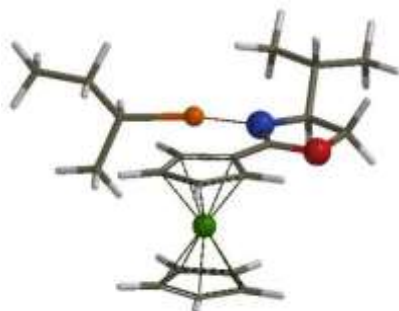
H	6.27250160	0.00002942	-0.32889552
H	4.50682462	-1.68276787	1.99444441
H	-4.50682545	1.68276780	1.99444412
H	-4.50681066	-1.68265301	1.99456062
H	4.50681148	1.68265294	1.99456033
O	0.00000000	0.00000068	0.52736126
C	-2.23945985	-0.00003462	-0.96727733
H	-2.26254885	-1.68550003	-2.21336101
C	2.23945985	0.00003507	-0.96727733
H	-2.26254357	1.68536458	-2.21345062
H	2.26254293	-1.68536426	-2.21345045
H	2.26254949	1.68550035	-2.21336118
C	-4.51515957	0.00001530	0.77865934
C	4.51515957	-0.00001559	0.77865934
H	-6.27250160	-0.00003076	-0.32889552

H	5.03706535	1.72734949	-3.01806129
H	2.66152572	2.10100268	-5.29909983
C	-5.83097473	0.45635044	6.16604599
C	-5.89253283	0.17567737	9.04860121
H	-7.25002242	-0.80647107	5.30275852
H	-6.40236020	2.39117149	5.63341795
H	-7.77091032	0.59534366	9.83720830
H	-4.53055474	1.46147719	9.95732805
H	-5.39092806	-1.76093778	9.62499121
C	5.48621332	-0.64200661	-6.29467558
C	7.17991539	1.18597769	-7.77147023
H	4.27105416	-1.70396560	-7.61723725
H	6.66221387	-2.07545975	-5.33758611
H	6.04630520	2.60338435	-8.79143393
H	8.35828944	0.20190307	-9.17484361
H	8.45913967	2.22070631	-6.49610434
C	-5.01692326	-6.67270365	-0.93439779
C	2.11844289	-9.63715327	1.13710622
C	-7.85455933	2.52727974	-3.03741783
C	-2.63928459	2.79678943	-8.85835074
C	-1.64688473	7.87996061	3.25099900
C	3.58849756	7.95220702	-2.07946111
H	-9.43746430	3.81903119	-2.64939195
H	-7.45464327	1.44230316	-1.31292463
H	-1.40707519	9.75134764	2.38198238
H	-0.77501308	3.67392186	-8.60466709
H	-4.03886300	4.29656451	-9.18567338
H	-3.56890418	7.20185589	2.85641066
H	-1.46295494	8.12330680	5.30696782
H	3.97013496	9.34316476	-3.57668596
H	4.24203244	8.77628325	-0.28896534
H	4.70260342	6.24736185	-2.47802905
H	-2.56982317	1.62414050	-10.57353482
H	-6.92092118	-7.26465941	-0.34482170
H	-5.12655844	-4.72661628	-1.64445870
H	-4.42567579	-7.91681220	-2.48887164
H	0.74818724	-10.77124009	2.21093637
H	3.29128525	-10.94992702	0.03043058
H	3.34868244	-8.64291023	2.48023654
H	-8.47222341	1.21938426	-4.52794814
O	3.41520755	-2.46347096	3.51258213
H	1.35009584	-4.54841883	5.94278703
C	5.17126012	-0.39107878	3.22041572
C	7.76156364	-1.25820739	2.31407266
H	4.31865574	0.86971589	1.80162542
H	7.58262930	-2.28617565	0.52040990
H	8.97974142	0.39531345	1.98540360
H	8.70267082	-2.49266406	3.69127518
C	5.19298842	-4.54333754	7.34749013
H	5.30356501	0.65208442	5.02257649
H	5.85176996	-6.16542079	6.23066875
H	6.79087869	-3.24872171	7.63337563
H	4.60908030	-5.23673201	9.21906644

2. THEORETICAL CALCULATION OF LITHIATION OF (S)-2.

2.1. The coordinates and energie of complexes C4-6.

(S)- Fc-oxazol...s-BuLi (C4a)
(RI-DFT: BP86/def2-TZVP)



E = -2180.84104085586 au
Imaginary frequencies: 0

Fe	-1.92333538	0.16833154	-5.10585123
C	-3.74043421	-3.02018242	-3.89908287
C	-5.55100210	-1.14446869	-4.59712623
C	-5.12370303	1.05772968	-3.07829230
C	-3.04484831	0.57544604	-1.42542212
C	-2.19197062	-1.97565417	-1.90398183
C	1.80256730	0.29067342	-6.23213626
C	0.89857753	2.78432220	-5.69254692
C	-1.20967990	3.26950714	-7.32270699
C	-1.60569962	1.07564703	-8.86434387
C	0.25779723	-0.77072221	-8.18698804
C	-0.13549828	-3.28566262	-0.64523515
N	1.17460786	-2.49066779	1.26774997
H	-6.97722100	-1.34210440	-6.06044068
H	-6.16491005	2.82274532	-3.19062724
H	0.44827455	-2.64937317	-8.99212150
H	-3.08024447	0.84181011	-10.27355315
H	3.36010002	-0.65393729	-5.28417531
H	-2.33515452	4.98585468	-7.35249116
H	-2.25478682	1.90654055	-0.05458251
H	-3.55245480	-4.90379689	-4.68833111
O	0.43335223	-5.62042187	-1.56408372
C	2.38561455	-6.64896442	0.07641307
C	3.06169805	-4.45666800	1.89608727
C	3.04901172	-5.22493445	4.70711304
C	3.39852185	-2.94788311	6.46200109
C	5.10220180	-7.21606166	5.19824480
H	6.99454737	-6.43328352	4.82594139
H	1.57326328	-8.28804792	1.06703044
H	3.95464541	-7.28059294	-1.12153924
H	4.96012118	-3.69488730	1.46250885
H	1.18402109	-6.07913391	5.09899549

(S)- Fc-oxazol...s-BuLi (C4b)
(RI-DFT: BP86/def2-TZVP)



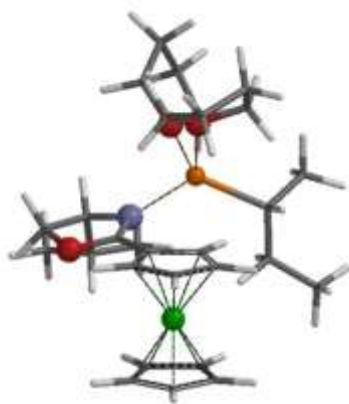
E = -2180.84093824976 au
Imaginary frequencies: 0

Fe	4.88864537	0.20458124	1.78702806
C	1.56570755	2.05603805	2.48606904
C	3.58975081	3.27640230	3.79011235
C	4.74852999	1.48433133	5.45907346
C	3.45191044	-0.86928326	5.20904208
C	1.44669128	-0.52135082	3.38469795
C	8.64572725	-0.18658460	0.89774893
C	7.46923726	1.63077752	-0.73294414
C	5.45605241	0.39460769	-2.05858188
C	5.39367252	-2.18574943	-1.24468717
C	7.35825003	-2.54961784	0.58394925
C	-0.34077225	-2.45286125	2.60762673
Li	-3.24546807	1.06249356	-0.52766361
N	-2.25198685	-2.18016790	1.09666798
H	4.17527061	5.22401372	3.51466147
H	6.36449204	1.83858755	6.67462513
H	7.77939652	-4.29743991	1.57473569
H	4.05042961	-3.60837600	-1.86764987
H	10.21435187	0.17370325	2.17230215
H	4.17075187	1.27844237	-3.39349664
H	3.85909266	-2.61153131	6.21143367
H	0.34067142	2.92744446	1.06606575
C	-3.18713357	4.50132754	-2.33467444
H	7.98422273	3.61030147	-0.90538301
O	0.00663721	-4.78048459	3.64696751
C	-1.89535411	-6.42222858	2.53089048
C	-3.58194392	-4.63546098	0.93784405
C	-4.01871871	-5.56199735	-1.79056687
H	-0.90406778	-7.83300922	1.36644837
H	-2.88754628	-7.38397388	4.07552342
H	-5.45982330	-4.40563450	1.82775058
H	-2.13684305	-5.86967835	-2.64284255

H	4.86843831	-8.90511351	4.00932993
Li	0.97863686	0.97383437	2.72631656
C	0.26892951	4.71482581	3.49036883
H	1.67193138	5.07558320	5.01994462
C	0.91242453	6.55347732	1.32957751
C	-2.34659333	5.28291924	4.63792995
H	-3.82182718	5.06132031	3.16539351
H	-2.81539525	3.84937790	6.08608408
C	-2.70061897	7.90797786	5.86398081
H	-2.38962834	9.44334201	4.49694620
H	-1.33850831	8.17485156	7.41627953
H	-4.61586842	8.15404404	6.65011220
H	1.79548194	-1.62865279	6.37460926
H	2.83106786	6.22026595	0.57874731
H	-0.39961275	6.32863363	-0.28592514
H	0.84438956	8.59564593	1.82571766
H	1.63446108	4.06185425	-4.26334219
H	3.55234362	-3.56598442	8.43912789
H	5.13721195	-1.89924502	6.00231592
H	5.05931658	-7.84035698	7.17794630

C	-0.90649502	5.02711166	-4.06014039
H	-4.83105497	10.78467826	-0.46457676
H	-1.04273610	6.76411802	-5.23680982
H	-0.57695825	3.46120264	-5.39888803
H	0.86026585	5.23851621	-2.95747210
C	-5.44465734	-8.08969555	-1.76009001
C	-5.44186077	-3.61312879	-3.39173621
H	-7.25362767	-3.09291358	-2.50756986
H	-5.87080898	-4.38664052	-5.27130951
H	-4.34226992	-1.87618190	-3.70120703
H	-5.70105790	-8.80936319	-3.69068301
H	-7.33432733	-7.86064569	-0.91811292
H	-4.44117392	-9.55451474	-0.67924240
C	-3.74406041	6.75352186	-0.57339255
C	-4.45114963	9.27877695	-1.85541822
H	-5.29773433	6.26650611	0.73975318
H	-2.08704341	7.10484130	0.66105723
H	-6.15946226	9.04752813	-3.02326692
H	-2.93388619	9.95658694	-3.10483309
H	-4.86341772	4.31353036	-3.59644468

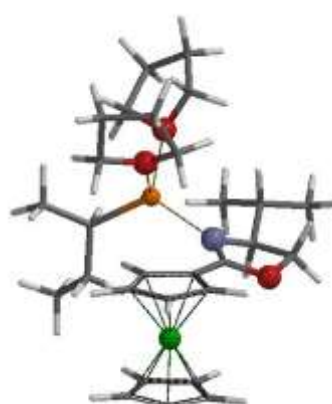
(S)-Fc-oxazol...s-BuLi...TMEDA (C5a)
(RI-DFT: BP86/def2-TZVP)



E = -2645.95156602992 au
Imaginary frequencies: 0

Fe	6.79394686	0.61839112	1.87281399
C	3.11878524	1.76564244	2.34777920
C	4.75462042	3.17169282	3.97457891
C	6.06466911	1.43340223	5.59417025
C	5.25089983	-1.06973834	4.98102411
C	3.39407745	-0.86982031	2.98547001
C	9.31126165	2.71642357	-0.20510149
C	7.69415616	1.29711878	-1.85168606
C	8.01699129	-1.32575215	-1.26990788
C	9.82553162	-1.53428737	0.73567785
C	10.63130850	0.96823361	1.39094080

(S)-Fc-oxazol...s-BuLi...TMEDA (C5b)
(RI-DFT: BP86/def2-TZVP)



E = -2645.94601806734 au
Imaginary frequencies: 0

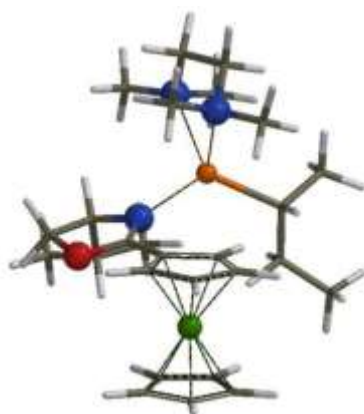
Fe	-6.61511063	1.63627822	0.20966482
C	-5.51283134	0.38205084	-3.26777230
C	-7.15446253	-1.42578487	-2.10817492
C	-6.03760915	-2.20342730	0.24030665
C	-3.69813782	-0.88896369	0.55871256
C	-3.34293378	0.69180138	-1.63430249
C	-10.12033175	3.17173429	0.89031004
C	-8.50022325	5.00675376	-0.26996619
C	-6.35071613	5.35404663	1.34125583
C	-6.62869320	3.73284139	3.48939653
C	-8.96077289	2.38179109	3.20958706

C	2.06418129	-2.95982729	1.80078414	C	-1.22301068	2.38418202	-2.04533594
Li	-2.53563546	0.28683381	-0.11892806	Li	2.24492257	-1.03228470	1.07817856
N	0.10287180	-2.82610980	0.34612025	N	0.94639960	2.33673340	-0.91057176
H	5.00415165	5.20926658	3.94249026	H	-8.95833766	-2.06138440	-2.85549775
H	7.46720927	1.92585107	7.01065660	H	-6.86515949	-3.51378545	1.58719386
H	11.97629349	1.45710630	2.86324215	H	-9.70022286	0.97640219	4.51070759
H	10.45020886	-3.27769137	1.62141089	H	-5.27571731	3.51058531	5.01734641
H	9.47649757	4.76192362	-0.15187223	H	-11.89477068	2.47351288	0.12910312
H	7.01568808	-2.88508264	-2.15342584	H	-4.75342194	6.58661800	0.96258048
H	5.88355342	-2.81728667	5.84919346	H	-2.37878132	-1.03194500	2.14249655
H	1.86096771	2.51281118	0.89743354	H	-5.81127181	1.34971079	-5.05190056
C	-1.71687622	3.81576023	-2.09530251	C	1.83278296	-1.16185999	5.12296811
H	6.40610149	2.07589019	-3.24770426	H	3.75487251	-0.33789902	5.43153468
O	2.99702654	-5.31831755	2.32947068	H	-8.82629765	5.94638190	-2.06573763
C	1.21206456	-7.07940293	1.20323447	O	-1.60383874	4.26677835	-3.79530565
C	-0.39148404	-5.42327375	-0.58951410	C	0.86300242	5.44659633	-4.08706882
C	0.32522961	-5.74008122	-3.41001917	C	2.22814451	4.73920460	-1.63164570
H	2.30922952	-8.55435346	0.24505370	C	5.12096268	4.59024304	-1.75812054
H	0.10211015	-7.93750479	2.73973167	H	1.78255435	4.62258130	-5.77044698
H	-2.42326377	-5.83478643	-0.38973747	H	0.56873358	7.47544927	-4.37330781
H	2.39425054	-5.47637576	-3.53976046	H	1.74183989	6.14459559	-0.15425183
C	-0.32513488	-8.41375776	-4.33053838	H	5.60591977	2.87095517	-2.83709570
C	-0.95350792	-3.76032391	-5.08716259	C	-0.02142515	0.68702821	6.37787853
H	-3.02067853	-3.98774148	-5.02392532	H	-0.14314141	2.44707803	5.25344094
H	-0.35218331	-3.98484313	-7.06378258	H	-1.95180210	-0.13107161	6.32469242
H	-0.50612043	-1.82507077	-4.48956759	C	0.53580645	1.44680278	9.14275629
H	0.25595648	-8.66368076	-6.30900751	H	0.59699533	-0.21232311	10.39501496
H	-2.37915550	-8.74071858	-4.23617010	H	2.38676546	2.39199947	9.27506305
H	0.60516853	-9.90368499	-3.21914237	C	6.24443009	4.38055945	0.90474966
C	0.20862791	3.61257219	-4.26275178	C	6.22861321	6.89215498	-3.13828171
C	1.30867169	6.10764834	-5.31245891	H	5.40102721	2.82593577	1.98612682
H	1.82398222	2.41465396	-3.67904175	H	8.29605221	4.06542420	0.81966669
H	-0.67112240	2.58272496	-5.86096801	H	8.30404494	6.80106941	-3.15209834
H	2.30113483	7.15503854	-3.80974015	H	5.59769324	7.01845959	-5.11467410
H	-0.18585338	7.35334881	-6.04595952	H	5.91864026	6.14449331	1.96150252
H	-0.81407400	5.02437158	-0.61536788	H	5.69348063	8.66060675	-2.17907275
C	-4.08464156	5.25550488	-2.97377942	C	1.79218137	-3.74114916	6.45059005
H	2.66446602	5.78530450	-6.86585858	H	3.21057420	-5.05492636	5.65725551
H	-3.76946226	7.22248524	-3.65647878	H	2.15005649	-3.72604171	8.52669364
H	-5.51989063	5.41622859	-1.46379998	H	-0.06385466	-4.67920545	6.21638377
O	-3.66879279	1.13361238	3.74726686	H	-0.89804386	2.75367895	9.91200633
C	-2.84080367	0.14075151	6.15101130	O	6.20930610	-1.88016869	0.22913427
C	-2.12492723	2.44424831	7.72855977	C	7.64106589	-3.06268663	2.22538663
C	-4.12065439	4.37694953	6.88177033	C	10.38576075	-2.98311147	1.30321785
C	-4.47633567	3.75116985	4.07301026	C	10.13197269	-3.10236114	-1.61820351
H	-1.26171066	-1.15517385	5.79050774	C	7.26059102	-2.85371809	-2.07935419
H	-4.40047992	-0.93023260	7.04429926	H	6.98312629	-5.02999075	2.47812255
H	-2.16934062	2.06374788	9.76826464	H	7.26148713	-2.01193432	3.96850611
H	-0.21443362	3.08258589	7.21979490	H	11.28994696	-1.20951708	1.88784243
H	-3.52344055	6.34232899	7.17008722	H	11.50792759	-4.54882461	2.07341874
H	-5.89157558	4.08946662	7.93337687	H	10.85728590	-4.88439574	-2.39556536
H	-3.29862145	4.91667861	2.82063895	H	11.17996928	-1.55738911	-2.52152594
H	-5.01466807	4.26412514	-4.56286567	H	6.39986405	-4.70969968	-2.49911559
H	-6.45558762	3.91348377	3.45671528	H	6.76237328	-1.53257500	-3.60002932
O	-5.95492838	-1.65245550	-1.00685317	O	1.12675429	-4.27273369	-1.16263841

C	-7.53211422	-2.93975692	0.82687063
C	-10.26749390	-2.45312811	0.02642572
C	-10.01674302	-2.15563080	-2.85048013
C	-7.51058357	-0.74541414	-3.08325555
H	-7.06772021	-2.19232909	2.70718146
H	-7.07950594	-4.97750276	0.77977024
H	-11.54208118	-3.99084497	0.58884627
H	-10.97064367	-0.69019464	0.87465123
H	-11.59154958	-1.11092191	-3.70623035
H	-9.90155417	-4.01870593	-3.76815977
H	-7.75211976	1.31218400	-2.89097413
H	-6.49156135	-1.11920644	-4.85238473

C	0.11926153	-6.43744827	0.15440895
C	0.67633288	-8.67473447	-1.59772906
C	0.57944001	-7.48427920	-4.27818229
C	0.41274881	-4.61365624	-3.76776078
H	-1.93608908	-6.18301883	0.42383894
H	1.02986771	-6.51492611	2.01224044
H	2.56338412	-9.44501040	-1.20537174
H	-0.69564048	-10.21203206	-1.35540604
H	-1.06501434	-8.13758139	-5.36160351
H	2.27480921	-7.96632868	-5.37206455
H	-1.53121877	-3.90969791	-4.04673376
H	1.70474787	-3.47313889	-4.92212942

(S)-Fc-oxazol...s-BuLi...TMEDA (C6a)
(RI-DFT: BP86/def2-TZVP)



E = -2528.73361184462 au
Imaginary frequencies: 0

Fe	7.05930312	0.27676268	1.56208502
C	3.53543701	1.75615375	2.18631471
C	5.34654892	2.95334674	3.79573558
C	6.52591810	1.05204078	5.32794533
C	5.45657256	-1.34281362	4.67734210
C	3.56794997	-0.91045170	2.74969747
C	9.69006304	2.18876378	-0.55467204
C	7.89685719	0.96384793	-2.17468354
C	7.99735528	-1.69157749	-1.66229373
C	9.84277311	-2.11330540	0.27457895
C	10.89477988	0.28867753	0.95656059
C	2.01622610	-2.83416890	1.55359799
Li	-2.39364390	0.83945344	0.09242732
N	-0.02078090	-2.48966072	0.24275992
H	5.79113879	4.95747432	3.80765631
H	8.00933519	1.36686007	6.71210601
H	12.32574248	0.61664712	2.39186890
H	10.33344351	-3.92779807	1.09964187
H	10.04397094	4.20877999	-0.46227218

(S)-Fc-oxazol...s-BuLi...TMEDA (C6b)
(RI-DFT: BP86/def2-TZVP)



E = -2528.72673116507 au
Imaginary frequencies: 0

Fe	-8.22934206	-0.80392901	-1.74076602
C	-6.95238003	1.72692884	-4.34596617
C	-8.01341767	-0.42497551	-5.59170704
C	-6.65802389	-2.62794412	-4.78295455
C	-4.73224205	-1.84677208	-3.05177119
C	-4.87881835	0.85796547	-2.79343992
C	-12.00605546	-1.02927806	-0.87861659
C	-10.85690797	1.03426666	0.45055335
C	-8.88415227	0.02614288	2.00746303
C	-8.80448079	-2.65329740	1.63964445
C	-10.73474158	-3.30711074	-0.14436092
C	-3.19831811	2.48849363	-1.34725077
Li	1.56694206	-0.93162321	0.05213788
N	-0.83188752	2.11130395	-0.84872256
H	-9.60490883	-0.39587219	-6.88841949
H	-7.05661777	-4.56214557	-5.34390509
H	-11.14136695	-5.19403611	-0.84416496
H	-7.47734498	-3.94480633	2.52456688
H	-13.54404950	-0.88756333	-2.23150618

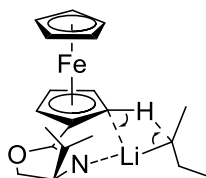
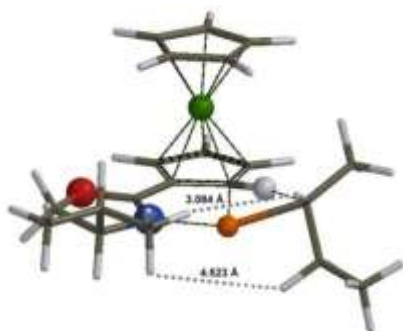
H	6.83052511	-3.13203845	-2.54452482	H	-7.62409651	1.10942645	3.21199450
H	5.94097830	-3.16651948	5.48180846	H	-3.44144162	-3.06760727	-2.02619035
H	2.33453013	2.66389027	0.78310552	H	-7.54868618	3.67977173	-4.54332433
C	-1.41465266	4.26960325	-1.98759950	C	0.89444750	-2.34319386	3.77526313
H	6.64318347	1.89110952	-3.50981711	H	2.38045461	-3.72059148	4.35215645
O	2.81805354	-5.27238811	1.89109490	H	-11.36644793	3.01551350	0.28141905
C	0.86682954	-6.85116725	0.77550914	O	-4.24160480	4.71268943	-0.53008797
C	-0.74687194	-4.99306391	-0.79776679	C	-2.33922974	5.84183971	1.10679857
C	-0.26687352	-5.17190385	-3.67969542	C	0.11502694	4.47127938	0.35873944
H	1.81294930	-8.31544633	-0.34583141	C	1.76305064	6.06482427	-1.46647746
H	-0.19379961	-7.75115596	2.32252497	H	-2.32195402	7.88271883	0.74221163
H	-2.77839139	-5.30024101	-0.46171705	H	-2.89966238	5.48533429	3.07769624
H	1.79269269	-4.96136654	-3.96133532	H	1.24042172	3.96422538	2.03590174
C	-1.08035797	-7.76452759	-4.69787501	H	0.46237350	6.91501091	-2.86392035
C	-1.60303508	-3.05793375	-5.13477093	C	0.88227330	-0.23254702	5.77001222
H	-1.12968719	-3.15376263	-7.15570760	H	2.61383989	0.93345422	5.60665721
H	-3.66967939	-3.25549832	-4.97466933	H	-0.70150627	1.08038186	5.36039472
H	-1.08074017	-1.17412123	-4.44094131	C	0.65797494	-1.04368889	8.56738501
H	-0.68368076	-7.90141740	-6.73204730	H	-1.08120284	-2.12991128	8.91159285
H	-3.12730541	-8.04594004	-4.44145289	H	2.26267500	-2.25813737	9.10099193
H	-0.10296811	-9.34628715	-3.76965964	C	3.69966130	4.47107555	-2.90729406
C	0.27499983	3.87788805	-4.32088786	C	3.06118158	8.20617812	-0.00367838
C	1.69234525	6.21525486	-5.35263126	H	2.75944317	3.10217995	-4.14946975
H	1.71032401	2.40406947	-3.92750604	H	4.90264749	5.68888944	-4.08739127
H	-0.88231011	3.09578643	-5.88149798	H	4.10068057	9.45731125	-1.29573226
H	2.94979834	7.00896219	-3.89339607	H	1.70833501	9.38267299	1.04910961
H	0.37688331	7.72344703	-5.91596641	H	4.93707822	3.40656297	-1.61332144
C	-7.79434805	-0.04073472	2.64026780	H	4.42444018	7.43633391	1.36720196
C	-6.41213862	2.24444237	3.72652577	N	7.84455212	-0.17725620	0.22103640
N	-6.96555189	-0.75471881	0.08338509	C	8.22997272	-2.53964465	-1.16259406
N	-3.66994060	1.87482552	4.03396970	C	7.54523421	-0.60636578	2.93819383
C	-7.94051322	1.01180183	-1.82436276	C	9.94794229	1.54664062	-0.25394174
C	-7.85069476	-3.31091248	-0.49978576	C	5.98148028	-4.34837571	-1.23938695
C	-3.09585140	-0.00827155	5.98596062	N	3.66619948	-3.42358015	-2.51256542
C	-2.49237137	4.30085907	4.70585406	C	4.17226050	-2.55754191	-5.09994009
H	-10.04162456	1.03461518	-1.85303195	C	1.84188785	-5.52405661	-2.57433353
H	-7.24327270	2.92900500	-1.47571968	H	9.20589603	-1.59552042	3.76907595
H	-7.25845801	0.44670430	-3.69994492	H	5.82818787	-1.70927197	3.31735985
H	-7.20627938	-3.86331024	-2.39384289	H	7.33936209	1.22065823	3.90098926
H	-9.94640407	-3.45691747	-0.46667283	H	11.79154393	0.77865677	0.40744687
H	-7.08944733	-4.66533767	0.87922032	H	9.61823217	3.34457537	0.73110130
H	-3.83012939	-1.87253040	5.45224469	H	10.10583822	1.93904880	-2.28825312
H	-7.50892317	-1.68577922	3.87936901	H	8.80335061	-2.05163208	-3.10172208
H	-9.85759937	0.36493077	2.67434979	H	5.08422916	-4.04303244	-6.26841900
H	-7.30713446	2.73301174	5.56628282	H	2.60671534	-7.18936128	-3.59598600
H	-3.90652514	0.51723198	7.85061360	H	9.83954603	-3.63243969	-0.34690368
H	-1.03849435	-0.17197933	6.19137464	H	5.42489060	-4.90017953	0.68592034
H	-3.26690782	5.07046287	6.49859287	H	6.65500261	-6.09075963	-2.20543282
H	-0.44767258	4.03988437	4.93253080	H	5.39325472	-0.88413486	-5.07689979
H	-6.67524365	3.88913925	2.48291466	H	2.37999824	-2.03121786	-6.00399752
H	-2.80397692	5.66969765	3.18098259	H	1.36816064	-6.08562898	-0.63323741
H	-0.20618978	5.22191512	-0.54128206	H	0.10800816	-4.91868431	-3.54139191
C	-3.54907784	6.14719050	-2.58789059	C	-1.63329595	-3.77342782	3.78021373
H	2.86010399	5.75865816	-7.02036048	H	-1.63413575	-5.37912248	2.44410946
H	-2.94186059	8.04740806	-3.25800557	H	-2.22519221	-4.59074657	5.62882278

H -4.76667867 6.52150407 -0.92818805
H -4.81066538 5.40931582 -4.08313923

H -3.19823664 -2.51900192 3.18902267
H 0.63949876 0.58987646 9.86414959

2.2. The coordinates and energies of transition states TS4-6.

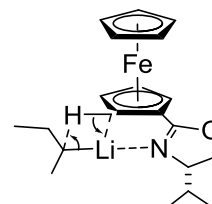
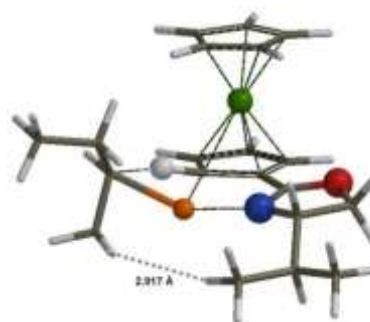
(S,R_p)-TS4 (preferred)
(RI-DFT: BP86/def2-TZVP)



E = -2180.823580892 au
Imaginary frequencies: 1 (-1159.80 cm⁻¹)

Fe	3.70538466	-1.53454021	-0.03983108
C	1.78404218	1.31213598	1.88976088
C	4.36190254	1.13921626	2.70902570
C	4.90299124	-1.35244260	3.64648248
C	2.65709669	-2.83055959	3.42881340
C	0.73304466	-1.19507126	2.37146914
C	6.03214362	-0.60413294	-2.99735394
C	3.44788242	-0.61987742	-3.81310713
C	2.45764248	-3.10205036	-3.37812618
C	4.42126867	-4.62257843	-2.29829930
C	6.63469174	-3.07743214	-2.06641669
C	-1.86461668	-1.89895636	1.86496590
Li	-2.07261854	3.00818195	0.86212234
N	-3.62259545	-0.36110217	1.09471351
H	5.74248593	2.65655669	2.57549984
H	6.71451747	-2.02430164	4.34660865
H	8.44089119	-3.66521306	-1.28690488
H	4.25282625	-6.58802896	-1.72960831
H	7.29818554	1.01100812	-3.04210618
H	0.53445070	-3.71415109	-3.75821458
H	2.41925663	-4.79845462	3.96364327
H	0.99460644	3.34763961	0.50827342
C	-0.02835449	5.88466358	-0.74307306

(S,S_p)-TS4 (non-preferred)
(RI-DFT: BP86/def2-TZVP)



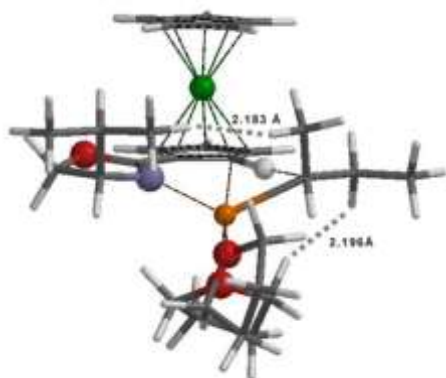
E = -2180.82326807978 au
Imaginary frequencies: 1 (-1091.78 cm⁻¹)

Fe	4.10075575	1.17040900	0.00792102
C	2.70615002	3.60200607	2.64399540
C	4.70808438	2.14132593	3.71346203
C	4.02737367	-0.48232271	3.52832712
C	1.59422323	-0.75160521	2.36670928
C	0.78355477	1.83039204	1.83471003
C	7.43866747	1.83630256	-1.85569666
C	5.43896662	3.28415645	-2.97203815
C	3.53864473	1.55383838	-3.82615995
C	4.35375187	-0.95999057	-3.23809029
C	6.76623207	-0.78467146	-2.01665137
C	-1.62846088	2.45200637	0.70058036
Li	-2.18197885	-2.48982884	1.42529540
N	-3.45839403	0.84981235	0.33465269
H	5.22644184	-2.04367908	4.12285543
H	6.46152516	2.89380599	4.47679284
H	7.87274360	-2.36028782	-1.30451777
H	3.30428255	-2.68754283	-3.59321923
H	9.14659538	2.59303618	-1.00367308
H	1.76281828	2.06552720	-4.72167942
H	0.87677271	-3.03117315	1.42721272
H	2.62362726	5.64703812	2.47961292
C	-0.11047440	-5.80820812	0.85324025

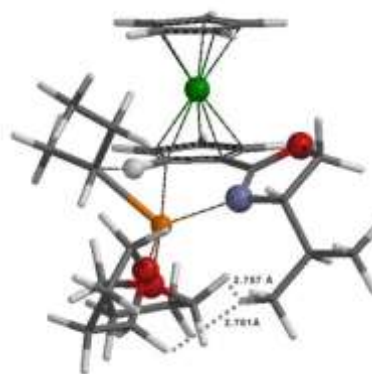
H	-1.49035400	5.93255946	-2.25767197
H	2.41258207	0.98222998	-4.56996501
O	-2.55916218	-4.33483924	2.30193975
C	-5.19464664	-4.53372561	1.53972051
C	-6.00742200	-1.78788103	0.90878702
C	-7.33120726	-1.52073005	-1.67328134
H	-5.27708001	-5.79023423	-0.11707472
H	-6.24417050	-5.39691852	3.10491467
H	-7.32110264	-1.05685399	2.36274629
H	-6.03896919	-2.31909127	-3.10691436
C	-9.79990882	-3.04459567	-1.69949670
C	-7.83445859	1.25108135	-2.34090766
H	-9.02961448	2.15962723	-0.89853803
H	-8.82677933	1.39907796	-4.16013377
H	-6.07230794	2.33518518	-2.50108658
H	-10.72640218	-2.91161803	-3.55331774
H	-11.13278741	-2.31478320	-0.27673086
H	-9.49030020	-5.06152182	-1.30309835
C	-0.97283432	7.46754642	1.50013766
C	-1.95439806	10.13749532	0.89838356
H	-2.52753704	6.49636281	2.56496293
H	0.56650180	7.61060574	2.90501838
H	-3.58053757	10.05299939	-0.39597107
H	-0.47923510	11.26924113	-0.02872732
C	2.44325985	6.88033648	-1.84318411
H	-2.55122259	11.16152946	2.61083928
H	3.98570115	6.75833163	-0.44178177
H	2.38165389	8.87307284	-2.48123562
H	3.04483058	5.75430543	-3.48713328

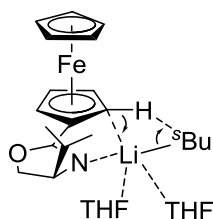
H	1.80031722	-6.53360241	1.28550156
H	5.36307099	5.33043958	-3.11892031
O	-2.05111367	4.88730031	-0.00802804
C	-4.67660291	4.99679124	-0.82314109
C	-5.54237991	2.20118345	-0.92993706
C	-8.14717612	1.73567235	0.28386659
H	-5.73115338	6.09856231	0.59461125
H	-4.73611075	5.98502712	-2.64328784
H	-5.64368489	1.53771725	-2.91182357
H	-8.03465595	2.42954607	2.25078982
C	-0.95154466	-6.89128077	-1.69623484
H	-2.89844154	-6.24957184	-2.13726224
H	0.23621195	-6.08843616	-3.21431156
C	-0.88762161	-9.79315747	-1.93923306
H	1.03561859	-10.50894753	-1.59408088
H	-2.14673010	-10.70157176	-0.55574209
C	-8.81957813	-1.07952831	0.34253939
C	-10.19372486	3.24411577	-1.11464182
H	-7.46265265	-2.17301978	1.46946096
H	-10.69990983	-1.36798719	1.17765272
H	-12.05130675	2.95604570	-0.23185817
H	-9.81318216	5.28748596	-1.10814184
H	-8.85313483	-1.87949019	-1.57847566
H	-10.33856245	2.62985063	-3.09825036
C	-1.86278338	-6.53235872	3.05145709
H	-1.78146308	-8.52240691	3.68506428
H	-1.45134534	-5.39827747	4.77035586
H	-3.88835189	-6.22011135	2.57962726
H	-1.47365469	-10.43307260	-3.83281745

(S,R_p)-TS5 (preferred)
(RI-DFT: BP86/def2-TZVP)



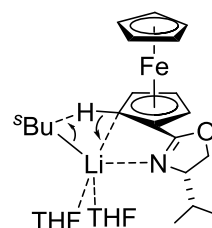
(S,S_p)-TS5 (non-preferred)
(RI-DFT: BP86/def2-TZVP)





E = -2645.93686400521 au
Imaginary frequencies: 1 (-1253.92 cm⁻¹)

Fe	5.98239462	0.22182427	-0.33771945
C	2.40206226	1.91399945	-0.15024418
C	4.38954551	3.72615872	0.23210347
C	5.97125766	3.01684098	2.33258553
C	5.00718657	0.70448188	3.33950006
C	2.80539260	0.05369232	1.83349257
C	8.13545966	0.52854415	-3.54747977
C	6.22768256	-1.36537478	-3.88595647
C	6.58837956	-3.25474345	-1.98153344
C	8.72092955	-2.54153184	-0.47093003
C	9.68069229	-0.20173762	-1.44224154
C	1.22744739	-2.14700874	2.23792273
Li	-2.64499481	0.65882061	-0.35853072
N	-0.95493478	-2.57979364	1.19983554
H	4.72461341	5.37153717	-0.95657075
H	7.64178095	4.01088777	3.00381529
H	11.27296963	0.85510399	-0.69095942
H	9.45591619	-3.57367391	1.14462704
H	8.35184832	2.23464804	-4.66880692
H	5.41779826	-4.91836155	-1.69944842
H	5.76267498	-0.36115238	4.92436212
H	0.37535050	2.15324832	-1.86386609
C	-1.53791590	2.74597690	-3.90927976
H	4.73427481	-1.33735469	-5.29295481
O	2.06706073	-3.88547858	3.96150331
C	0.03184203	-5.70038392	4.26126629
C	-1.82691843	-5.08272506	2.08561233
C	-1.83250052	-7.11427826	-0.02005330
H	0.85949256	-7.59919063	4.14310375
H	-0.79335556	-5.43526603	6.15232466
H	-3.77945877	-4.90509305	2.79857780
H	0.15894928	-7.42121475	-0.57135679
C	-2.91187569	-9.61233991	0.98561238
C	-3.29686051	-6.25091734	-2.35868409
H	-5.28500362	-5.86486659	-1.87716038
H	-3.27244722	-7.72435227	-3.82432568
H	-2.48187019	-4.52304631	-3.16194698
H	-2.83260899	-11.08669085	-0.47549717
H	-4.90702618	-9.38053359	1.53518155
H	-1.87934725	-10.32527922	2.64258445
C	-0.29019037	5.20618363	-4.79616288
C	-1.51109429	6.54148687	-7.07121239
H	-0.21925781	6.56842607	-3.21194257
H	1.71038551	4.80413674	-5.25297482



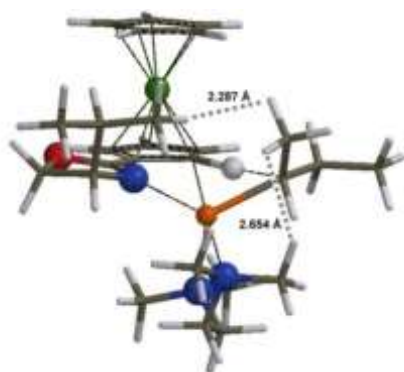
E = -2645.93403005217 au
Imaginary frequencies: 1 (-1251.6 cm⁻¹)

Fe	-6.12663555	-0.06518970	0.16747287
C	-4.97420645	1.73132284	-3.00233218
C	-6.01108872	-0.68357749	-3.63580793
C	-4.54469092	-2.57924181	-2.33899330
C	-2.53725100	-1.43740219	-0.90375858
C	-2.82867724	1.24768089	-1.36008603
C	-9.88848264	0.07798404	1.09701626
C	-8.61978738	2.30542767	1.97498818
C	-6.66385648	1.52868924	3.68177279
C	-6.72359110	-1.16969659	3.86363461
C	-8.70975377	-2.07016178	2.25771687
C	-1.13945487	3.17521381	-0.37406639
Li	2.58654896	-0.91042399	-0.01904756
N	1.24680491	2.87644059	0.11398780
H	-7.65933298	-1.00192956	-4.82423928
H	-4.97073031	-4.59224177	-2.38314437
H	-9.21446208	-4.03671690	1.95185437
H	-5.45014059	-2.33434053	4.97290060
H	-11.44109567	0.02321890	-0.24604125
H	-5.33526058	2.77004946	4.63556784
H	-0.66680735	-2.52690214	0.65824892
H	-5.63724850	3.56617603	-3.64562545
C	0.97709118	-3.88100650	2.56482023
H	3.00676956	-4.37128034	2.30328033
H	-9.03828141	4.23635036	1.41700720
O	-2.12627324	5.53292219	-0.00432669
C	-0.15221354	6.99216938	1.21849546
C	2.26000694	5.36582239	0.90163977
C	4.13037315	6.52218008	-1.03134578
H	-0.05317769	8.83697281	0.27475139
H	-0.70088075	7.26955293	3.20481939
H	3.26096700	5.14705835	2.71810445
H	3.02855377	6.93943072	-2.75734318
C	0.67979038	-2.44927182	5.06824978
H	1.82035729	-0.69507459	5.02022570
H	-1.29404031	-1.77765000	5.21416811
C	1.33652610	-3.87562786	7.52028224
H	0.13236338	-5.54991641	7.77586201
H	3.31047098	-4.54300838	7.49955994
C	6.27148594	4.71358411	-1.73871429
C	5.22256015	9.00928208	-0.00969739
H	5.54665739	2.95190745	-2.55216791
H	7.54211683	5.60106216	-3.12438714
H	6.47101559	9.89433216	-1.41449985

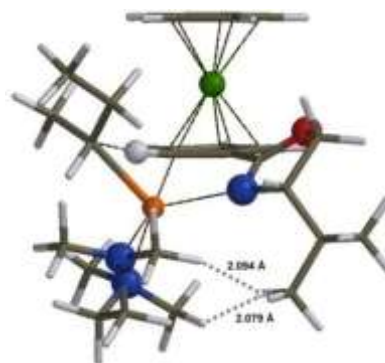
H	-3.56891336	3.17795291	-3.55599657
C	-1.33858513	0.66130737	-5.90429894
H	-0.47485722	8.26733161	-7.60831440
H	-1.99045665	1.18895377	-7.82439070
H	-2.41623965	-1.04467034	-5.38077248
H	0.64782482	0.05019174	-6.10705263
O	-3.24186175	3.19521165	2.63655155
C	-2.56920761	2.76296142	5.26305726
C	-1.14787549	5.12261488	6.11897673
C	-2.41944119	7.19683346	4.53576308
C	-2.83957241	5.85275158	2.01720113
H	-1.43115340	1.03167699	5.36187260
H	-4.32332439	2.48327884	6.36098163
H	-1.30115345	5.43920975	8.16389778
H	0.86321461	4.96119923	5.62415812
H	-1.24772815	8.89549551	4.32575903
H	-4.23165433	7.76104817	5.38742367
H	-1.17007989	5.98181239	0.78462843
H	-4.50480785	6.52379548	0.97348172
O	-6.53181855	-0.23276890	-0.96168531
C	-8.39674905	0.01714630	1.02441694
C	-10.79453451	0.94601179	-0.27973552
C	-10.64101243	-0.42455519	-2.83471562
C	-7.80231449	-0.39136849	-3.39880738
H	-7.62746240	1.33147109	2.43236577
H	-8.70144452	-1.84439965	1.92279068
H	-12.51285932	0.49136773	0.79079786
H	-10.71967155	3.00629685	-0.54738276
H	-11.74445773	0.49971818	-4.32810849
H	-11.33030275	-2.37700508	-2.64571215
H	-7.23740667	1.26666632	-4.52174832
H	-7.14295288	-2.10228388	-4.37475366
H	-3.47215212	7.09293062	-6.63980295
H	-1.56726565	5.31007091	-8.74553578

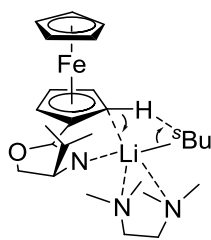
H	3.75183628	10.39519383	0.47382549
H	7.40110434	4.21472111	-0.06477409
H	6.35223666	8.66303243	1.70459095
C	-0.53359797	-6.34611255	2.49549551
H	-0.19280220	-7.39154443	0.72446987
H	-0.13189461	-7.68257078	4.05191034
H	-2.58364092	-5.94965452	2.55801924
H	1.09350495	-2.67366910	9.20491337
O	6.51314415	-1.01651772	1.04840654
C	7.39974545	-1.10688481	3.65085738
C	10.15484588	-1.99612764	3.54951754
C	10.25299878	-3.46263814	1.04493718
C	8.50286706	-1.88643953	-0.61539244
H	6.18413104	-2.43748889	4.68796270
H	7.18611307	0.78359900	4.49060873
H	11.45219775	-0.37292865	3.48269941
H	10.66173679	-3.15140718	5.19572128
H	9.48704829	-5.37977894	1.28744414
H	12.16932203	-3.61783056	0.26437723
H	7.60559724	-2.92812459	-2.16703561
H	9.50528877	-0.23648281	-1.41389712
O	3.03102355	-2.15867089	-3.68079726
C	2.40919456	-0.59714846	-5.85790043
C	0.76574698	-2.23646091	-7.57255707
C	1.77103279	-4.90260614	-7.01557163
C	2.28849702	-4.76472671	-4.18092531
H	4.18907950	-0.04194700	-6.79416017
H	1.44237640	1.10566420	-5.17121646
H	-1.22669810	-2.08247388	-7.00734535
H	0.93146009	-1.69906861	-9.56985724
H	3.52655995	-5.26250671	-8.07222834
H	0.41383612	-6.39859643	-7.48800982
H	3.83509756	-6.00020207	-3.54939654
H	0.58664354	-5.18009792	-3.06079834

(S,R_p)-TS6 (preferred)
(RI-DFT: BP86/def2-TZVP)



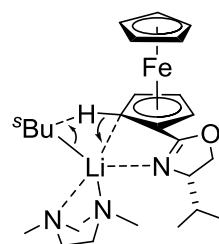
(S,S_p)-TS6 (non-preferred)
(RI-DFT: BP86/def2-TZVP)





E = -2528.71840132797 au
Imaginary frequencies: 1 (-1247.57cm⁻¹)

Fe	5.63482450	0.15228330	0.74078568
C	2.08847688	1.89321462	0.76212386
C	4.00802976	3.52357840	1.78341544
C	5.25814329	2.35339445	3.89993022
C	4.14257440	-0.07581428	4.27220159
C	2.18040082	-0.33540226	2.37027159
C	9.45050967	-0.16241854	0.09080065
C	8.22171668	1.03556241	-2.00863080
C	6.37118910	-0.68213875	-2.99127117
C	6.45164101	-2.93296272	-1.48951727
C	8.35238800	-2.61762059	0.41426095
C	0.57727138	-2.52822823	2.05076083
Li	-2.75751135	0.98749843	-0.38652742
N	-1.38569756	-2.69592826	0.57916860
H	4.52062036	5.36089063	1.01389405
H	6.81831943	3.13398172	4.98825312
H	8.84796904	-3.98400540	1.86431916
H	5.24584641	-4.57902957	-1.72267663
H	10.92582161	0.66365085	1.25585258
H	5.09098479	-0.31394965	-4.55212909
H	4.65219376	-1.46209943	5.69905690
H	0.38844213	2.53103753	-1.17031063
C	-1.20715706	3.60944741	-3.31293655
H	8.60142511	2.92742546	-2.70962057
O	1.14480335	-4.60878307	3.48142297
C	-0.92551515	-6.36452124	3.08150805
C	-2.23696721	-5.36345536	0.67589329
C	-1.49153180	-6.88233983	-1.71749133
H	-0.11404025	-8.26181865	2.88534021
H	-2.15102245	-6.31174170	4.76366149
H	-4.31081898	-5.42930270	0.87085816
H	0.59285723	-7.02347833	-1.70357167
C	-2.59869439	-9.56143297	-1.60837250
C	-2.28118556	-5.56271565	-4.16602844
H	-4.35412238	-5.43006990	-4.29812870
H	-1.62346420	-6.63857100	-5.81788942
H	-1.49856766	-3.64820132	-4.28588614
H	-1.98109778	-10.67626045	-3.24862703
H	-4.67970289	-9.49751823	-1.64348215
H	-2.02749522	-10.60139966	0.09787720
C	0.45325482	5.96057744	-3.65076888
C	-0.33399472	7.82900018	-5.73303416
H	0.54437960	7.00329881	-1.84182435
H	2.41726244	5.34134794	-4.01575650



E = -2528.71104348502 au
Imaginary frequencies: 1 (-1216.91cm⁻¹)

Fe	-6.96561441	-0.58375029	-0.83777351
C	-5.58781043	0.82734008	-4.10870505
C	-6.38555746	-1.73060693	-4.47324938
C	-4.95710904	-3.29652889	-2.76548638
C	-3.19362515	-1.79841004	-1.33630797
C	-3.61374372	0.76042653	-2.20568491
C	-10.79312483	-0.86296457	-0.28135801
C	-9.96393476	1.68136942	0.14632814
C	-8.13261362	1.63425793	2.14088808
C	-7.83167341	-0.93067221	2.95044227
C	-9.46920498	-2.47753067	1.44741325
C	-2.15326151	2.92716381	-1.35751028
Li	1.53133244	-1.03996111	0.08009459
N	0.24097947	2.91673588	-0.80909684
H	-7.86271112	-2.34799476	-5.76386801
H	-5.24249314	-5.32228595	-2.54398738
H	-9.65177373	-4.51850342	1.57502412
H	-6.55088226	-1.59417070	4.40886195
H	-12.15346442	-1.46739921	-1.69594364
H	-7.11513992	3.25935255	2.87434783
H	-1.65141116	-2.48351344	0.68215649
H	-6.29060449	2.49006382	-5.08947616
C	-0.27281400	-3.35361698	3.09543040
H	1.71472892	-4.03268175	3.08197303
H	-10.58258148	3.34513511	-0.88541170
O	-3.38668234	5.19236021	-1.17856837
C	-1.62975675	6.85920149	0.11437817
C	0.95372328	5.60003868	-0.33910960
C	2.32875660	6.84112291	-2.61899365
H	-1.82715252	8.75009057	-0.70903338
H	-2.16308620	6.91584940	2.12561885
H	2.17102632	5.71684921	1.34578337
H	0.90789069	6.98229244	-4.14370142
C	-0.53632268	-1.38112603	5.20479838
H	0.76366483	0.22042281	4.83636459
H	-2.44651034	-0.53553588	5.10639491
C	-0.08287673	-2.27253827	7.94145997
H	-1.43743881	-3.74771738	8.49613024
H	1.82447398	-3.07990271	8.16081965
C	4.54711652	5.29209055	-3.63367432
C	3.21749583	9.51739947	-1.93506357
H	3.97248017	3.33879294	-4.01845837
H	5.26619028	6.11957409	-5.39929214
H	4.08368019	10.44480777	-3.57992641

H	-2.23470517	8.59450391	-5.36179246	H	1.66926013	10.73801790	-1.28093655
H	-0.38670569	6.92184038	-7.60311567	H	6.12820553	5.26612932	-2.28175503
C	-8.28582432	1.50031616	1.32732227	H	4.65002786	9.45146875	-0.42583509
C	-6.84982826	3.74335158	2.43067103	N	5.92949762	-0.96932531	1.45517892
N	-7.32896266	0.70697435	-1.16571605	C	7.09256607	-1.58381645	-1.00032927
N	-4.17537589	3.17920353	2.96856029	C	6.60136514	-2.84740685	3.38649272
C	-8.10496100	2.48711640	-3.15244961	C	6.75802003	1.52728842	2.32760128
C	-8.30931941	-1.80889323	-1.79089948	C	5.86416243	-3.86343058	-2.27688083
C	-3.91368931	1.65853289	5.27798654	N	3.19515149	-3.42192068	-2.95896186
C	-2.75012950	5.54985007	3.26420686	C	2.98828145	-2.11369805	-5.40052732
H	-10.19455162	2.58020846	-3.32941816	C	1.80906564	-5.82997388	-3.09115938
H	-7.38709129	4.39020443	-2.76153171	H	8.67630321	-2.91758552	3.69970156
H	-7.30899984	1.88672887	-4.97044829	H	5.94805422	-4.73798194	2.85023706
H	-7.56183870	-2.41170806	-3.62938207	H	5.67495852	-2.35843189	5.17516159
H	-10.40571079	-1.83813246	-1.89644010	H	8.83403757	1.61704170	2.62765490
H	-7.70887873	-3.18183314	-0.35587439	H	5.82626794	1.97478954	4.12750747
H	-4.90749502	-0.15147267	5.08218188	H	6.23322550	2.97103639	0.93835362
H	-8.13041175	-0.13006710	2.60884877	H	6.90828178	0.08887640	-2.22215855
H	-10.32869157	1.98397943	1.23022859	H	3.70835371	-3.29834631	-6.97509466
H	-7.84285070	4.39882184	4.16139004	H	2.61647267	-7.11599696	-4.53712198
H	-4.68157077	2.65892306	6.95503406	H	9.15249592	-1.95010183	-0.79173584
H	-1.90677476	1.25606430	5.60923889	H	5.92917914	-5.49494111	-0.99368322
H	-3.48821237	6.70779917	4.84925452	H	6.99496712	-4.39794183	-3.96065949
H	-0.75497271	5.11457782	3.61754489	H	4.07487154	-0.34818164	-5.37188533
H	-6.89835945	5.33153359	1.09154553	H	1.00162788	-1.64587989	-5.76994194
H	-2.86548854	6.65452428	1.51268176	H	1.86103989	-6.76977893	-1.24328036
H	-3.17382363	4.29535513	-3.01298202	H	-0.17269819	-5.44697682	-3.56217416
C	-1.16082983	1.89308579	-5.64154825	C	-1.95873659	-5.67258135	3.48385204
H	0.97864549	9.44109460	-5.86617875	H	-1.65794302	-7.07727252	1.97277295
H	-2.56506730	0.35492936	-5.51669925	H	-1.68190224	-6.68380992	5.29315276
H	-1.52340435	2.85167791	-7.47013932	H	-3.97716874	-5.15146337	3.38900103
H	0.70125729	0.96498752	-5.83078688	H	-0.27174504	-0.71124160	9.30864567

2.3. The coordinates and energies of intermediates Int3-5.

(S,R_p)-Int3 (preferred)
(RI-DFT: BP86/def2-TZVP)



E = -2022.35358058818 au
Imaginary frequencies: 0

Fe	-4.34698649	1.17133405	-1.15808850
C	-1.44638829	2.90630283	-3.32398844
C	-3.88894358	3.18055187	-4.47074977
C	-5.06585373	0.76837110	-4.93991252
C	-3.38466468	-1.15451216	-4.06497309
C	-1.18155989	0.15544650	-3.10469696
C	-7.79598237	0.91254599	0.59911148
C	-6.65854891	3.32685682	1.07869276
C	-4.28935020	2.90359485	2.32719351
C	-3.96048551	0.22834454	2.59935502
C	-6.12559621	-1.00379134	1.53565836
C	1.04146383	-0.95907907	-1.96070713
N	2.94787830	0.33121865	-1.06297443
H	-4.79818202	4.98129730	-4.88302825
H	-6.92467232	0.44832120	-5.75887444
H	-6.43104524	-3.03146336	1.43084442
H	-2.33510422	-0.70732854	3.43788848
H	-9.59029860	0.59321230	-0.34672360
H	-2.97408032	4.35746184	2.93686184
H	-3.69077961	-3.18456556	-4.12890240
H	-7.44217296	5.15346878	0.56435869
O	1.24266656	-3.52081044	-1.87094213
C	3.56046852	-4.06571405	-0.49956520
C	4.88641893	-1.46951874	-0.20554634
C	5.86271106	-0.95370922	2.49012452
H	3.03025909	-4.89741406	1.33475171
H	4.63559959	-5.45813013	-1.59539723
H	6.52927808	-1.33691594	-1.49679416
H	4.22889643	-1.14263349	3.77749239
C	7.86288152	-2.91778280	3.23717851
C	6.92383804	1.72764948	2.74996852
H	8.50318533	2.03502904	1.42888284
H	7.63836217	2.05692072	4.67300097
H	5.47343469	3.16194182	2.36476889
H	8.53675783	-2.58645006	5.17372339
H	9.51137743	-2.81156832	1.97032447

Int-(S,S_p)- Int3 (non-preferred)
(RI-DFT: BP86/def2-TZVP)



E = -2022.35385331343 au
Imaginary frequencies: 0

Fe	-4.79211544	0.97766527	-0.00130993
C	-2.86511875	4.02765717	-1.33262003
C	-5.13837729	3.68305745	-2.74802851
C	-5.04297011	1.21050424	-3.88855969
C	-2.74371698	-0.09348092	-3.28160145
C	-1.40992752	1.73599780	-1.68066324
C	-7.92035237	1.37460896	2.25853888
C	-5.66432224	1.69054183	3.72479649
C	-4.21239893	-0.58662350	3.51795779
C	-5.56711852	-2.31320986	1.92929390
C	-7.85726434	-1.09486198	1.14047891
C	1.01756802	1.12828324	-0.57249175
N	2.24432345	-0.97907048	-0.97119317
H	-6.68002425	5.03734417	-2.88127532
H	-6.57869327	0.42384832	-5.01196410
H	-9.28150598	-1.89269377	-0.10454852
H	-4.96547588	-4.20305647	1.39785001
H	-9.40013971	2.77490297	2.00279410
H	-2.38489662	-0.92945829	4.39138017
H	-2.33250989	5.68065554	-0.23583734
H	-5.13272255	3.36910088	4.78088788
O	2.15355956	2.84678237	0.96682509
C	4.62598616	1.81759677	1.58260649
C	4.58193390	-0.91779525	0.53430766
C	6.96484591	-1.62876650	-0.98239742
H	6.05544848	3.00420790	0.64163614
H	4.87720520	1.94448188	3.63612227
H	4.40543902	-2.29754093	2.09996954
H	7.16006446	-0.21304936	-2.50540394
C	6.71817294	-4.24530227	-2.19716362
C	9.31874232	-1.50475846	0.70854233
H	5.12618322	-4.31793268	-3.52717361
H	8.44086119	-4.73675142	-3.24974415
H	11.03052062	-1.96703619	-0.37322336
H	9.59633452	0.38213625	1.53463626
H	6.42363465	-5.71366963	-0.75061818

H	7.12719471	-4.86001179	3.15883109
Li	1.79634753	3.83416419	-1.65199714

H	9.17676816	-2.86914765	2.27455843
Li	-0.22341042	-2.87661824	-3.03334515

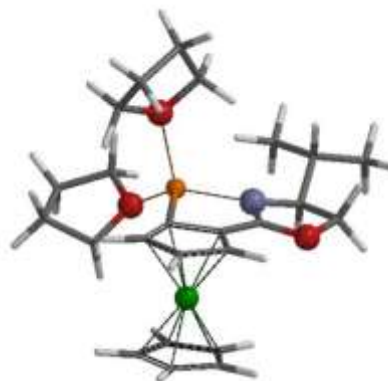
(S,R_p)-Int4 (preferred)
(RI-DFT: BP86/def2-TZVP)



E = -2487.48002893094 au
Imaginary frequencies: 0

Fe	5.56527532	0.38624294	-1.46151527
C	2.05901568	2.22136432	-0.63466028
C	4.10558674	3.97629048	-1.00891287
C	6.17925995	3.52425188	0.70406946
C	5.51667721	1.40147581	2.23621887
C	3.01470165	0.63579148	1.41958864
C	6.74237564	0.10009477	-5.14372172
C	4.95072354	-1.85568656	-4.58051692
C	5.94563921	-3.32932916	-2.53579086
C	8.35244542	-2.29856473	-1.84288159
C	8.84685265	-0.17895632	-3.45661856
C	1.56454891	-1.47654031	2.38842894
Li	-1.68039750	0.84226539	-0.88226045
N	-0.72653787	-2.04448453	1.70095403
H	4.14982918	5.44310333	-2.45685729
H	7.95636380	4.55695516	0.79148851
H	10.50489316	1.03066264	-3.38741376
H	9.56867336	-2.98001054	-0.33531215
H	6.53577118	1.55474743	-6.57850901
H	5.01891808	-4.92853583	-1.64009041
H	6.65451840	0.54466469	3.71688597
H	3.14620827	-2.15361038	-5.51019445
O	2.63832677	-2.95764535	4.21459052
C	0.83484576	-4.95356567	4.74805775
C	-1.52245836	-4.29667014	3.12675820
C	-2.41472024	-6.49363935	1.42734325
H	1.70642229	-6.76106065	4.19532787
H	0.48221019	-4.97168212	6.79296972
H	-3.13769773	-3.77875114	4.35510476
H	-0.77448482	-7.06426401	0.26655786

(S,S_p)-Int4 (non-preferred)
(RI-DFT: BP86/def2-TZVP)



E = -2487.47957405204 au
Imaginary frequencies: 0

Fe	-6.26326384	-0.42573230	0.62336343
C	-5.46449044	-3.79378176	-1.02633185
C	-6.18036598	-4.17398934	1.54959500
C	-4.40821647	-2.80035287	3.10264322
C	-2.50721610	-1.53339332	1.62297554
C	-3.23132663	-2.20577512	-0.96074090
C	-9.31280450	1.05101300	-1.28528774
C	-7.17949132	2.70673223	-1.48931929
C	-6.43683129	3.44153019	1.01093771
C	-8.10835057	2.22573076	2.76577759
C	-9.88952418	0.75475548	1.34552607
C	-1.85453839	-1.24786158	-3.12457427
Li	0.98125763	0.26784901	0.89731069
N	0.27721470	-0.02580396	-3.01035629
H	-7.80671620	-5.25660564	2.19403007
H	-4.56826048	-2.69507995	5.15538578
H	-11.38681859	-0.41155098	2.12977403
H	-8.02865834	2.37046395	4.81273540
H	-10.29366867	0.14912122	-2.84751264
H	-4.86647794	4.67372116	1.48526626
H	-6.39940253	-4.55020753	-2.69220845
H	-6.26048131	3.27226925	-3.23687453
O	-2.84157400	-1.64869982	-5.48472686
C	-0.94393423	-0.74650112	-7.24737257
C	0.90794240	0.79690669	-5.59734514
C	3.70481633	0.44133045	-6.30828633
H	-0.02452715	-2.40877020	-8.10986454
H	-1.90520933	0.34530164	-8.72340786
H	0.48269512	2.84373352	-5.75264561
H	4.13132189	-1.59315461	-6.09972624

C	-3.24093795	-8.75698203	3.04282719
C	-4.54634311	-5.67331809	-0.35050491
H	-6.20310641	-5.02738611	0.73436419
H	-5.15977549	-7.26324796	-1.54133799
H	-3.94362098	-4.12645221	-1.59337714
H	-3.82418766	-10.34788577	1.84085051
H	-4.86454090	-8.24990057	4.24418518
H	-1.72233794	-9.44130740	4.28659055
O	-4.16865541	3.35033625	0.86673976
C	-4.82159277	2.95670427	3.49271156
C	-3.35594256	4.96756286	4.94466525
C	-3.50922404	7.23121955	3.12946977
C	-3.39173028	5.97817594	0.51601048
H	-4.29050191	1.00984976	3.97313876
H	-6.88387868	3.18770684	3.73999702
H	-4.17180028	5.36522267	6.81105303
H	-1.38399890	4.36526668	5.19665274
H	-1.96748836	8.59076391	3.40407455
H	-5.30825966	8.24146402	3.38668587
H	-1.46280587	5.92878938	-0.26059442
H	-4.67651074	6.86828486	-0.85755515
O	-3.35819699	0.35331714	-4.28503600
C	-5.97784362	0.88860206	-4.91559830
C	-5.95634390	2.17920503	-7.52026916
C	-3.21115376	3.10124960	-7.78236557
C	-1.75849473	1.03026477	-6.40738315
H	-6.73460125	2.11305623	-3.41564256
H	-7.04750110	-0.89607840	-4.92097448
H	-6.39638465	0.80710468	-9.01778999
H	-7.34620616	3.71443754	-7.64273002
H	-2.94247211	4.92115724	-6.81459345
H	-2.61766803	3.32088843	-9.75840417
H	0.06365278	1.61457312	-5.60094337
H	-1.48691169	-0.64250444	-7.62887612

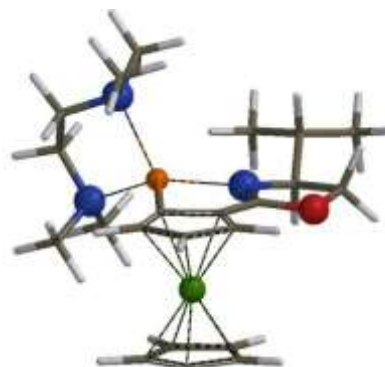
C	5.44535983	1.93228699	-4.53967842
C	4.16431039	1.19983071	-9.07121462
H	5.17146055	1.37763786	-2.56054572
H	7.44120789	1.62279920	-5.03197597
H	6.16178579	0.94655988	-9.58389280
H	3.03238967	0.07007844	-10.39871540
H	5.06868222	3.97441254	-4.68823754
H	3.68860657	3.20392389	-9.37475701
O	1.97995446	3.46786845	2.72088164
C	0.14405173	4.39363010	4.53210821
C	1.59616783	4.58465915	7.01166674
C	4.20088414	5.50575620	6.10516847
C	4.49949895	4.20989240	3.52020126
H	-1.42542316	3.03481040	4.52409311
H	-0.54998382	6.26610197	3.91798857
H	0.70601333	5.88152281	8.36475000
H	1.73986308	2.71179291	7.90196367
H	5.73770941	5.01337867	7.40864034
H	4.19281267	7.57258469	5.88843183
H	5.65136232	2.48154693	3.61670278
H	5.31630230	5.47608998	2.08542190
O	3.88325569	-2.18225392	2.02242444
C	3.15729988	-3.45478836	4.34932151
C	2.88334541	-6.23480715	3.65013122
C	4.96626381	-6.55851054	1.65353901
H	1.37806002	-2.59242543	4.98382246
H	4.65406096	-3.16002143	5.77564263
H	3.11555255	-7.49474683	5.28245681
H	1.00651818	-6.56213260	2.82133173
H	4.64112567	-8.16962162	0.38748770
H	6.81475753	-6.82424439	2.56872395
C	4.87649738	-4.03224383	0.24441489
H	6.74697025	-3.38745358	-0.39539383
H	3.59206669	-4.09522322	-1.39164326

(S,R_p)-Int5 (preferred)
(RI-DFT: BP86/def2-TZVP)



E = -2370.26198245523 au
Imaginary frequencies: 0

(S,S_p)-Int5 (non-preferred)
(RI-DFT: BP86/def2-TZVP)



E = -2370.26149128287 au
Imaginary frequencies: 0

Fe	5.61180281	-0.78199252	-1.85861876	Fe	-5.11748376	-0.29794638	-0.18027017
C	2.10287426	1.01192409	-2.74400085	C	-4.35269730	1.35925558	-3.55506418
C	3.93219251	1.22977309	-4.74603725	C	-5.39447318	-1.10042670	-3.94812434
C	6.23510345	2.43027802	-3.91215809	C	-3.73368878	-2.89559359	-2.74021050
C	5.94901430	2.99917364	-1.28828826	C	-1.58986883	-1.69244295	-1.57337608
C	3.43608622	2.14537092	-0.60543891	C	-2.04345008	0.97750806	-2.12879302
C	8.67901294	-3.06930672	-2.50844804	C	-7.80330749	1.90924666	1.56494720
C	6.38760859	-4.30590124	-3.26624362	C	-5.55840278	1.78234220	3.07447919
C	4.78183727	-4.50048184	-1.08966398	C	-5.08894771	-0.81871340	3.67258575
C	6.07779193	-3.36909770	1.00387230	C	-7.04115115	-2.30462517	2.51862184
C	8.48600489	-2.48825336	0.13097713	C	-8.72210289	-0.61669420	1.22297634
C	2.29330338	2.27427740	1.87887277	C	-0.36181041	2.92990677	-1.20786760
Li	-1.42934519	0.31955413	-1.10429082	Li	2.04895612	-1.45304007	-0.01794470
N	0.03287757	1.48267322	2.44468554	N	1.78502847	2.53476951	-0.06829492
H	3.67404548	0.51859812	-6.66378688	H	-7.15441796	-1.51339434	-4.93010888
H	7.91677700	2.79231390	-5.04040039	H	-4.13166792	-4.91751083	-2.67600747
H	9.89920061	-1.51892176	1.26217993	H	-10.37721107	-1.16276082	0.13700185
H	5.34603236	-3.17906124	2.91385547	H	-7.20677571	-4.35011438	2.58983512
H	10.26459120	-2.61551924	-3.73193942	H	-8.63790571	3.61574343	0.78557142
H	2.90468585	-5.32920264	-1.03838412	H	-3.51759469	-1.53447231	4.78185091
H	7.33094482	3.89831575	-0.06246087	H	-5.13080417	3.14735909	-4.20178508
H	5.94171549	-4.95772008	-5.16180509	H	-4.39498507	3.37978830	3.63405170
O	3.64616952	3.39808784	3.77443713	O	-1.05274801	5.39979116	-1.56302932
C	2.14291718	3.13010342	6.04915875	C	1.09767970	6.89607108	-0.75937843
C	-0.43225583	2.07957365	5.12476449	C	2.76969753	5.02070255	0.72665743
C	-1.38289651	-0.18793228	6.68889340	C	5.62146188	5.36782883	0.28100678
H	3.13032440	1.80176404	7.31453085	H	2.05608712	7.61474965	-2.46748800
H	2.03115643	4.98534521	6.96941485	H	0.39115251	8.49561981	0.35278623
H	-1.90857038	3.56250562	5.23043005	H	2.43247253	5.23156889	2.78563388
H	0.10505234	-1.65080775	6.59829102	H	5.96095425	5.04289875	-1.75411923
C	-1.77163231	0.57083532	9.46176526	C	7.16127853	3.43927332	1.79320072
C	-3.81731855	-1.29577091	5.58602277	C	6.45090567	8.06933447	0.93918965
H	-5.35507254	0.10778069	5.63532805	H	6.57523935	1.50084725	1.34505455
H	-4.44100479	-2.95020704	6.67892936	H	9.19147173	3.61976672	1.38505706
H	-3.54137889	-1.88304120	3.61652473	H	8.49216160	8.30937663	0.63468122
H	-2.42181085	-1.04989588	10.58728574	H	5.47759484	9.49694933	-0.21523991
H	-3.21286781	2.06518662	9.62192973	H	6.90023398	3.73411165	3.83774788
H	-0.02572601	1.27743071	10.34039709	H	6.06172879	8.49441323	2.93984252
C	-6.16167443	-1.36570423	-3.55856362	N	3.37355141	-4.16607991	2.89337234
C	-5.56720031	1.32267457	-4.43236494	C	5.38465208	-5.57961059	1.57671665
N	-3.89611809	-2.76210014	-2.73036166	C	1.13407698	-5.76308899	3.30519113
N	-4.41485399	2.87334254	-2.42968833	C	4.28725589	-3.19196227	5.32446181
C	-2.36440942	-3.57686419	-4.90541150	C	4.88774111	-5.84065888	-1.25690292
C	-4.62167630	-4.97783688	-1.22839208	N	4.83837835	-3.38265822	-2.56500105
C	-6.26844708	3.63382940	-0.51649078	C	7.38853422	-2.34819838	-2.88856328
C	-3.18576605	5.11786493	-3.50972152	C	3.60579120	-3.62227153	-5.04501717
H	-3.45311962	-4.84551301	-6.17494988	H	1.59200235	-7.43631886	4.48644557
H	-1.68681997	-1.93544403	-5.96997420	H	0.34473654	-6.38249877	1.49377719
H	-0.68155143	-4.57536740	-4.22453368	H	-0.33882754	-4.65221689	4.24801172
H	-2.91665218	-5.94976480	-0.55402720	H	4.86014440	-4.72675910	6.63471018
H	-5.75940695	-6.35099980	-2.33375545	H	2.78453714	-2.09057130	6.23813819
H	-5.73475419	-4.38717098	0.42115153	H	5.91816599	-1.94453725	5.02137257
H	-7.13860173	1.97270657	0.36996671	H	8.58664262	-3.57926435	-4.09520028
H	-7.48712050	-1.30714514	-1.95749057	H	4.61611789	-4.97049298	-6.29541635
H	-7.15143974	-2.37859189	-5.10952439	H	5.63334488	-7.49104964	2.40850746

H	-7.32869637	2.20138425	-5.16686317	H	7.17558575	-4.56932929	1.88414573
H	-7.79593041	4.82381264	-1.32726393	H	3.03997796	-6.74126067	-1.56195882
H	-5.31155301	4.71761337	0.97080407	H	6.32952003	-7.12176355	-2.08991974
H	-4.54732929	6.35424828	-4.51918591	H	8.33518351	-2.11852247	-1.05764163
H	-2.30416726	6.21725654	-1.98718466	H	7.26623616	-0.47883592	-3.77942130
H	-4.22596953	1.26342170	-6.01820473	H	1.64296963	-4.23512491	-4.78041485
H	-1.68422850	4.52251005	-4.80993738	H	3.56888142	-1.76794796	-5.97513498

2.4. The coordinates and energies of starting materials and product of lithiation of (S)-2.

s-BuLi

(RI-DFT: BP86/def2-TZVP)



E = -165.38014452742 au

Imaginary frequencies: 0

C	-3.04250393	0.18985941	1.01197914
C	-1.23710354	-0.13219283	-1.24553551
C	1.26032642	-1.36664016	-0.42901850
C	3.09020057	0.38829674	0.98369066
Li	-0.58874184	3.16685920	-3.07984609
H	-4.93702883	0.81632652	0.41221710
H	2.24609589	-2.13659114	-2.09964985
H	-2.37434127	1.59537468	2.40150188
H	-3.31561859	-1.59588957	2.09258906
H	-2.16078241	-1.45195126	-2.58041780
H	2.19659040	1.22275824	2.66672357
H	4.80735783	-0.60267356	1.61867762
H	3.70789175	1.97078860	-0.23746633
H	0.90040246	-3.02354987	0.82346909

THF

(RI-DFT: BP-86/def2-TZVP)



E = -232.54810052377 au

Imaginary frequencies: 0

H	2.36347164	1.69076431	-2.33698140
H	3.91518289	-1.20455364	-1.52007459
H	2.28654706	-1.02927730	2.74136530
H	2.07789089	2.25651648	2.12815592
H	-2.43759647	1.88224784	2.10573641
H	-2.10470397	-1.39102601	2.73008780
H	-2.60168146	1.26593416	-2.35649208
H	-3.64417007	-1.84989706	-1.54284549
O	0.14158705	-1.57072800	-2.32643095
C	2.16789118	-0.11103005	-1.28681843
C	1.43597388	0.38924721	1.48920957
C	-1.49095024	0.14521050	1.47838343
C	-2.10944236	-0.47529816	-1.30140576

TMEDA

(RI-DFT: BP86/def2-TZVP)



E = -347.88026888527 au

Imaginary frequencies: 0

C	-1.12434284	0.71115266	-0.57348441
C	1.12434400	-0.71105992	0.57373162
N	3.54085461	0.02121289	-0.55914736
N	-3.54088608	-0.02136342	0.55917272
C	5.50506302	-1.83274959	-0.01467076
C	4.35458601	2.54122794	0.20667160
C	-5.50510595	1.83266145	0.01495292
C	-4.35455022	-2.54125020	-0.20714273
H	4.92569917	-3.70138910	-0.71253183
H	7.26157365	-1.29573534	-0.98632069
H	6.13751523	3.01327332	-0.74846419
H	2.95153401	3.96642007	-0.34318022
H	4.66623325	2.69885007	2.28358688
H	5.93302488	-2.00654901	2.03961505
H	0.89107610	-2.74944930	0.23793008
H	-4.92581105	3.70118336	0.71318595
H	-7.26164882	1.29543151	0.98642531
H	-5.93298063	2.00683112	-2.03931947
H	-6.13749635	-3.01351060	0.74785541
H	-4.66613685	-2.69848541	-2.28409605
H	-2.95148718	-3.96652031	0.34247622
H	1.11017908	-0.43474130	2.66044954
H	-1.11003311	0.43503698	-2.66022816
H	-0.89120393	2.74952214	-0.23746744

(S)-Fc-oxazol (2)

(RI-DFT: BP86/def2-TZVP)



E = -2015.42769707072 au

Imaginary frequencies: 0

Fe	-2.65233547	2.62516963	-2.82469399
C	-4.14543353	-0.80636312	-1.81954942
C	0.09672147	1.92912779	-5.47749355
C	-1.11111034	-0.55166198	1.98024777
N	-0.09826682	-2.74992824	1.82180546
H	-7.20563798	0.37838601	-4.51014374
H	-7.47439569	4.62055333	-1.65354754
H	0.64375412	0.07408868	-6.16511915
H	-3.02736437	3.06335112	-8.13394815
H	2.63015800	2.47643997	-2.11109804
H	-3.29421372	7.31819104	-5.29411344
H	-3.98752970	4.22897142	2.09411403
H	-3.54925161	-2.64117934	-2.51565370
H	0.21229650	6.95887994	-1.57211913
O	-0.33271183	1.02737544	3.89976546
C	1.74413015	-0.29582504	5.12020847
C	1.71889470	-2.97287391	3.92147930
C	4.33241328	-3.92110554	3.05714037
C	4.12181082	-6.46046649	1.68271604
C	6.15449361	-4.10272922	5.30625367
H	5.45379752	-5.46879549	6.71257579
H	3.49935535	0.74584917	4.70017066
H	1.40771373	-0.26574528	7.16583685
H	0.95875456	-4.37936404	5.27185886
H	5.07453800	-2.50402001	1.71262263
H	2.81341933	-6.33121237	0.08011904
H	5.97937785	-7.07651852	0.98240365
H	3.41162184	-7.93575691	2.96900367
H	8.02915800	-4.74884867	4.68616493
H	6.41184704	-2.27726231	6.26792613
C	-6.07277316	0.78431361	-2.84672637
C	-6.21428573	3.03104251	-1.33599030
C	-4.37299166	2.84096591	0.63408857
C	-3.09621498	0.44954426	0.35473303
C	1.15407093	3.20623878	-3.33714178
C	-0.13247577	5.57184860	-3.04560224
C	-1.98735585	5.75998046	-5.01229548
C	-1.84620912	3.50872758	-6.51478431

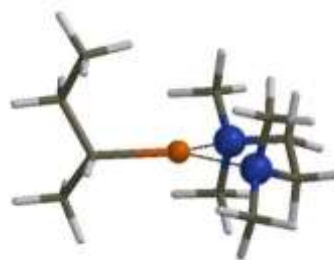
s-BuLi...2THF
(RI-DFT: BP86/def2-TZVP)



E = -630.52146284901 au
Imaginary frequencies: 0

Li	-0.47121933	0.44826862	-0.25523057
C	3.37858619	1.39438139	-0.14332663
C	5.01763317	0.02014286	1.80775257
C	4.09009646	0.29523240	4.53737539
H	5.12529379	-2.02377928	1.34752924
C	0.15903773	-4.81247746	-1.33997506
H	-5.60795426	-4.02096602	-0.24548878
H	-3.91390907	-3.38858413	2.61047491
C	4.62119983	1.21254654	-2.76365485
H	5.33447423	-0.66642238	5.90265597
H	6.65002653	1.79441260	-2.79589514
H	3.65001792	2.39051129	-4.18578574
H	4.60008304	-0.74083408	-3.51570404
O	-1.82391383	-3.01071314	-0.69501648
C	-3.79470546	-4.28690151	0.73637915
C	-3.00208870	-7.06867774	0.91439523
C	-0.11895443	-6.93876019	0.57977287
H	-3.57956628	-7.93062244	2.71063520
H	-3.85698488	-8.17025361	-0.62712284
H	0.70058049	-8.72377082	-0.08721535
H	0.81142338	-6.41943457	2.36393610
H	-0.15525469	-5.48843650	-3.28822899
H	1.95969335	-3.78488618	-1.24496427
O	-3.27205576	2.94178225	-0.16807862
C	-2.52760438	5.42145957	0.76828968
H	7.03013327	0.66385691	1.74664732
H	2.16885981	-0.48520119	4.76257074
H	3.99833737	2.30374425	5.08138858
H	3.45239275	3.43102493	0.39300713
C	-3.36638993	7.26658057	-1.27534330
C	-5.85456890	6.06682458	-2.17634503
C	-5.29939686	3.22688600	-2.00514683
H	-0.47863873	5.35232295	1.08826923
H	-3.50470433	5.78119294	2.57634050
H	-3.61233758	9.19590255	-0.55401642
H	-1.96848808	7.31657713	-2.81239519
H	-6.39237149	6.64197602	-4.09531927
H	-7.40772444	6.58442901	-0.89576305

s-BuLi...TMEDA
(RI-DFT: BP86/def2-TZVP)



E = -513.30297277634 au
Imaginary frequencies: 0

Li	0.58004535	0.38817264	-0.30099376
C	4.31455424	1.41538554	-0.91009776
C	6.18337167	0.70234842	1.18298542
C	5.50756504	1.76402869	3.79126668
H	6.32846130	-1.38201775	1.33176489
H	8.15016816	1.33204051	0.73090104
H	3.66670371	1.03244524	4.44850853
H	5.34980769	3.83987205	3.72171016
C	-4.07453731	-2.39278359	0.34639148
C	-4.86502482	0.25934770	-0.49549432
N	-1.52682059	-3.06893606	-0.55813634
N	-3.01370513	2.20145878	0.26041943
C	-1.51531015	-3.69305150	-3.26675392
C	-0.46267533	-5.17857779	0.90126338
C	-3.18070046	2.79379737	2.97010523
C	-3.31827388	4.52308713	-1.23383881
H	-2.68508586	-5.38261155	-3.68244852
H	-2.24109881	-2.10600028	-4.38883231
H	0.43195025	-4.05793140	-3.87958852
H	1.47491265	-5.54802721	0.26082492
H	-1.58371203	-6.93675188	0.68690081
H	2.86010399	5.75865816	-7.02036048
H	-0.39438124	-4.67999233	2.91474886
H	-2.88709598	1.08818161	4.11422111
H	-4.04727364	-2.49234035	2.42274063
H	-5.51915258	-3.77324117	-0.29425393
H	-6.77857138	0.67576034	0.25771017
H	-5.04315931	3.61348125	3.47593440
H	-1.69561728	4.15289852	3.46955480
H	-5.18597542	5.42409452	-0.92713031
H	-1.83528995	5.87519000	-0.71043677
H	-5.02361622	0.32048523	-2.56730608
H	-3.11384697	4.09306227	-3.25375700
H	4.35833406	3.51441464	-1.04047182
C	5.28071045	0.41547593	-3.46167110
H	6.93010102	1.29068057	5.23700163
H	7.26977637	0.96875435	-3.90354144
H	4.12300085	1.07837977	-5.06668563

H -4.63618045 2.44972987 -3.81857173
H -6.93775720 2.11797478 -1.36590999

H 5.26277484 -1.67562744 -3.54349613

3. THEORETICAL CALCULATION OF LITHIATION OF (S)-3.

3.1. The coordinates and energie of complexes C7-8.

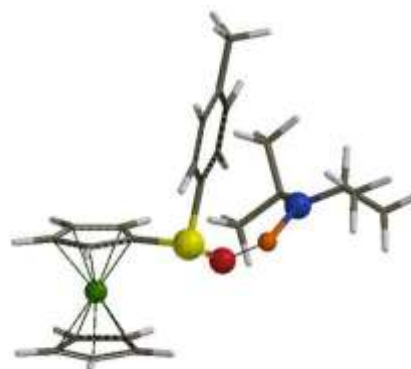
(S)- Fc-sulfoxid...LDA (C7a)
(RI-DFT: BP-86/def2-TZVP)



E = -2694.68047128002 au
Imaginary frequencies: 0

Fe	-0.51764671	-7.03510495	-2.07400883
C	-1.35830336	-3.94490735	0.10759247
C	-3.24099561	-5.85221457	0.44612218
C	-4.35620489	-6.40181436	-1.96011493
C	-3.16647449	-4.84922131	-3.82273839
C	-1.31385436	-3.30958804	-2.53990040
C	2.91163504	-7.87012159	-3.73314662
C	0.96193894	-9.44517476	-4.75192975
C	-0.13041767	-10.84460873	-2.70678425
C	1.14499508	-10.12872038	-0.42531963
C	3.02410719	-8.28401821	-1.05884148
S	0.41145653	-0.94086109	-4.20963072
H	-5.81885174	-7.79701456	-2.31885753
H	-3.71263285	-6.76193367	2.22520789
H	0.73278334	-10.83333756	1.45820450
H	4.28866400	-7.34249978	0.25510270
H	4.08041414	-6.56656838	-4.80274520
H	0.39279256	-9.54038033	-6.72180919
H	-1.67692575	-12.18664533	-2.85357123
C	2.89206782	-0.27225662	-1.97043895
C	6.93604013	0.86999849	1.26926654
C	5.32880830	-1.09377922	-2.57104076
C	2.45089837	1.17439563	0.20166887
C	4.47679124	1.72328619	1.79498502
C	7.32796918	-0.54099689	-0.94155900
H	9.22889563	-1.19199335	-1.41110664
H	4.12967279	2.85712331	3.48423065
H	0.57857961	1.95853826	0.63606736
C	9.10176019	1.52568904	2.99736177
H	5.66789407	-2.14513886	-4.31285174

(S)- Fc-sulfoxid...LDA (C7b)
(RI-DFT: BP-86/def2-TZVP)



E = -2694.68178622841 au
Imaginary frequencies: 0

Fe	6.19014629	0.35405678	0.18538848
C	4.81716905	3.94923129	0.27613455
C	6.17811636	3.43890128	2.55744052
C	5.03284657	1.30764887	3.77658440
C	2.93919608	0.47771235	2.27851695
C	2.79921924	2.12254703	0.11874421
C	6.53780705	-1.75983436	-3.07210578
C	6.67185828	-3.35498750	-0.89057270
C	8.75863560	-2.52639424	0.62431588
C	9.91108239	-0.41362444	-0.62042871
C	8.53503670	0.06172879	-2.90538241
S	0.58660856	2.04897740	-2.41676067
H	5.67394663	0.43215557	5.51964657
H	7.83167580	4.46017943	3.21902726
H	11.52409275	0.65697578	0.06271277
H	8.92315053	1.55508892	-4.25950962
H	5.12353588	-1.87839074	-4.55483820
H	5.38899474	-4.89321879	-0.44371954
H	9.34214706	-3.33503447	2.41865092
H	5.21232892	5.43430622	-1.08480311
C	-2.03132040	3.65338154	-0.92868710
C	-6.05937849	6.33338102	1.23653344
C	-3.67708380	2.41170463	0.72773725
C	-2.39367410	6.19414608	-1.54534942
C	-4.39027013	7.52244114	-0.44484324
C	-5.67440897	3.76243613	1.78507854
H	-6.96824959	2.78775094	3.06368316
H	-4.67014616	9.51029599	-0.92131776
H	-1.12766720	7.13094723	-2.87863113
C	-8.24299867	7.74859241	2.39215901

H	-3.58482483	-4.80121189	-5.83202475
O	-1.30298462	1.37432636	-4.31888751
H	9.71485881	3.49232814	2.69909178
H	8.55457801	1.35624794	4.99348704
H	10.74237543	0.30063785	2.66305296
Li	-2.72342712	3.80453687	-2.18351516
N	-3.14411969	5.52369162	0.80741800
C	-2.03567580	8.00695281	1.17771490
C	-4.79287194	4.70118898	2.83804475
H	-1.06492574	8.16535102	3.04854609
H	-6.18396760	6.19545036	3.36783126
C	-3.96544867	10.20176452	1.07912585
C	0.00237571	8.46030778	-0.83452050
C	-6.35360972	2.42390728	1.95457258
C	-3.37927948	4.00813329	5.30432777
H	-3.05671575	12.04088160	1.44710700
H	-5.47088565	9.95775639	2.49011497
H	-4.86187106	10.26839587	-0.79985833
H	0.91034162	10.31839533	-0.61730253
H	-0.84540060	8.41433256	-2.74405655
H	1.48174548	7.00068574	-0.74209640
H	-2.14573127	2.35971988	4.98170550
H	-5.09309933	0.85252275	1.40517957
H	-7.61527047	1.71253882	3.44769089
H	-7.52094368	2.93051697	0.30756896
H	-4.69620974	3.54503637	6.85244421
H	-2.18413411	5.58161486	5.94936113
H	-0.16640410	-3.12992057	1.56279263

H	-3.47410647	0.39657857	1.14711074
H	1.70410780	-1.11376187	2.66764955
O	-0.19169076	-0.69754152	-2.77630604
H	-8.11445417	9.78449906	2.01704879
H	-10.05558834	7.07417897	1.62476167
H	-8.31531275	7.47124944	4.45027297
N	-5.01213234	-4.90038523	-0.23429818
C	-7.59048955	-4.99038606	-1.17018879
C	-4.57971388	-6.37043522	2.03610112
C	-5.76035310	-5.20152393	4.44389626
C	-1.73053984	-6.71772555	2.43713903
C	-7.93556154	-2.97914134	-3.23032897
H	-9.86851959	-2.97002616	-3.99634732
H	-7.52268163	-1.07827373	-2.49111757
H	-6.64866210	-3.35943534	-4.83340106
H	-0.87778596	-7.70519013	0.81659762
H	-0.80861270	-4.85225686	2.62550212
H	-1.30431804	-7.79668402	4.16351371
H	-4.85803093	-3.37019693	4.86156285
H	-7.79511223	-4.86374699	4.18956763
H	-5.53209823	-6.44016071	6.10497348
Li	-2.60151868	-3.14475425	-2.00476282
H	-5.38775115	-8.31222253	1.87410621
C	-8.37325940	-7.59433158	-2.24522819
H	-10.36719089	-7.60914708	-2.85147588
H	-8.14020755	-9.10043964	-0.83308860
H	-7.17746843	-8.06967345	-3.88291995
H	-8.99193772	-4.53283246	0.34301986

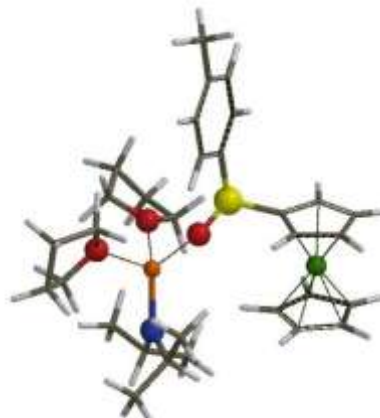
(S)- Fc-sulfoxid...LDA...2THF (C7a)
(RI-DFT: BP-86/def2-TZVP)



E = -3159.78535276285 au
Imaginary frequencies: 0

Fe	5.30855360	4.07678028	-0.75051762
C	2.26873757	3.64554671	1.63651013
C	3.77554482	5.75953009	2.39763051
C	6.29457444	4.90074319	2.90881381

(S)- Fc-sulfoxid...LDA...2THF (C7b)
(RI-DFT: BP-86/def2-TZVP)



E = -3159.78780875342 au
Imaginary frequencies: 0

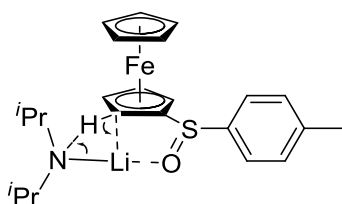
Fe	5.01122242	4.34142441	-0.34447426
C	2.54248582	5.97312451	-2.80413215
C	4.04482338	7.88498135	-1.61650645
C	3.67927705	7.71341430	1.06331689

C	6.38926659	2.23206140	2.46178025	C	1.93703516	5.70574124	1.56969772
C	3.89782565	1.46118830	1.66729752	C	1.22316024	4.63860052	-0.82686483
C	5.14164412	2.76641214	-4.42370926	C	7.04903738	1.64224318	-2.27021322
C	7.71569698	3.12331749	-3.65849670	C	5.96712063	0.55710208	-0.03690892
C	8.02530138	5.72744282	-2.97811304	C	6.89725486	1.94351828	2.08900490
C	5.63923075	6.96857689	-3.31721271	C	8.55435366	3.88223797	1.17942911
C	3.85621273	5.13591938	-4.20658004	C	8.65057384	3.69673804	-1.52226709
S	2.64786706	-1.68946232	1.58245218	S	-0.98326545	2.15898639	-1.43822352
H	7.88265290	6.07592089	3.47076106	H	4.61382670	8.87163539	2.47840915
H	3.12403281	7.70443306	2.49724750	H	5.29470225	9.19848694	-2.58012057
H	5.23915030	8.94320932	-2.92271354	H	9.53702003	5.27122188	2.32882915
H	1.86315304	5.46485011	-4.57672535	H	9.72299577	4.91589345	-2.77930808
H	4.29079170	0.99770560	-5.01668716	H	6.70416457	1.02548191	-4.19780383
H	9.16551542	1.67212382	-3.58232343	H	4.65190472	-1.02771679	0.05303042
H	9.75333058	6.60006629	-2.29344185	H	6.39215905	1.59939556	4.04772487
C	5.22755092	-3.37325094	0.09569126	H	2.41045219	5.59084449	-4.81697070
C	9.09267184	-6.22362577	-2.15757059	C	-3.84998010	4.03082922	-1.17374988
C	7.25435076	-4.21792437	1.56205515	C	-8.31941324	6.87010696	-0.83057591
C	5.06977253	-3.98919447	-2.46103794	C	-5.14737785	4.14682536	1.11792828
C	7.00241220	-5.39988211	-3.56931418	C	-4.77558115	5.27709657	-3.30790728
C	9.18365702	-5.60905745	0.42191188	C	-6.99295120	6.69247088	-3.12148650
H	10.77884246	-6.25167967	1.56305966	C	-7.36411687	5.56558794	1.27411427
H	6.88483240	-5.87540855	-5.57463528	H	-8.38264235	5.65576385	3.06760037
H	3.42129882	-3.38087707	-3.53855379	H	-7.71875072	7.66282863	-4.79229836
C	11.14131800	-7.79632525	-3.35936118	H	-3.77781057	5.14189703	-5.10919150
H	7.32734956	-3.80505912	3.58249477	C	-10.68520418	8.44344959	-0.62745169
H	8.03522550	1.02181386	2.65531331	H	-4.42061121	3.10410424	2.74070365
O	0.46474697	-1.71793844	-0.27000298	H	1.29320926	5.06016440	3.40685251
H	10.69214535	-9.82535410	-3.23138147	O	-0.98204264	0.39773863	0.81935694
H	11.36410645	-7.34144438	-5.37218259	H	-11.68949022	8.54619724	-2.44108250
H	12.97002692	-7.50960512	-2.42045429	H	-11.98822128	7.67781116	0.79541447
Li	-3.15328641	-0.30557059	0.70407290	H	-10.23122581	10.39515974	-0.06124959
N	-4.21732807	3.12401919	-0.17059145	N	2.18715238	-5.56097119	1.99045974
C	-3.84150402	4.09870089	-2.71283196	C	3.50812629	-7.54486048	0.62142882
C	-5.56807680	4.87316645	1.46496930	C	3.48131353	-4.85848709	4.31080538
H	-2.50991430	5.75607689	-2.74504402	C	1.67892617	-9.02799703	-1.07387909
H	-7.47710942	5.34920385	0.69221872	C	2.24401983	-2.51100003	5.47926239
C	-6.25505664	5.04881867	-4.06945998	C	5.75999939	-6.57927506	-0.98388613
C	-2.61106162	2.07137280	-4.38090874	H	0.23195096	-9.98728699	0.06915789
C	-6.04798684	3.65581178	4.04634762	H	0.69850897	-7.73453675	-2.37815975
C	-4.23906303	7.44760487	1.88982033	H	2.66819406	-10.46206222	-2.21423060
H	-5.81544783	5.68204197	-6.00459596	H	6.85383709	-8.13935327	-1.83518600
H	-7.14221146	6.64497353	-3.07961539	H	5.07036299	-5.35408548	-2.52325507
H	-7.66460983	3.51742968	-4.18845144	H	7.06647343	-5.45620367	0.17937737
H	-2.15423905	2.81498631	-6.27104974	H	2.21789468	-0.91618211	4.14863475
H	-3.91521860	0.46475644	-4.63351520	H	0.26471658	-2.93169641	5.98645597
H	-0.86814152	1.34194645	-3.51694239	H	3.22186546	-1.91703656	7.21798145
H	-2.42019847	7.16593757	2.86602679	Li	-0.64447343	-3.55602753	0.71745315
H	-4.24051662	3.32191836	5.02354931	H	4.33635998	-8.96636078	1.93701517
H	-7.21396609	4.87798769	5.26176033	C	-0.41350770	-3.56043696	-5.47212487
H	-7.01890486	1.82716390	3.84047122	C	-4.32127554	-5.04009116	-3.85153791
H	-5.40715467	8.72286101	3.05280309	C	-4.48682081	-5.00887079	-6.73368517
H	-3.85268601	8.41930250	0.09318897	C	-1.69010991	-5.18192763	-7.49375121
C	-2.14183578	-1.09967286	6.97826456	O	-1.96773202	-3.78294355	-3.22265924
C	-1.27828854	-3.37001914	8.53974302	H	-1.31479575	-4.49184109	-9.41417820

C	-2.91976262	-5.50084155	7.44942983	H	-5.63581513	-6.56906553	-7.47600051
C	-2.98339675	-4.82529305	4.64243805	H	-5.31480836	-3.22099051	-7.39961894
O	-2.82620685	-2.09218835	4.51620498	H	-5.86285945	-4.02447326	-2.90457990
H	-3.81415701	-0.18408760	7.81927223	H	-1.02690175	-7.14800304	-7.37054611
H	-1.55060205	-3.07813766	10.57579823	H	1.50814607	-4.18878208	-4.99602443
H	-4.83271390	-5.43061198	8.26180712	H	-0.34379373	-1.55066433	-6.02532095
H	-4.71904690	-5.40847883	3.66736376	H	-4.25899424	-6.98853250	-3.11284439
H	-1.34961392	-5.63299084	3.62605266	C	-3.99159577	-7.08910414	3.58565140
H	-0.66735628	0.33895740	6.71359224	O	-4.10443566	-4.61237577	2.38502492
H	0.73553930	-3.76237400	8.20227347	C	-5.73454707	-2.95704835	3.83342041
H	-2.14320842	-7.39467677	7.79037577	C	-7.04124811	-4.62773828	5.79954601
C	-8.11367054	-2.26183535	-1.09568415	C	-5.06951611	-6.71528743	6.23261597
C	-8.86405916	-3.21379289	-3.71303732	H	-3.58207229	-6.05671222	7.52797952
C	-7.37958165	-5.70218242	-3.91320623	H	-7.52538446	-3.57993201	7.52477125
C	-4.90468069	-5.04152671	-2.57372005	H	-8.79388511	-5.43625816	5.02429932
O	-5.54507463	-3.16710650	-0.68180726	H	-7.05852083	-2.02744962	2.52727090
H	-8.04378264	-0.18974307	-0.92051996	H	-5.88184140	-8.45810069	7.01254662
H	-8.23729063	-1.87378611	-5.17373401	H	-1.99147021	-7.66613678	3.53359301
H	-7.07352230	-6.32132547	-5.87039248	H	-5.15196866	-8.41964932	2.47114164
H	-3.51411521	-4.21494994	-3.88688790	H	-4.55610551	-1.49158354	4.73195891
H	-4.02189176	-6.66138463	-1.61557057	C	3.54263498	-6.95275147	6.36224555
H	-9.34143208	-3.05885248	0.39141153	H	4.38623867	-8.71335666	5.65242614
H	-8.37436716	-7.22474906	-2.90391281	H	4.65392151	-6.35875566	8.02348116
H	-10.91436802	-3.46775140	-3.90549322	H	1.60440433	-7.38550843	6.99279746
H	0.26277943	3.64922897	1.09571309	H	5.51174372	-4.34898813	3.96632089

3.2. The coordinates and energie of transition states TS7-8.

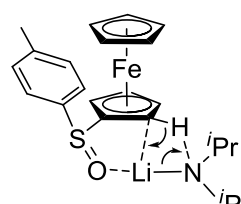
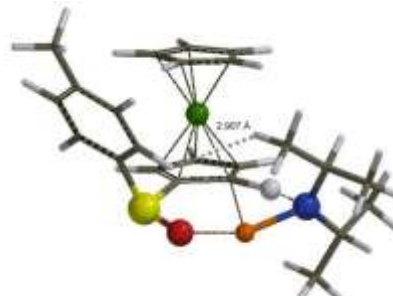
(S,S_p)-TS7 (preferred)
(RI-DFT: BP-86/def2-TZVP)



E = -2694.65817799206
Imaginary frequencies:1 (-1075.15 cm⁻¹)

Fe	0.19561571	-3.63676521	-1.02238353
C	-2.22536029	-1.30807238	-2.91734976
C	-0.47648382	-2.43711033	-4.64062428
C	2.03197500	-1.72514666	-3.86679228
C	1.98372766	-0.15232458	-1.64246931
C	-0.70035948	0.07991735	-1.12584564
C	-1.90146555	-6.39886600	0.75468553
C	-0.38768799	-5.05905828	2.56009229
C	2.21021150	-5.32466833	1.84647487
C	2.30422302	-6.82756375	-0.40579917
C	-0.23590208	-7.49532776	-1.07783863
S	-1.65584139	1.90470919	1.54030240
H	3.74864227	-2.36209777	-4.80802372
H	-0.97363574	-3.65610012	-6.22019925
H	4.00045823	-7.34335412	-1.44074975
H	-0.80021020	-8.60551123	-2.71016302
H	-3.94961112	-6.54414471	0.75892309
H	-1.07889473	-4.00683520	4.18297673
H	3.81762473	-4.48539624	2.80639364
H	-4.27184871	-1.46001538	-2.95500333
C	-5.03507194	1.96063503	1.09383544
C	-10.30756077	2.10191796	0.54755300
C	-6.51059571	0.05204533	2.16647757
C	-6.15457551	3.95867589	-0.21071141
C	-8.77695122	4.01142238	-0.47774870
C	-9.12961946	0.12435134	1.86684763
H	-10.28315641	-1.37557018	2.69078191
H	-9.65600466	5.57094618	-1.50534506

(S,R_p)-TS7 (non-preferred)
(RI-DFT: BP-86/def2-TZVP)



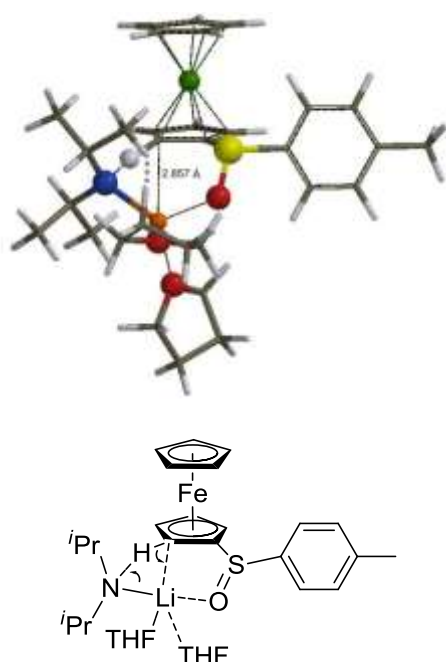
E = -2694.65557330048
Imaginary frequencies:1 (-1238.50 cm⁻¹)

Fe	0.30327400	-3.42836604	0.66880520
C	-2.39726683	-1.17863742	-1.19553744
C	-3.18742082	-3.77573566	-0.97653591
C	-1.40576931	-5.46331938	-2.13640308
C	0.59695140	-3.95963888	-3.14655754
C	-0.01683237	-1.36350502	-2.55585068
C	2.92458507	-1.90541380	3.14402633
C	3.70224685	-4.36790222	2.32955208
C	1.76875446	-6.12949632	3.03348802
C	-0.20667041	-4.74970774	4.27425863
C	0.51288633	-2.13922393	4.34651749
S	1.54727820	1.21264675	-4.14441376
H	-1.51631765	-7.51502143	-2.19570924
H	-4.88469250	-4.39167814	0.01125458
H	-1.95757721	-5.53871408	4.99987176
H	-0.59807642	-0.60786750	5.13995437
H	3.96818314	-0.16037104	2.86707381
H	5.44319185	-4.81825050	1.33952787
H	1.77742097	-8.14811665	2.65789537
H	-4.09841242	0.70645616	-0.27968639
C	4.25844682	1.93359508	-2.19502109
C	8.60124740	3.13814675	0.60191224
C	6.41690736	0.42894094	-2.41949668
C	4.25835964	4.06505098	-0.64977727
C	6.42441326	4.64559938	0.74246983
C	8.56061887	1.02822960	-1.00985555
H	10.24687489	-0.14897774	-1.18340040
H	6.42554705	6.31588588	1.95483463

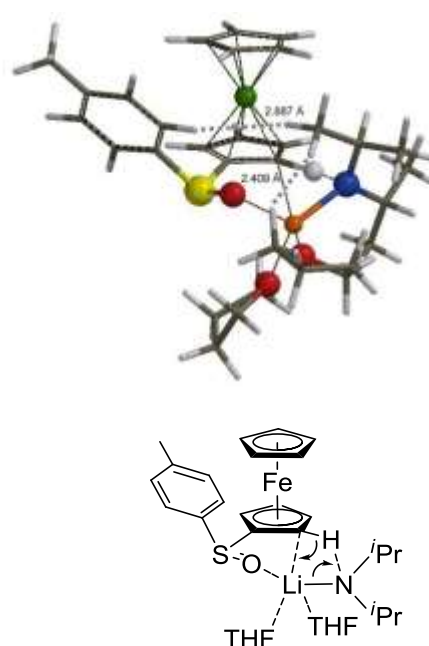
H	-4.96460294	5.45327759	-0.98343857
C	-13.14324527	2.21040248	0.30206457
H	-5.62394760	-1.48348131	3.21851827
H	4.08059853	1.43141270	-0.83436207
O	-0.76428587	4.63063866	0.99049541
H	-13.97791931	0.31013379	0.27874059
H	-13.98842751	3.23679170	1.90436967
H	-13.71734445	3.19571348	-1.43218202
Li	2.58544900	4.99333520	0.11857627
N	5.71279010	3.11077738	-0.05544688
C	7.51062024	3.73272289	-2.07383374
C	6.67493130	1.90822782	2.26848139
H	8.58738925	2.02940521	-2.66383896
H	5.03847521	0.79563323	2.97008682
C	9.46366044	5.76795662	-1.36808429
C	6.00136582	4.61811517	-4.39011807
C	8.82003537	-0.01385077	1.86404133
C	7.34732660	3.78116661	4.39325875
H	10.65448259	6.24361661	-3.00855862
H	10.72392610	5.14777584	0.15846200
H	8.50539617	7.50592188	-0.73643234
H	7.25137120	4.95030398	-6.01624477
H	5.03491790	6.42791939	-3.99441624
H	4.57141357	3.21975046	-4.94897879
H	9.02535557	4.91488357	3.93152771
H	10.59256506	0.89744165	1.27210585
H	9.21258444	-1.03370507	3.63279963
H	8.30217326	-1.41440481	0.41990690
H	7.73358090	2.77390240	6.17468507
H	5.77324914	5.09558612	4.74093867

H	6.43332601	-1.19545767	-3.69098462
H	2.24001811	-4.64063997	-4.17787036
H	2.58187881	5.25898112	-0.56513995
C	10.91480030	3.74914878	2.14641061
O	-0.18823680	3.51771865	-3.91195639
H	12.65929363	3.33404617	1.09953448
H	10.94999897	5.74766583	2.70259132
H	10.96132636	2.61554480	3.89194716
Li	-3.30277193	3.42035431	-2.37078598
N	-5.74703219	2.64063829	0.19901072
C	-5.40997942	3.56987282	2.78767970
C	-8.33681074	1.91431587	-0.48393086
H	-5.72334172	2.03138150	4.19150330
H	-9.61579507	3.54984944	-0.20295193
C	-7.20378245	5.74030239	3.50859963
C	-2.66483566	4.44968099	3.10063652
C	-8.43153062	1.26710559	-3.31041554
C	-9.43298359	-0.28056725	1.08911714
H	-6.74923289	6.45569306	5.40844308
H	-9.19486517	5.15193612	3.52857658
H	-7.01258520	7.31322060	2.15695070
H	-2.25527376	4.96219466	5.07345428
H	-2.30998146	6.13942596	1.92968378
H	-1.33043466	2.96200202	2.53201492
H	-8.34501940	-2.02628125	0.78484446
H	-7.18231280	-0.33548363	-3.75726912
H	-10.35533833	0.74806795	-3.90014019
H	-7.85241081	2.90036075	-4.46867431
H	-11.41115023	-0.65685711	0.56573983
H	-9.39459155	0.14529430	3.12236108

(S,S_p)-TS8 (preferred)
(RI-DFT: BP-86/def2-TZVP)



(S,R_p)-TS8 (non-preferred)
(RI-DFT: BP-86/def2-TZVP)



E = -3159.77609751968 au

Imaginary frequencies: 1 (-1151.83 cm⁻¹)

Fe	-5.39011748	-3.42621470	-0.36155577
C	-4.97534045	-0.29252543	-2.57434609
C	-5.10693922	-2.51475211	-4.10810450
C	-3.05259244	-4.14741012	-3.38323605
C	-1.56709616	-3.05078949	-1.38302032
C	-2.81209159	-0.65101265	-0.94442018
C	-6.58037353	-3.45690576	3.35586186
C	-5.41653714	-5.81648379	2.71727953
C	-6.79844086	-6.89151896	0.64984942
C	-8.82265839	-5.20116351	0.02096061
S	-1.51608067	1.35482989	1.42709902
C	-8.68643040	-3.07485233	1.69242467
H	-2.72142259	-6.00692835	-4.20278088
H	-6.54660413	-2.90547332	-5.52435324
H	-10.19519977	-5.46825360	-1.48259047
H	-9.95160351	-1.45732146	1.68423228
H	-5.95899384	-2.18611045	4.84544628
H	-3.75492653	-6.62321380	3.61001081
H	-6.36808472	-8.66223031	-0.29568270
H	-6.24520432	1.31960587	-2.62567495
C	-3.62802936	4.03909649	1.21565508
C	-6.77661032	8.31882909	1.10554635
C	-6.02394627	3.93736754	2.33074087
C	-2.77387382	6.26368504	0.09704678
C	-4.35255818	8.38061825	0.04100645
C	-7.58009616	6.06082868	2.25212511
H	-9.45454563	5.97014026	3.11264986
H	-3.68100838	10.12065237	-0.84411749
H	-0.87316643	6.31435858	-0.69816144
C	-8.47470091	10.60619091	1.05352374
H	-6.67275415	2.20479011	3.23798836
H	0.97302136	-3.59382553	-0.66359226
O	1.03422365	2.31401584	0.43099649
H	-8.93623374	11.24792603	2.97755619
H	-7.58097578	12.18859134	0.05312335
H	-10.27700880	10.18630303	0.10475426
Li	4.02408735	0.11110009	-0.22113676
N	3.46101087	-3.79333827	-0.22714308
C	4.53730141	-5.24177820	-2.34556035
C	3.68933177	-5.10911636	2.22060264
C	7.39222647	-5.73615618	-2.08535485
C	2.54255353	-7.79398802	2.27513949
H	8.11548259	-6.78424032	-3.73206873
H	7.84923135	-6.84930374	-0.39155565
H	8.42839448	-3.93249932	-1.96157582
H	3.52323804	-9.09515061	0.98736997
H	2.66913386	-8.60396427	4.18761309
H	0.54054195	-7.73327917	1.71850686
O	5.41314938	2.25994110	-3.25165315
C	3.75840331	3.44135406	-5.08282086
C	5.28198528	5.64670457	-6.13833044
C	7.95830863	4.51755827	-6.23252417

E = -3159.76896639066 au

Imaginary frequencies: 1 (-1187.17 cm⁻¹)

Fe	4.53375113	3.33201285	-0.38730859
C	0.69011794	3.20124119	0.70641499
C	1.93829688	5.47380948	1.54392462
C	4.09353515	4.91546113	3.10383356
C	4.28885622	2.22325154	3.28553933
C	2.21824332	1.21400866	1.80843157
C	5.82964730	1.31311871	-3.47475067
C	7.89042270	2.01151460	-1.86177881
C	7.92204247	4.71408058	-1.67473512
C	5.87293475	5.67940945	-3.16468839
C	4.58225776	3.57496265	-4.27975806
S	1.11123470	-1.98173088	2.11181714
H	5.39705856	6.27059509	3.93757649
H	1.38070054	7.38062930	1.00180037
H	5.36488293	7.65698458	-3.38080197
H	2.91766725	3.67800549	-5.47510410
H	5.29194324	-0.60348262	-3.97006205
H	9.18291348	0.71862562	-0.92742524
H	9.24020409	5.83342503	-0.56709616
H	-1.56390259	3.14021494	-0.83617404
C	3.81130716	-3.84233477	1.13962982
C	7.86721012	-6.95618058	-0.28473793
C	5.74798824	-4.33992381	2.86233119
C	3.83605132	-4.93697979	-1.25757571
C	5.85896170	-6.47956156	-1.95215395
C	7.77021579	-5.86838951	2.13253646
H	9.28786685	-6.24985203	3.47853110
H	5.87497041	-7.34169818	-3.82800427
H	2.25621511	-4.58597094	-2.53436346
C	10.07404988	-8.57468869	-1.07590062
H	5.67413072	-3.56384755	4.77239888
H	5.72855809	1.17482887	4.31150888
O	-0.90263650	-2.42856306	0.10458899
H	10.97112837	-9.49011285	0.55676778
H	9.49214478	-10.05301275	-2.41219143
H	11.53250235	-7.42899279	-2.02235179
Li	-3.98477858	-0.26970897	-0.07773017
N	-3.72674512	3.02710470	-2.14573700
C	-3.05498472	2.83463121	-4.83856930
C	-5.24099641	5.29131104	-1.56536027
H	-1.73620130	4.38656668	-5.38220380
H	-7.05783322	5.20792587	-2.61271161
C	-5.31562583	3.01553900	-6.66162059
H	-2.20982210	8.09566003	-1.25850147
H	-4.20776934	5.50177572	2.41407478
H	-7.14857090	6.95759702	1.68612595
H	-6.92017888	3.60214710	1.80735000
H	-5.24794088	9.42189155	-1.84322493
H	-3.56076689	7.93017211	-4.32591654
C	-3.93759789	1.14532462	5.96979323
C	-3.40547659	-0.62948928	8.18049148
C	-5.42187209	-2.68214586	7.79932185

C	8.02213708	2.80194936	-3.89111687	C	-1.64682899	0.35355484	-5.33187660
H	3.27888541	2.06520409	-6.57805982	C	-5.92089452	5.33713433	1.24846436
H	2.02610054	3.96643891	-4.07409671	C	-3.99074372	7.82658948	-2.29641751
H	5.20852613	7.26557574	-4.83533137	H	-4.68031642	2.75094035	-8.62548307
H	9.45566528	5.95281204	-6.19445222	H	-6.28575575	4.84878530	-6.56522675
H	8.89279877	3.73301534	-2.24637501	H	-6.71226194	1.52994446	-6.23442313
H	9.02261461	1.01070992	-4.23766677	H	-0.93676166	0.28615763	-7.28656171
H	8.19881547	3.39344021	-7.96371486	H	-2.91926897	-1.27330674	-5.06036752
H	4.60098183	6.27418951	-7.99505486	H	-0.04821012	0.12693417	-4.03256705
O	6.72979779	1.47869483	2.31028752	C	-5.49483113	-2.92828711	4.92112214
C	8.64526642	0.06249947	3.65450350	O	-4.83913259	-0.45694779	3.92604177
C	8.71924619	1.20489932	6.29984577	H	-5.42684897	2.52647466	6.44019931
C	8.22610039	4.01309392	5.74297622	H	-3.54551149	0.32952239	10.01497903
C	6.34524031	3.90905903	3.54131940	H	-7.36168928	-3.45119889	4.17724297
H	8.09878970	-1.93811329	3.60273908	H	-7.26052801	-2.03700105	8.52610157
H	10.48034054	0.28431827	2.68159937	H	-4.09236648	-4.30609001	4.22902474
H	6.64725571	5.41476767	2.13957474	H	-2.26731901	2.17216832	5.28948154
H	9.98883878	4.94972391	5.16100966	H	-1.50018211	-1.44247844	8.01046383
H	4.36512096	3.99155284	4.16719047	H	-4.95529368	-4.47650125	8.73086735
H	7.46479823	5.04679476	7.37227514	C	-9.18510352	-1.93351104	-2.01059419
H	7.19617008	0.40813421	7.46822621	C	-9.96300552	-3.71954468	-4.13846651
H	10.52472900	0.86907243	7.26542076	C	-8.73313389	-6.21582791	-3.30714953
C	2.45346884	-3.50685299	4.29667378	C	-6.23607829	-5.31783700	-2.16218501
H	5.71738904	-5.32247777	2.73878394	O	-6.72116005	-2.80179909	-1.17694483
H	2.71746714	-4.37885994	6.16626111	H	-8.98707770	0.04802642	-2.59682749
H	3.26243700	-1.59226828	4.35875463	H	-9.16301400	-3.08041224	-5.94757628
H	0.41155260	-3.32228487	3.95845804	H	-8.44585225	-7.54791586	-4.87132162
H	3.61582043	-7.12545891	-2.49883852	H	-4.72837693	-5.18575383	-3.59288049
C	4.01629135	-3.87776245	-4.84880378	H	-5.55413756	-6.50649429	-0.60217220
H	1.99077245	-3.49117199	-5.08379607	H	-10.51298097	-2.03482491	-0.40373973
H	4.64902738	-5.03333844	-6.45814792	H	-9.90370961	-7.15621269	-1.86835234
H	5.03135256	-2.06321015	-4.91741709	H	-12.02246421	-3.85109234	-4.35098243

3.3. The coordinates and energies of intermediates Int6-7.

(S,S_p)-Int 6 (preferred)
(RI-DFT: BP-86/def2-TZVP)



E = -2402.12911720469 au
Imaginary frequencies: 0

(S,R_p)-Int6 (non-preferred)
(RI-DFT: BP-86/def2-TZVP)

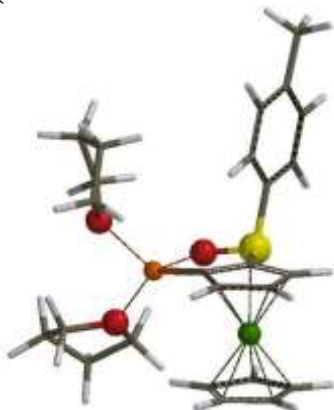


E = -2402.12351107344 au
Imaginary frequencies: 0

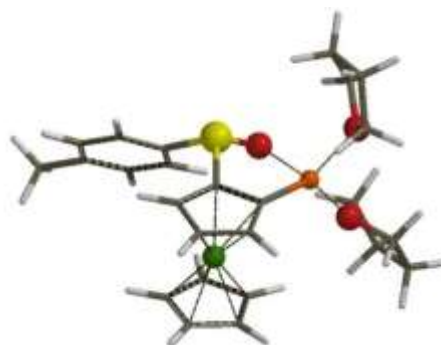
Fe	-1.32037344	4.73191619	0.15078508
C	1.01371007	2.42152889	2.12960458
C	2.43759747	4.45295185	1.04820569
C	2.11639037	4.34788699	-1.65269107
C	0.53299223	2.26661467	-2.41771146
C	-0.09167310	1.11335802	0.00284760
C	-3.95003058	6.10448684	2.67052948
C	-5.19054863	4.82807121	0.62977347
C	-4.49519878	6.06745815	-1.67921248
C	-2.81163014	8.10089850	-1.06562636
C	-2.48310312	8.12808968	1.62455386
S	-2.21936346	-1.48020582	0.23213569
H	2.91409683	5.74157986	-2.94173115
H	3.50528741	5.85600491	2.10685560
H	-1.92857080	9.38336467	-2.40357091
H	-1.30025178	9.43247313	2.68042167
H	-4.07794771	5.60780013	4.65863264
H	-6.43031196	3.19925220	0.79688884
H	-5.15818434	5.58425817	-3.56330270
H	0.84046734	1.95736424	4.12365321
H	4.21169499	-12.12151203	1.17448891
H	4.97179547	-11.42096049	-2.02276807
H	6.80440864	-10.11347032	0.44803328
Li	-2.24428718	0.83545513	-4.53538563
C	-0.03059799	-4.10435968	0.10922159
C	3.14326325	-8.35855891	-0.02451637
C	-0.53804663	-6.17316549	1.66592495
C	2.05691383	-4.13137225	-1.51727323
C	3.61588505	-6.24856316	-1.57442411
C	1.04834193	-8.28370657	1.59226760
H	0.64913011	-9.89902705	2.81299819
H	5.25006232	-6.26669419	-2.83631745
H	2.45274103	-2.48658451	-2.69927096
C	4.86556113	-10.62530811	-0.10443835
H	-2.16748584	-6.13421563	2.93122306
O	-3.62490712	-1.52174467	-2.32403753

Fe	-1.84388696	3.14274568	1.45699240
C	1.08837845	5.83031603	0.87664505
C	-1.38386381	6.85436377	0.37663771
C	-2.70341910	5.43644467	-1.53505100
C	-1.09753081	3.40023589	-2.31294187
C	1.17285867	3.67023836	-0.82598844
C	-1.74560516	2.14714118	5.22983976
C	-1.45378800	-0.05396321	3.67755323
C	-3.63747663	-0.25840490	2.09020968
C	-5.28379594	1.81478674	2.66362741
C	-4.11079017	3.30935465	4.59678320
S	4.17561837	2.15403904	-1.19995152
H	-4.60823004	5.78277020	-2.22925205
H	-2.21018963	8.45506156	1.37391781
H	-7.08740473	2.20920339	1.76514910
H	-4.87049024	5.02870301	5.42234685
H	-0.42756309	2.81182856	6.65899096
H	0.14315353	-1.34114890	3.69041412
H	-3.97310278	-1.71698195	0.68511991
C	3.37841258	-1.11464381	-1.75801451
C	2.41120803	-6.23691195	-2.74778555
C	3.80699622	-2.90748678	0.12197235
C	2.54883080	-1.85041759	-4.15691356
C	2.04618088	-4.39434770	-4.62448384
C	3.31714807	-5.45113960	-0.38408046
H	3.66050015	-6.85819398	1.08663226
H	1.38649211	-4.96639387	-6.49470968
H	2.31569739	-0.45462982	-5.65819125
C	1.83555722	-8.97803305	-3.26619055
H	4.55216552	-2.29471074	1.94317822
O	5.40428423	2.25561182	1.43628041
H	2.79919517	-10.22403013	-1.91580434
H	-0.20682040	-9.35088871	-3.11162232
H	2.41388314	-9.52739313	-5.18374909
H	-1.53345888	1.96054937	-3.71151615
Li	3.90659924	4.93031933	3.21629395

(S,S_p)-Int7 (preferred)
(RI-DFT: BP-86/def2-TZVP)



(S,R_p)-Int7 (non-preferred)
(RI-DFT: BP-86/def2-TZVP)



E = -2867.25430077504 au
Imaginary frequencies: 0

Fe	-1.40746448	5.44336058	0.98913659
C	-4.42104084	3.25932623	1.88672495
C	-3.38219596	4.36629548	4.12901872
C	-0.79194693	3.54076908	4.32561342
C	-0.07034036	1.86967356	2.28687471
C	-2.39832914	1.74512364	0.84178400
C	-0.62468923	6.73613163	-2.59249499
C	1.55963807	6.96764664	-1.00206018
C	0.89800230	8.55419073	1.09326960
C	-1.68845336	9.31028581	0.79144413
H	8.95658460	3.19248137	-1.19794909
H	8.40199895	-0.01561723	-0.25090310
H	4.00517501	0.30447390	-5.72939312
H	7.85196541	1.03600308	-8.12022722
H	4.12673215	3.65498041	-5.39071377
H	8.51352945	3.86811309	-6.44411355
H	11.43905464	0.94571281	-4.38398426
H	9.20322097	-1.56697048	-4.51894625
C	-2.62993097	8.18495075	-1.48664140
S	-2.59227384	0.01515397	-2.03716468
H	0.48422530	4.19098666	5.80772565
H	-4.37150468	5.65019776	5.39640932
H	-2.75679223	10.49811556	2.08172713
H	-4.53507129	8.37316064	-2.22971555
H	-0.75404148	5.62883192	-4.31794071
H	3.36648793	6.03471803	-1.28330078
H	2.12857311	9.06343987	2.65608948
H	-6.33278710	3.48705707	1.16673097
C	-4.20327810	-2.81407218	-0.93618139
C	-6.70378015	-7.29441984	0.46483722
C	-5.66230891	-4.12384811	-2.70526876
C	-3.99001225	-3.72111473	1.53784129
C	-5.23203705	-5.94289399	2.21630172
C	-6.89222817	-6.35134417	-2.00414115
H	-8.02686999	-7.36937773	-3.39602485
H	-5.07458870	-6.64085460	4.15366626
H	-2.87476722	-2.66374199	2.91301673
C	-8.08989358	-9.65771215	1.24542011
H	-5.83360378	-3.40008701	-4.63058198
O	0.12394389	-0.80282529	-2.63889930
H	-9.83808817	-9.18906403	2.27444577
H	-8.62426703	-10.80373050	-0.39979434
H	-6.93529856	-10.83345646	2.51005179
Li	2.68292888	0.20752264	-0.08799208
O	4.59076186	-2.81739886	1.48416915
C	4.36120332	-3.03655338	4.21589051
C	3.20453224	-5.63503346	4.69160674
C	4.29381157	-7.19934539	2.50063433
C	4.29518663	-5.29408854	0.32635460
H	6.26409811	-2.88119670	5.05904267
H	3.18080933	-1.44988942	4.85147634
H	1.13360986	-5.53639637	4.54997190

E = -2867.250281005 au
Imaginary frequencies: 0

Fe	1.95776377	-3.58657727	-0.99645297
C	-1.62742833	-2.07911702	-2.06762313
C	-1.01063054	-4.39748920	-3.36920520
C	1.32981442	-4.21248315	-4.75241531
C	2.32501299	-1.72728911	-4.34396616
C	0.51512416	-0.49282868	-2.71130266
C	3.82822028	-2.63188855	2.29050063
C	5.49032623	-3.95057158	0.60670563
C	4.41268526	-6.38537472	0.10740162
C	2.07814444	-6.56440080	1.47516946
C	1.71809555	-4.24342903	2.82882925
S	0.23919446	2.79593985	-1.96832848
H	2.23673595	-5.69641330	-5.85217681
H	0.79148301	-8.16475837	1.45612174
H	-2.12406296	-6.12863915	-3.26632027
H	0.09848176	-3.75635225	3.99207670
H	4.11117441	-0.73049005	3.00615057
H	7.24531957	-3.22255505	-0.17182259
H	5.20298820	-7.82762238	-1.12256697
C	3.44317142	3.73679969	-1.24036589
C	8.33300098	5.49061913	-0.13933238
C	5.15608638	4.16762577	-3.20576454
C	4.11703271	4.24588900	1.25339820
C	6.55244528	5.11251001	1.78716332
C	7.58805680	5.01222959	-2.64232402
H	8.92797282	5.33444911	-4.17932568
H	7.07810379	5.51466762	3.74278401
H	2.71378563	3.98036894	2.73967925
C	10.97696962	6.37250825	0.45153673
H	4.59277035	3.86495529	-5.16735416
H	4.08369703	-0.97396420	-5.09277218
O	-1.24885519	2.93357283	0.51064704
H	11.07714119	7.27100981	2.31932362
H	12.31138784	4.77434606	0.45625837
H	11.65919246	7.73429484	-0.96071608
Li	-3.60146651	-0.05275543	0.72464646
C	-8.21096329	-0.24889587	-2.52529834
C	-9.15237820	1.67516218	-4.48334789
C	-7.62901624	4.06518015	-3.84090031
C	-7.42169697	3.87830347	-0.97276598
O	-7.11609309	1.20976025	-0.45393417
H	-9.74489527	-1.43039433	-1.76322520
H	-11.18668519	2.03464288	-4.24792319
H	-8.55620395	5.81338868	-4.46658158
H	-9.15735107	4.57453061	-0.03918492
H	-5.77062703	4.85306682	-0.17942977
H	-6.69584448	-1.47277076	-3.25501735
H	-8.84324195	1.01777161	-6.42615473
H	-5.73626498	3.98357900	-4.69461212
C	-6.09409322	-2.55077249	5.36403589
C	-5.74945953	-2.64755081	8.26090856
C	-4.08614682	-0.30533995	8.86313757

H	3.16995882	-8.88701668	2.06147012	C	-4.02902417	1.14471811	6.35845942
H	2.50164097	-5.30663762	-0.73059225	O	-4.22739687	-0.78668310	4.44935428
H	5.86142820	-5.57781188	-1.01075428	H	-5.74989741	-4.35620353	4.40504803
H	6.23172625	-7.81216050	2.94151183	H	-4.81026820	-4.39811088	8.85353766
H	3.69514377	-6.39249481	6.56003892	H	-2.16780463	-0.89012464	9.39427746
O	5.53981387	1.57688382	-2.35401435	H	-2.28041631	2.19311507	5.99251168
C	8.20721313	1.34118818	-1.80848170	H	-5.65123540	2.45368814	6.19978125
C	9.41778301	0.48750089	-4.28239912	H	-7.99562363	-1.86408557	4.84655162
C	7.82184025	1.91817692	-6.24308620	H	-4.85265611	0.84379684	10.41087193
C	5.17352192	1.88966217	-5.06710200	H	-7.58435486	-2.56580940	9.22549830

3.4. The coordinates and energies of starting materials and product of lithiation of (S)-3.

(*i*Pr)₂NH

(RI-DFT: BP-86/def2-TZVP)



E = -292.53712621932 au

Imaginary frequencies: 0

N	0.07655836	0.17106365	-1.18996692
C	2.27484968	-0.70809632	0.26760717
C	-2.24503399	0.79974511	0.20972248
C	4.19805189	-1.82658532	-1.57926251
C	3.44057593	1.47718018	1.76737737
C	-4.11565224	2.01764452	-1.63051129
C	-3.46623532	-1.44383009	1.60234056
H	3.39789978	-3.44736917	-2.61027330
H	4.77644831	-0.39562822	-2.97224268
H	5.88972189	-2.49057961	-0.57484786
H	4.02070195	3.00048117	0.47734426
H	5.10797733	0.82444171	2.82198417
H	2.10737880	2.27420638	3.14588669
H	1.75748853	-2.21871607	1.63471134
H	-4.67324612	0.66243473	-3.11096831
H	-3.25880656	3.66331575	-2.55926071
H	-5.84583036	2.62307548	-0.65270335
H	-5.13429621	-0.83544476	2.68483224
H	-2.14894221	-2.33784434	2.93655058
H	-1.71757070	2.23427042	1.62628617
H	-4.08652664	-2.89379938	0.24236783
H	-0.35494518	-1.15015480	-2.53697394

LDA

(RI-DFT: BP-86/def2-TZVP)

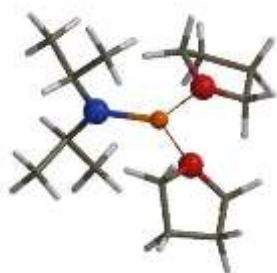


E = -299.45174414033 au

Imaginary frequencies: 0

C	-3.19082385	2.03152846	1.81368598
H	-2.02901505	1.76739631	-2.06565742
H	-1.72963324	3.37604978	2.42434695
H	-3.62380982	0.78976090	3.42864948
H	-4.89578090	3.13175108	1.34371867
C	4.38162197	-1.30237303	1.35654769
H	6.17624252	-0.30486307	1.67887241
H	4.75934692	-2.78521104	-0.07092327
H	3.82715108	-2.21483204	3.14576643
H	2.03098199	1.92894905	1.91448894
N	0.00107134	-1.00467412	0.04111895
C	-2.28138247	0.43336392	-0.45294784
C	2.28460598	0.46604584	0.41804567
Li	-0.03153674	-4.35569371	0.16347806
C	3.19681124	1.87127650	-1.97201280
H	4.90190596	3.00576262	-1.59285841
H	1.73700207	3.16149202	-2.69339722
H	3.63092811	0.50009205	-3.47829220
C	-4.38119556	-1.40484936	-1.24012027
H	-6.17597980	-0.43695592	-1.64146358
H	-4.75972856	-2.76424105	0.30582634
H	-3.83067293	-2.46181197	-2.94970476

LDA...2THF
(RI-DFT: BP86/TZVP)



E = -764.58921219487 au
Imaginary frequencies:0

H	-5.29105165	1.01270028	4.21864213
H	-7.07037367	2.23927731	-1.17445344
H	-8.85231757	2.51289943	1.66826837
H	-9.39586465	-1.79648080	-1.14931619
H	-9.05625792	-2.07411483	2.17965579
H	-5.44228309	-4.54910639	1.07955948
H	-5.06514152	-2.97225720	-1.88883469
H	-0.37313866	-5.85787447	-2.41374067
H	0.22358986	-7.23276580	0.61642750
H	4.84380578	-1.33387525	-0.65322014
H	5.49123709	-3.92721473	1.44508826
H	4.75775513	-4.20770089	-4.31435610
H	7.22433601	-5.61982463	-2.51029537
H	4.32519900	-8.64356319	-0.58610372
H	3.08632124	-8.50646376	-3.70186134
C	1.34367610	4.19312959	-2.20260257
N	1.44119418	2.80100921	0.15594758
Li	-0.02287502	-0.41501028	0.48594860
C	2.72747469	4.11984445	2.18693091
C	-0.38624394	6.55419112	-2.14193099
C	2.26831921	2.72664853	4.68928409
C	5.61151317	4.42920563	1.79067076
O	-3.68678497	-1.02262964	1.22775912
C	-5.54908516	-2.70733032	0.11956582
C	-8.12332004	-1.41345685	0.44378998
C	-7.40514334	1.39085713	0.69364338
C	-4.94273137	1.24094511	2.17407156
O	1.81395065	-3.67526271	-0.00118375
C	4.53003894	-3.36008972	-0.31853958
C	5.21370804	-5.10938815	-2.49758815
C	3.47227483	-7.38303877	-2.00110445
C	1.06982286	-6.14458402	-0.94128857
H	3.24842084	4.89592256	-2.79133890
C	0.45317557	2.43277941	-4.32948015
H	1.97673238	6.07697714	2.46377558
H	6.48237139	5.57024872	3.30244043
H	6.03006120	5.36634381	-0.01644213
H	6.53600385	2.56203882	1.76814434
H	0.33612228	3.41239142	-6.16067672

(S)-Fc-sulfoxid (3)
(RI-DFT: BP-86/def2-TZVP)



E = -2395.19634196059
Imaginary frequencies: 0

Fe	-3.04719092	1.83874914	-3.29211736
C	0.20067246	-0.19837790	-3.65823005
C	-1.90132156	-1.65999080	-4.53957362
C	-3.67073921	-1.91653712	-2.50193350
C	-2.68009624	-0.62955768	-0.33708070
C	-0.27859383	0.42042269	-1.04910826
C	-2.62146908	5.10933930	-5.35046700
C	-3.12420381	5.69447691	-2.75373350
C	-5.50876988	4.59787751	-2.09612220
C	-6.48693587	3.33822567	-4.28646879
C	-4.70055026	3.65335019	-6.30008939
S	1.78472252	2.31653587	0.87146380
H	-5.48155618	-2.88058364	-2.59940989
H	-2.13709192	-2.39973196	-6.44057960
H	-8.25335643	2.29732643	-4.39346930
H	-4.87776077	2.89712651	-8.20067704
H	-0.94414504	5.64696716	-6.40520663
H	-1.88709302	6.70811985	-1.46748865
H	-6.38703787	4.66817796	-0.24269595
H	1.85043337	0.35807762	-4.74639470
C	3.12915913	-0.26138501	2.72795863
C	5.33466208	-4.04171654	5.72392860
C	2.56704562	-0.37752589	5.29539887
C	4.80814190	-1.98262042	1.63409215
C	5.88612083	-3.86250353	3.13044111
C	3.66449698	-2.27359441	6.77210928
H	3.21695628	-2.37425169	8.78497721
H	7.18657515	-5.21755561	2.27310202
H	5.26491782	-1.86935957	-0.37519047
C	6.54656103	-6.06007684	7.32904632
H	1.28087690	1.02047444	6.09855295
H	-3.56908596	-0.43003032	1.50083966
O	0.20580196	3.84926474	2.66856285
H	5.68228926	-6.14791347	9.21292910
H	6.36962905	-7.93528967	6.45034007
H	8.57970570	-5.69614916	7.58451631

H	1.74715312	0.81607091	-4.53969776
H	-1.45246383	1.69326551	-3.89710339
H	2.99559298	0.77314070	4.57144510
H	0.23651909	2.63648416	5.12851541
H	3.23088441	3.65153371	6.28448952
H	0.14468712	7.83655997	-0.59517427
H	-0.28360043	7.64039831	-3.91859988
H	-2.36695494	5.98020630	-1.83924196
H	-3.61954803	2.81291711	1.85810535

3.5. The energies of LDA and (*i*-Pr)₂NH conformers.

Table S1: Searching of the most stable conformer of LDA.

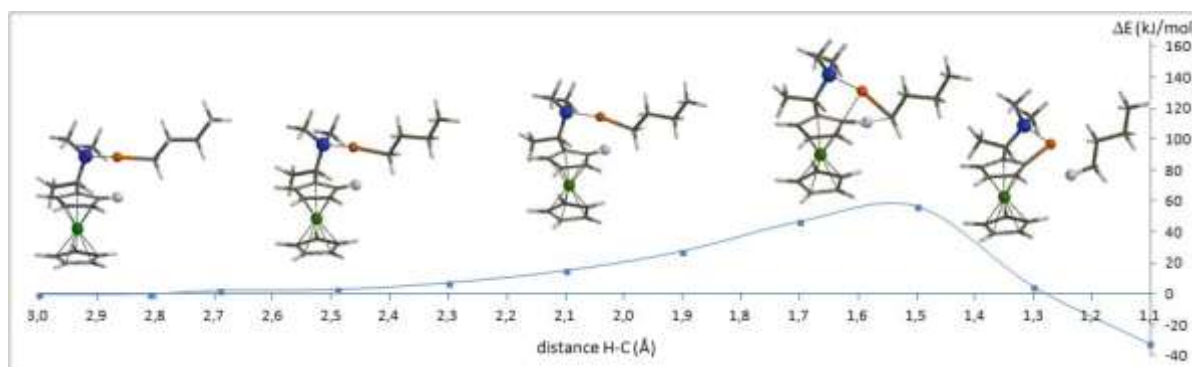
(HF, 6-31G*)			(RI-DFT, BP-86, def2-TZVP)			
$\alpha^{(H,H)}$	$\beta^{(H,Li)}$	E (au)	$\alpha^{(H,H)}$	$\beta^{(H,Li)}$	E (au)	$\Delta E(\text{kJ/mol})$
0.3°	-0.3°	-259.582369	-	-	-	-
-171.1°	-165.1°	-259.593557	-	-	-	-
170.9°	3.9°	-259.593555	-	-	-	-
82.4°	-135.8°	-259.600081	96.8°	-126.6°	-299.4517441	0.000

Table S2: Searching of the most stable conformer of (*i*-Pr)₂NH.

(HF, 6-31G*)			(RI-DFT, BP-86, def2-TZVP)			
$\alpha^{(H,H)}$	$\beta^{(H,NH)}$	E (au)	$\alpha^{(H,H)}$	$\beta^{(H,NH)}$	E (au)	$\Delta E(\text{kJ/mol})$
35.9°	51.3°	-288.769284	-	-	-	-
166.2°	-158.5°	-288.777651	-	-	-	-
-166.8°	37.2°	-288.777652	-	-	-	-
82.5°	-88.3°	-288.781222	96.5°	-75.9°	-292.5371183	0.0017
-4.8°	-177.7°	-288.779598	-	-	-	-
-86.4°	-179.7°	-288.781245	-96.5°	179.6°	-292.5371247	0.000

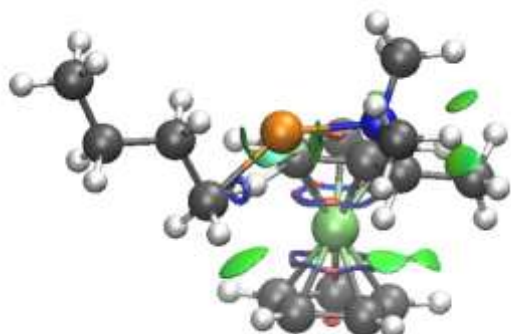
4. Potential energy scan for the formation of intermediate (*R,R*)Int1 and *n*-BuH. .

Figure S1: The energy dependence of calculated molecules on distance between acid hydrogen and *n*-BuLi.

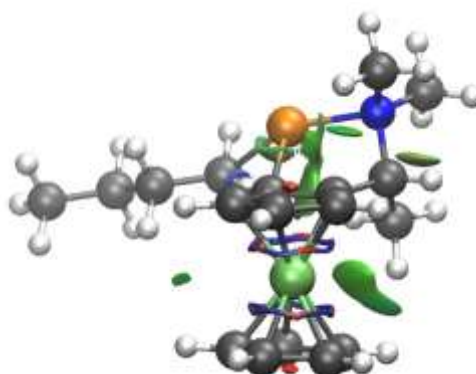


5. NCI plot of TS1-2, 4-7¹.

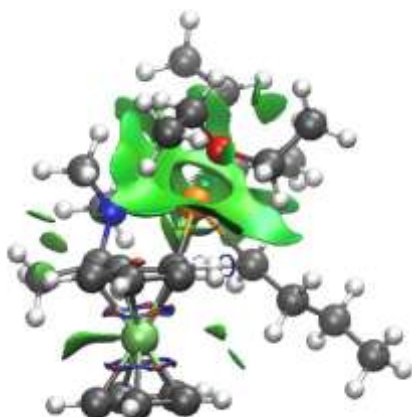
(*R,R*)-TS1 (preferred)^a



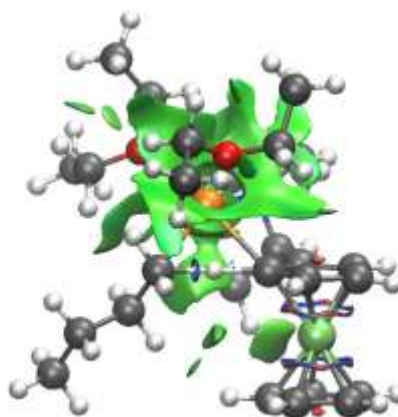
(*R,S*)-TS1 (non-preferred)



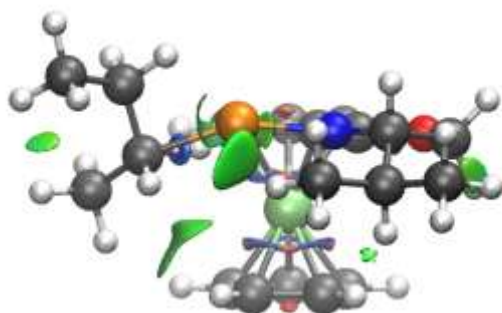
(*R,R*)-TS 2 (preferred)



(*R,S*)-TS 2 (non-preferred)



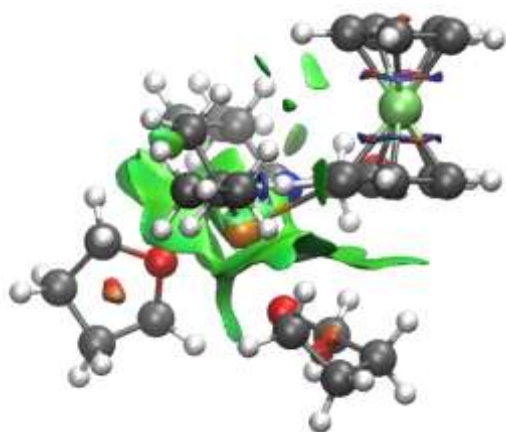
(*S,R*)-TS4 (preferred)



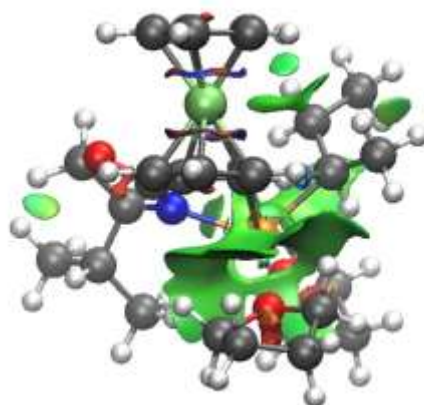
(*S,S*)-TS4 (non-preferred)



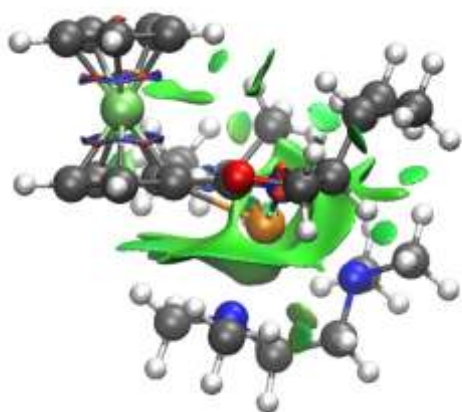
(*S,R*_p)-TS5 (preferred)



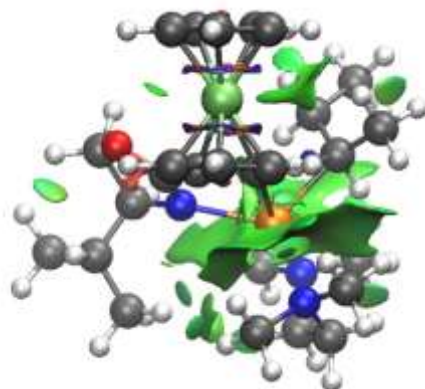
(*S,S*_p)-TS5 (non-preferred)



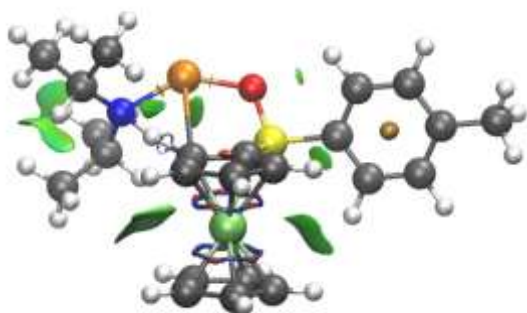
(*S,R*_p)-TS6 (preferred)



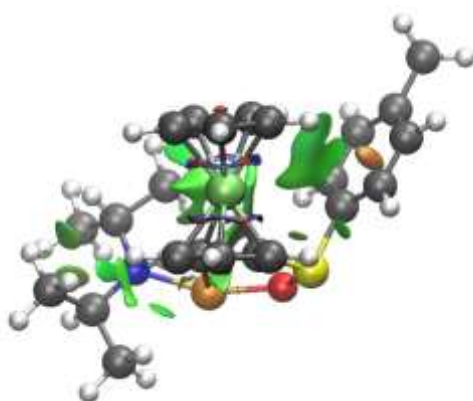
(*S,S*_p)-TS6 (non-preferred)



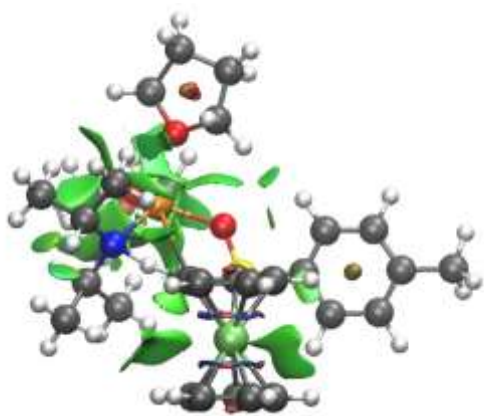
(*S,S*_p)-TS7 (preferred)



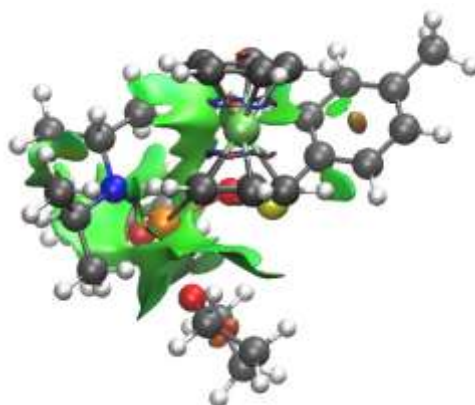
(*S,R*_p)-TS7 (non-preferred)



(*S,S*)-TS8 (preferred)



(*S,R*)-TS8 (non-preferred)



1, NCI surfaces correspond to $s=0.1$ au and a color scale of $-0.75 < \rho < 0.75$ au.