9 Details zu den quantenchemischen Rechnungen (Anhang)

Quantenchemische Studien zur Thermodynamik der Methoxy/Amino-Substitution[58]

Tabelle 9.1 Standardorientierung von **85b** [B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
C	1.18339800	–0.77024500	2.50260600
C	2.63432900	–1.73659700	–1.09724400
C	2.53741500	2.16825800	–0.53845700
H	0.11245300	–0.80438900	2.74137600
H	1.73192400	–0.43388200	3.38776300
H	1.52038200	–1.78133100	2.23876100
H	3.27584700	–1.66871700	–0.20841000
H	2.62972000	–2.77224000	–1.45062600
H	2.71328800	2.20111200	0.54210600
H	2.36775100	3.18339700	–0.91112500
H	3.04791100	–1.09679600	–1.88732900
H	3.42476400	1.75580600	–1.03569600
O	1.44623700	0.15355900	1.45218400
O	1.29132000	–1.37072400	–0.80258500
O	1.38636500	1.39123800	–0.85319300
Si	0.81872700	0.04714800	–0.08630000
C	–1.04148900	0.03286700	–0.13707600
C	–1.76650200	1.21321000	0.11520600
C	–1.76542800	–1.14630000	–0.39492300
C	–3.16333100	1.21670300	0.11362300
H	–1.23409100	2.14267500	0.30436800
C	–3.16327400	–1.14793300	–0.39589700
H	–1.22863000	–2.06698600	–0.60775200
C	–3.86431200	0.03384500	–0.14084900
H	–3.70408800	2.14031900	0.30589400
H	–3.70382500	–2.06916700	–0.60017700
H	–4.95179200	0.03470100	–0.14414200

Tabelle 9.2 Standardorientierung von $HN(C_4H_8)$ [B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
C	–1.16393000	–0.44931800	0.17082400

C	1.16534400	–0.44591200	0.17064500
C	0.77783000	1.03119800	–0.05674300
C	–0.78096000	1.02880700	–0.05695400
H	–2.07381900	–0.74633400	–0.36207000
H	–1.32607400	–0.63280100	1.25078600
H	1.32823500	–0.62910800	1.25054600
H	2.07599600	–0.74014600	–0.36247300
H	1.19638200	1.68029800	0.71958200
H	1.16068500	1.38171800	–1.02063800
H	–1.20167300	1.67698000	0.71897800
H	–1.16461000	1.37774900	–1.02110400
N	0.00171300	–1.17175000	–0.35051600
H	0.00318200	–2.15476300	–0.08662800

Tabelle 9.3 Standardorientierung von $LiN(C_4H_8)$ [B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
C	0.25284800	–1.13510100	0.32014200
C	0.25283900	1.13512600	0.32009100
C	–1.16430300	0.77718100	–0.21529700
C	–1.16425800	–0.77721400	–0.21535000
H	0.63843800	–2.07376800	–0.10583500
H	0.18048700	–1.29104900	1.42009100
H	0.18053300	1.29116300	1.42002900
H	0.63839100	2.07376300	–0.10598300
H	–1.96308100	1.19806000	0.40922000
H	–1.30067200	1.16810500	–1.23088400
H	–1.96308400	–1.19819400	0.40903800
H	–1.30047200	–1.16806800	–1.23098600
N	1.10081000	0.00000700	–0.01041300
Li	2.70700800	–0.00000200	–0.72310700

Tabelle 9.4 Standardorientierung von $[LiN(C_4H_8)]_4$ [B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
Li	1.25879100	–0.25264400	0.56087600
Li	0.32030300	0.90851500	–1.34487700
Li	–0.76632400	0.99417600	0.77331500
Li	–0.68557900	–1.09831100	–0.50281800
C	0.33427100	–1.96988200	2.13415700

C	–1.55666200	–0.74632200	2.39785500
C	–0.69002200	–3.00627000	2.67522800
H	0.90185200	–1.56209000	3.00041800
H	1.06790100	–2.43771800	1.45761700
C	–1.98645100	–2.16959000	2.84977900
H	–2.39457000	–0.19103700	1.94626900
H	–1.24133800	–0.17818500	3.30147800
H	–0.83749100	–3.81483900	1.94979800
H	–0.35419700	–3.46494600	3.61294300
H	–2.78870200	–2.54908200	2.20632000
H	–2.36019200	–2.17970000	3.88069100
C	–2.91595100	–0.05066100	–1.12172400
C	–1.91932800	1.87557100	–1.78399800
C	–4.05691300	0.99787700	–1.00848000
H	–3.02261200	–0.85233600	–0.37289600
H	–2.98620100	–0.53211700	–2.12255400
C	–3.37805500	2.31485100	–1.47422100
H	–1.85238500	1.64732900	–2.87155600
H	–1.19748700	2.68273800	–1.57728400
H	–4.92671500	0.73052500	–1.62052000
H	–4.39815400	1.07907000	0.03006300
H	–3.86896400	2.75618500	–2.34982500
H	–3.39078100	3.06771600	–0.67762300
C	0.67882200	–1.73031700	–2.51666000
C	2.54993200	–1.22743900	–1.33264800
C	1.39082000	–3.10423100	–2.36862600
H	0.96935100	–1.28573400	–3.49157300
H	–0.42070700	–1.82907300	–2.56031800
C	2.66801100	–2.76052200	–1.55601300
H	3.02563300	–0.91426700	–0.38444100
H	3.12178700	–0.70577500	–2.12805500
H	0.75810200	–3.81425800	–1.82270800
H	1.61860100	–3.55454700	–3.34214300
H	2.67625700	–3.29162500	–0.59708000
H	3.59049500	–3.02819400	–2.08484500
C	2.04181200	2.50900300	–0.40430600
C	1.02709700	2.49590800	1.62509700
C	3.17697300	2.93755800	0.56733600
H	1.56528500	3.43046400	–0.80654500
H	2.43409300	1.94687900	–1.26731300
C	2.48411700	2.92143900	1.95727100
H	0.57197100	1.92318000	2.45016500

H	0.41859300	3.41859600	1.49433800
H	4.00435600	2.21946700	0.53128700
H	3.58663200	3.92220800	0.31198700
H	2.95357300	2.18733600	2.62236300
H	2.52514700	3.89429800	2.46162100
N	1.12115200	–0.90437500	–1.38508500
N	1.10631300	1.70559000	0.38998100
N	–1.66369200	0.69152500	–0.95286400
N	–0.45256600	–0.93524400	1.45084700

Tabelle 9.5 Standardorientierung von $N(C_4H_8)^-$ [B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
C	–1.10660300	–0.52326600	0.15633900
C	1.10661200	–0.52325400	0.15632500
C	0.77780600	1.00134700	–0.05811900
C	–0.77782100	1.00133300	–0.05813500
H	–2.06151900	–0.81329200	–0.31382600
H	–1.25542200	–0.65191100	1.27980000
H	1.25545600	–0.65191200	1.27978000
H	2.06152300	–0.81326100	–0.31386300
H	1.19692900	1.64982700	0.73118000
H	1.17701800	1.34838600	–1.02164600
H	–1.19697600	1.64983400	0.73112900
H	–1.17701400	1.34832700	–1.02168600
N	0.00000500	–1.25756500	–0.36133300

Tabelle 9.6 Standardorientierung von **86b** [B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
C	0.34323400	2.57923200	1.93201100
C	–1.31265700	2.52605400	–1.69576200
H	1.37048800	2.23071600	2.10224300
H	–0.07214600	2.93096500	2.88160100
H	0.36845600	3.41789800	1.22364400
H	–1.57333700	3.30341900	–0.96494800
H	–1.04367800	3.00813300	–2.64110400
H	–2.19168400	1.88842100	–1.85959900
O	–0.48779700	1.52512400	1.46012500
O	–0.19447000	1.76395000	–1.25931300

Si	–0.23405000	0.70690900	0.03138000
C	1.44824800	–0.11477900	–0.03864200
C	1.80175800	–1.06222800	0.94226900
C	2.39270500	0.17653500	–1.04065000
C	3.04855100	–1.69258100	0.92756400
H	1.09229000	–1.31281800	1.72917200
C	3.64120200	–0.45292500	–1.06260600
H	2.14339600	0.90325600	–1.80899900
C	3.97158000	–1.38808600	–0.07788400
H	3.29946800	–2.41987300	1.69625600
H	4.35512700	–0.21346900	–1.84741800
H	4.94234000	–1.87814000	–0.09355200
C	–1.60399200	–1.51251500	–1.00757300
C	–2.70395500	–0.44435500	0.87781200
C	–2.98160400	–2.16105000	–0.77160200
H	–0.79561600	–2.24031200	–0.83952600
H	–1.50044900	–1.14558900	–2.03794900
C	–3.26030300	–1.86504600	0.70975900
H	–3.46331500	0.29760400	0.57847300
H	–2.41292600	–0.21495000	1.90721100
H	–3.74093200	–1.67581000	–1.39863800
H	–2.98394400	–3.22949800	–1.01247200
H	–4.32151600	–1.93545400	0.97311400
H	–2.70505400	–2.56495400	1.34791600
N	–1.53439300	–0.41262800	–0.02134500

Tabelle 9.7 Standardorientierung von **A1** [B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
C	0.15075200	–1.25620400	2.81159700
H	–0.89330400	–1.59371700	2.73974900
H	0.36767500	–1.01594800	3.85775000
H	0.80764700	–2.07972600	2.49857500
O	0.38025900	–0.09033500	2.03872800
Si	0.20512800	–0.00025800	0.37383000
C	–1.64174500	–0.04883700	–0.01269000
C	–2.58426700	0.31953700	0.96787200
C	–2.13017400	–0.35657100	–1.29743300
C	–3.95193400	0.36981400	0.68347500
H	–2.24178200	0.57329500	1.96885100
C	–3.49591300	–0.30622000	–1.59124400

H	–1.43311600	–0.64339700	–2.08210600
C	–4.41154800	0.05564100	–0.59885400
H	–4.65796300	0.65344700	1.46083100
H	–3.84522700	–0.54968700	–2.59220600
H	–5.47498400	0.09286600	–0.82327200
C	1.07876400	2.03831800	–1.35570200
C	1.39124800	2.50896100	1.00452900
C	1.96359500	3.28447000	–1.20340700
H	0.08937400	2.32300200	–1.75347700
H	1.50885200	1.30281300	–2.04753600
C	1.56971900	3.80140900	0.18833900
H	2.33701200	2.21989600	1.48748400
H	0.64723400	2.62304100	1.80098600
H	3.02332500	2.99728400	–1.21494500
H	1.80181900	4.01519900	–2.00342500
H	2.31339800	4.47416100	0.62966000
H	0.61833600	4.34626100	0.12842200
N	0.98278900	1.49353400	0.00935600
C	2.39476300	–1.34259600	–0.82192800
C	0.42352900	–2.59217800	–0.84575100
C	2.82082800	–2.73835600	–0.31153200
H	2.93783900	–0.52013600	–0.34824800
H	2.56828500	–1.27358900	–1.91033300
C	1.52229300	–3.59013000	–0.39076500
H	0.25888800	–2.69326400	–1.93231200
H	–0.53954600	–2.76104300	–0.35619600
H	3.63833900	–3.15911800	–0.90789900
H	3.17325900	–2.66860600	0.72374600
H	1.61441500	–4.42507400	–1.09447800
H	1.27728900	–4.01856600	0.58747200
N	0.95858500	–1.26145600	–0.54072600

Tabelle 9.8 Standardorientierung von **A2** [B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
Si	0.05696300	0.05571100	–0.08901100
C	–1.82861500	0.21535100	–0.13722700
C	–2.67641400	–0.86297400	0.18443000
C	–2.43975300	1.42868600	–0.50426200
C	–4.06754900	–0.74177200	0.13212700
H	–2.24168700	–1.81397800	0.48789500

C	–3.83124700	1.56135700	–0.55857600
H	–1.81867200	2.28759600	–0.74780000
C	–4.64919000	0.47391500	–0.24177500
H	–4.69743000	–1.59162000	0.38594200
H	–4.27548700	2.51196600	–0.84543400
H	–5.73147400	0.57293600	–0.28180100
C	1.11470400	2.41658900	–1.32344400
C	1.31790800	2.32227500	1.07040200
C	2.33306000	3.26395600	–0.93475600
H	0.26187100	3.08164500	–1.55641200
H	1.28481600	1.79017000	–2.20449700
C	2.04396300	3.58513300	0.54123400
H	1.98926300	1.69258800	1.66942300
H	0.47875400	2.60765900	1.72366700
H	3.24667300	2.66290200	–1.02824100
H	2.44815200	4.16024800	–1.55483800
H	2.94568400	3.81733300	1.11821400
H	1.38045700	4.45662200	0.60727000
N	0.87213200	1.59296600	–0.13432800
C	1.96836500	–0.90915300	–1.97599800
C	–0.17798200	–1.75580500	–2.31237100
C	2.18382000	–2.40674000	–2.32227200
H	2.67869800	–0.53135400	–1.23427000
H	2.09617100	–0.30095000	–2.88966500
C	0.74844800	–2.98290500	–2.47856200
H	–0.38987100	–1.31109500	–3.30135000
H	–1.13901900	–2.00195800	–1.85527800
H	2.78046500	–2.52023000	–3.23454800
H	2.72338000	–2.91905600	–1.51791700
H	0.59660800	–3.48104600	–3.44292700
H	0.54244000	–3.71877100	–1.69303600
N	0.58964800	–0.81878900	–1.49160500
C	1.67858000	–1.50643400	1.62650400
C	–0.24400000	–0.51524200	2.70096900
C	1.43509800	–2.24401800	2.94948800
H	2.56397100	–0.84929200	1.72225900
H	1.86692700	–2.18920400	0.79035300
C	0.64681600	–1.20298200	3.75879700
H	–1.25145000	–0.95349200	2.68777500
H	–0.36614000	0.55400200	2.92580700
H	0.82165800	–3.13661700	2.77076000
H	2.36340500	–2.55996700	3.43853500

H	0.06019400	–1.63832000	4.57516400
H	1.33991600	–0.47590700	4.20146900
N	0.43938800	–0.74820400	1.40898900

Tabelle 9.9 Standardorientierung von MeOH [B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
C	–0.66901300	–0.02081700	0.00000000
H	–1.02889500	–0.54669400	0.89609400
H	–1.02889400	–0.54670400	–0.89608800
H	–1.08099200	0.99121400	–0.00000600
O	0.74964600	0.12298300	0.00000000
H	1.15569300	–0.75677800	0.00000000

Tabelle 9.10 Standardorientierung von MeOLi [B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
C	–0.93653900	–0.00078600	0.00000000
H	–1.35504200	–0.51429000	0.88798400
H	–1.35504200	–0.51429900	–0.88797800
H	–1.35808200	1.02372700	–0.00000600
O	0.44399500	0.00214500	0.00000000
Li	2.04514600	–0.00252900	0.00000000

Tabelle 9.11 Standardorientierung von $[MeOLi]_4$ [B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
Li	–0.00081200	0.86624700	1.22412300
Li	–0.00081200	0.86624700	–1.22412300
Li	–1.22338200	–0.86684300	0.00000000
Li	1.22430600	–0.86510500	0.00000000
O	–1.44030500	1.01769100	0.00000000
O	0.00049000	–1.01773200	1.44035200
O	1.43927400	1.01801900	0.00000000
O	0.00049000	–1.01773200	–1.44035200
C	–2.59027200	1.81617700	0.00000000
H	–2.34860200	2.89522100	0.00000000
H	–3.22456400	1.63284200	–0.88709100
H	–3.22456400	1.63284200	0.88709100

C	2.58956400	1.81604500	0.00000000
H	2.34831500	2.89518200	0.00000000
H	3.22381500	1.63252300	0.88709300
H	3.22381500	1.63252300	–0.88709300
C	0.00049000	–1.81625800	–2.59025800
H	0.88613600	–1.63113300	–3.22605600
H	0.00328500	–2.89526800	–2.34839100
H	–0.88808800	–1.63508100	–3.22310800
C	0.00049000	–1.81625800	2.59025800
H	–0.88808800	–1.63508100	3.22310800
H	0.00328500	–2.89526800	2.34839100
H	0.88613600	–1.63113300	3.22605600

Tabelle 9.12 Standardorientierung von MeO^- [B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
C	0.54359600	0.00000500	0.00000000
H	1.03682100	–0.51552300	–0.89225900
H	1.03679500	–0.51498800	0.89257700
H	1.03674200	1.03052500	–0.00030500
O	–0.79649100	–0.00000600	–0.00000200

Tabelle 9.13 Standardorientierung von **Pent** [B3LYP/6-31+G(d)].

Atomsymbol	x	y	z
Si	0.28087100	0.61318400	0.23706900
O	0.36718200	–0.02039600	1.90699200
C	–0.37689300	0.49240200	2.97018100
H	–0.03242500	1.49419800	3.27406100
H	–1.45632400	0.57264600	2.73994300
H	–0.27679700	–0.18720100	3.83532600
O	0.26728600	2.20682900	0.92318900
C	–0.21415300	3.40125400	0.37552100
H	–0.83916600	3.91511900	1.12601300
H	0.61559500	4.08139100	0.11402600
H	–0.81883200	3.24563900	–0.52849200
O	0.21287200	1.25634000	–1.45176300
C	1.20996300	2.05358300	–2.01579600
H	1.62486800	1.58126000	–2.92522500
H	0.80570000	3.03737800	–2.31982400

H	2.05574500	2.24059600	–1.33157500
C	2.75275200	–0.84813500	0.80352100
C	2.16475000	–0.83159200	–1.42083200
C	2.92287200	–2.32657300	0.36555900
H	2.40770000	–0.73366900	1.82999800
H	3.73224000	–0.33217300	0.70159800
C	2.52908000	–2.31514100	–1.13817000
H	3.06148800	–0.31857100	–1.83024700
H	1.35928900	–0.71976100	–2.14881400
H	3.94570900	–2.69380000	0.53219200
H	2.24390200	–2.96856600	0.93991800
H	3.34003300	–2.66872600	–1.79073000
H	1.65917300	–2.95876900	–1.31722200
N	1.78965100	–0.28046300	–0.12776300
C	–1.43384400	–0.24744400	–0.10025900
C	–2.37415000	0.23808600	–1.03324700
C	–1.79876600	–1.42068300	0.59143000
C	–3.60358100	–0.39445700	–1.25408700
H	–2.11763100	1.12145300	–1.60985700
C	–3.01502700	–2.07660400	0.36648900
H	–1.10537700	–1.81869300	1.32777700
C	–3.93074400	–1.56192900	–0.55666800
H	–4.30382600	0.02001800	–1.97959500
H	–3.25036800	–2.98726900	0.91747000
H	–4.88273000	–2.06262100	–0.73057700

Tabelle 9.14 Standardorientierung von **85b** [B3LYP/6-31+G(d); PCM-Rechnung; Lösungsmittel: THF].

Atomsymbol	x	y	z
C	1.22581600	–1.03193500	2.39083100
C	2.66863100	–1.61047300	–1.19965000
C	2.51208300	2.23246900	–0.36581600
H	0.15728200	–1.14465100	2.61234600
H	1.75256200	–0.77673000	3.31430700
H	1.61496300	–1.98448300	2.01101500
H	3.26088800	–1.63460200	–0.27682800
H	2.68882000	–2.60189300	–1.65990800
H	2.67005800	2.20964000	0.71673900
H	2.35219900	3.26542000	–0.68737600
H	3.11335600	–0.88843300	–1.89485300
H	3.40221500	1.83799500	–0.86985400

O	1.44808000	0.02658400	1.45536700
O	1.30200600	–1.27969500	–0.93367000
O	1.35484000	1.47700900	–0.73507000
Si	0.81465900	0.05931800	–0.08404100
C	–1.04699100	0.04120400	–0.13182400
C	–1.77532600	1.21124300	0.16092100
C	–1.76966900	–1.13213700	–0.42196900
C	–3.17314900	1.21087200	0.16352000
H	–1.24606400	2.13534900	0.38184900
C	–3.16830100	–1.13825200	–0.42031300
H	–1.23440200	–2.04756800	–0.65920900
C	–3.87225900	0.03437300	–0.12775700
H	–3.71530400	2.12623200	0.38764400
H	–3.70673600	–2.05435200	–0.65128300
H	–4.95949100	0.03226600	–0.12869300

Tabelle 9.15 Standardorientierung von $N(C_4H_8)^-$ [B3LYP/6-31+G(d); PCM-Rechnung; Lösungsmittel: THF].

Atomsymbol	x	y	z
C	–1.11275000	–0.52070400	0.16299100
C	1.12130500	–0.50888600	0.15280700
C	0.77004600	1.00434300	–0.05199400
C	–0.78396100	0.99217200	–0.06492200
H	–2.06668500	–0.81548400	–0.30227500
H	–1.25363200	–0.65213700	1.27613700
H	1.28215100	–0.65038300	1.26171000
H	2.07154400	–0.78613500	–0.33053900
H	1.17819700	1.64536000	0.74419900
H	1.17289400	1.36856800	–1.00620600
H	–1.21768500	1.64561400	0.70748800
H	–1.17443100	1.32494300	–1.03560800
N	0.00568700	–1.26884200	–0.35831400

Tabelle 9.16 Standardorientierung von **86b** [B3LYP/6-31+G(d); PCM-Rechnung; Lösungsmittel: THF].

Atomsymbol	x	y	z
C	0.38054600	2.62100700	1.86477700
C	–1.35966000	2.49297700	–1.67403700
H	1.41991200	2.29071600	1.98789100
H	0.01151800	2.98789500	2.82685600

H	0.35318400	3.44273700	1.13821700
H	–1.60324900	3.26954200	–0.93771800
H	–1.12792500	2.97347400	–2.62914300
H	–2.23377400	1.84288700	–1.80593400
O	–0.46031900	1.54012900	1.45823500
O	–0.21398500	1.74248500	–1.26904800
Si	–0.23069800	0.69718900	0.03543600
C	1.45597600	–0.11928700	–0.04229800
C	1.81097100	–1.06837600	0.93755000
C	2.40183600	0.17430700	–1.04301600
C	3.05958800	–1.69695100	0.92333100
H	1.10169700	–1.32379400	1.72293500
C	3.65273400	–0.45253200	–1.06542800
H	2.15495100	0.90049700	–1.81255400
C	3.98419900	–1.38908900	–0.08104500
H	3.31046300	–2.42530600	1.69082700
H	4.36658800	–0.21038000	–1.84931200
H	4.95573400	–1.87723300	–0.09638200
C	–1.60923100	–1.52198100	–0.98172700
C	–2.69110400	–0.45398200	0.91653900
C	–3.01461800	–2.11691900	–0.78292700
H	–0.83593600	–2.28340700	–0.79600400
H	–1.46472100	–1.15350900	–2.00610100
C	–3.29903400	–1.84759800	0.70211800
H	–3.42313100	0.32542100	0.64882000
H	–2.39040200	–0.27851700	1.95410600
H	–3.74305100	–1.58333500	–1.40711100
H	–3.05692300	–3.17804900	–1.05018900
H	–4.36489600	–1.88113700	0.95228000
H	–2.77981300	–2.58596400	1.32710300
N	–1.52274900	–0.42907700	0.01268400

Tabelle 9.17 Standardorientierung von MeO^- [B3LYP/6-31+G(d); PCM-Rechnung; Lösungsmittel: THF].

Atomsymbol	x	y	z
C	–0.56772600	0.00006300	–0.00008500
H	–1.02381600	–0.15454800	1.01160000
H	–1.02438600	–0.79944200	–0.63877000
H	–1.02585600	0.95289400	–0.37183400
O	0.81005200	0.00009000	–0.00006100

Tabelle 9.18 Standardorientierung von **Pent** [B3LYP/6-31+G(d); PCM-Rechnung; Lösungsmittel: THF].

Atomsymbol	x	y	z
Si	0.26358100	0.63328400	0.23160700
O	0.29191700	0.04773300	1.93342300
C	–0.67215900	0.45877800	2.86012800
H	–0.55447700	1.51787100	3.14262300
H	–1.70438600	0.33518900	2.48348000
H	–0.58375800	–0.15333600	3.77261700
O	0.19853900	2.24733400	0.87733400
C	–0.34052800	3.40852800	0.29241900
H	–1.00861100	3.89982600	1.01745600
H	0.45434100	4.12551600	0.03091700
H	–0.91333600	3.19676900	–0.61866500
O	0.19756700	1.22933400	–1.47998600
C	1.17728500	2.07258700	–2.02737900
H	1.63485800	1.61431000	–2.92087500
H	0.73950700	3.03533900	–2.34278100
H	1.99380700	2.29547400	–1.32124300
C	2.73530600	–0.76480600	0.92334600
C	2.28364200	–0.72256700	–1.33501400
C	2.99083800	–2.22381500	0.46473700
H	2.32218500	–0.69230700	1.92766300
H	3.69720000	–0.21173700	0.89934900
C	2.67696600	–2.19707800	–1.05628600
H	3.18308200	–0.17114700	–1.67852600
H	1.52194100	–0.62573100	–2.10971800
H	4.01752100	–2.54883900	0.67817800
H	2.31389800	–2.90940700	0.98900200
H	3.52945700	–2.51557500	–1.67024000
H	1.83758600	–2.86223800	–1.29161700
N	1.81051800	–0.20344900	–0.05610100
C	–1.39748200	–0.29652600	–0.12384400
C	–2.51330400	0.30637600	–0.73711700
C	–1.54460300	–1.64765600	0.24842500
C	–3.70823900	–0.38996200	–0.96443000
H	–2.44552700	1.34423800	–1.05422100
C	–2.72288300	–2.36527800	0.00934600
H	–0.71364600	–2.14377500	0.74535400
C	–3.81649900	–1.73601600	–0.59766500
H	–4.55090100	0.11521800	–1.43447900
H	–2.79111800	–3.41239300	0.30123700

H	–4.73762300	–2.28569700	–0.78147100

Quantenchemische Studien zum Mechanismus der stereokontrollierten Substitution an Aminodimethoxysilanen

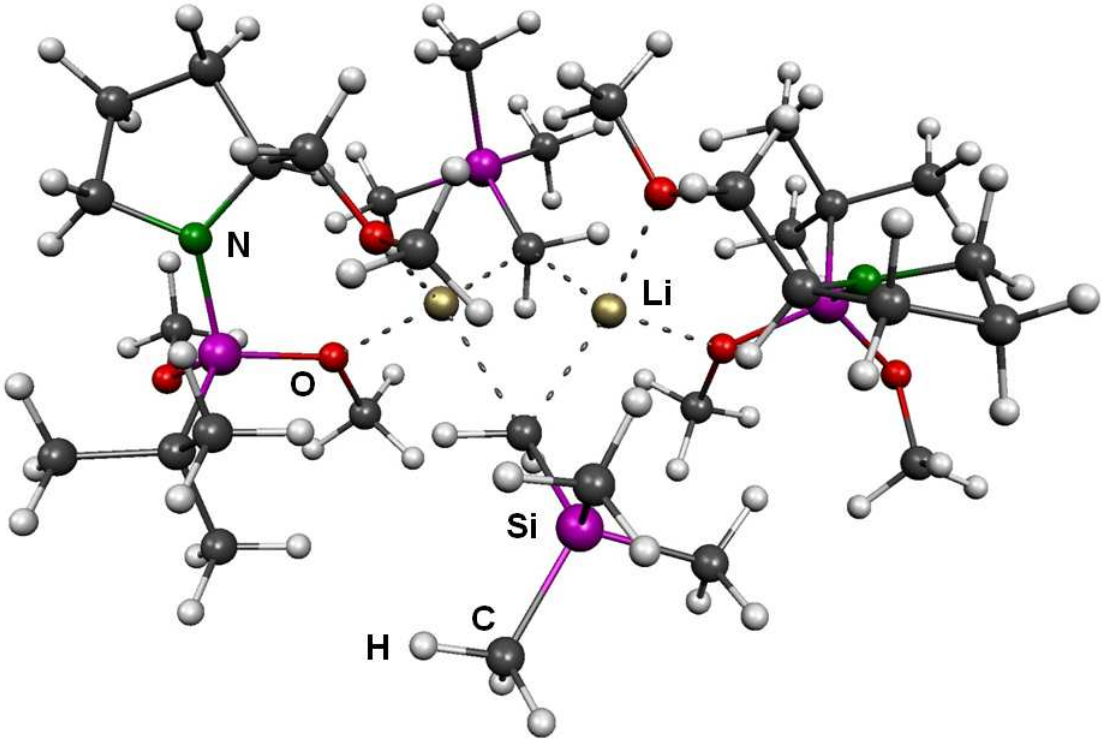

Abbildung 9.1 Molekel-Darstellung von [(S_C)-**92**·Me_3SiCH_2Li]$_2$ [M052X/6-31+G(d)].

Tabelle 9.19 Standardorientierung von [(S_C)-**92**·Me_3SiCH_2Li]$_2$ [M052X/6-31+G(d)].

Atomsymbol	x	y	z
C	4.25386600	3.03601900	–1.74729400
C	0.16449800	4.86493200	–1.43970200
C	6.16520800	2.63193500	–0.17356400
C	–2.53362700	3.49428700	–1.39171300
C	4.67940300	2.34290900	–0.44319600
C	2.60988400	0.05952500	–2.57865000
C	–5.76345000	1.32029500	–2.12882200
C	5.76340600	–1.32032200	–2.12893600
C	3.84514500	2.89508400	0.71859200
C	–0.01432700	1.78014600	–0.77865500
C	–2.60993800	–0.05954500	–2.57858900
C	–0.97334400	4.01661700	1.20701600

C	–5.89152700	2.12097800	1.86708600
C	5.95356900	–0.65473200	1.43573800
C	–4.45596000	2.24423500	2.38866300
C	–5.95354000	0.65473500	1.43586900
C	–3.63909500	1.22824100	1.55081000
C	–4.25385400	–3.03604300	–1.74714700
C	0.01430200	–1.78012100	–0.77864400
C	5.89156700	–2.12097800	1.86694400
C	3.63912800	–1.22824300	1.55072100
C	2.53356600	–3.49427900	–1.39181300
C	1.18734200	1.37303600	2.44826600
C	–4.67939900	–2.34291300	–0.44306100
C	2.76558800	–0.38732700	2.46471400
C	–2.76553400	0.38731700	2.46477800
C	–6.16520200	–2.63194300	–0.17342800
C	4.45601100	–2.24424200	2.38854900
C	–3.84514200	–2.89506100	0.71874100
C	–0.16456400	–4.86491400	–1.43965200
C	–1.18730800	–1.37306800	2.44826800
C	0.97341100	–4.01656300	1.20700300
H	4.43742800	4.11432600	–1.66797000
H	4.82077100	2.66232900	–2.60446300
H	0.26466000	4.68252900	–2.51408600
H	–0.32681100	5.83387200	–1.30352600
H	3.18646200	2.90028200	–1.94524900
H	–2.45159500	3.44831600	–2.48289500
H	6.31706800	3.71460700	–0.08881200
H	6.79948100	2.25850800	–0.97994500
H	–3.03926300	4.43237000	–1.14211400
H	1.17511900	4.93802900	–1.02407200
H	–6.70808000	1.37923600	–2.66806400
H	6.70802900	–1.37927200	–2.66818900
H	3.49248800	0.32135700	–3.16367300
H	1.81470300	0.77683400	–2.77668000
H	4.03349800	3.96989900	0.82871700
H	–5.80259700	1.97689000	–1.25606100
H	–4.95564200	1.65960900	–2.78207300
H	–3.17092200	2.66617600	–1.07234400
H	6.50021000	2.17997300	0.76543600
H	5.80256100	–1.97690700	–1.25616800
H	2.27689100	–0.94413200	–2.84028800
H	2.77572600	2.75669400	0.54758300

H	–0.10121600	1.50667700	–1.84459800
H	–2.27692700	0.94410200	–2.84023900
H	–3.49256200	–0.32135900	–3.16359100
H	4.95558800	–1.65964000	–2.78217400
H	–1.54341500	4.95008500	1.25104600
H	–6.03557900	2.76429100	0.99608400
H	1.06453500	1.93967600	–0.61203700
H	4.10557700	2.40503200	1.66193800
H	6.75084200	–0.44841400	0.71789300
H	–1.81477900	–0.77687500	–2.77663300
H	0.00911800	4.21578600	1.64791700
H	–4.05245600	3.25310200	2.30178700
H	–6.63953100	2.37966000	2.61807600
H	–1.47949700	3.28126100	1.83928000
H	–2.98376700	1.73788600	0.84071200
H	–6.75082700	0.44842300	0.71803800
H	6.11369000	–0.01010900	2.31212300
H	–4.82075900	–2.66237000	–2.60432400
H	0.10115100	–1.50665300	–1.84459100
H	2.45147700	–3.44832800	–2.48299100
H	0.45172800	1.82300400	1.78710800
H	3.17088000	–2.66616400	–1.07249300
H	–3.18645100	–2.90030300	–1.94510100
H	6.03560500	–2.76428400	0.99593400
H	1.88247500	2.13014800	2.82301500
H	–4.42101400	1.96232900	3.44660100
H	–6.79947700	–2.25851400	–0.97980500
H	2.98378300	–1.73788400	0.84063700
H	–6.11364700	0.01010800	2.31225300
H	6.63958800	–2.37966400	2.61791700
H	3.39833100	0.26638700	3.07959700
H	–1.06455300	–1.93964800	–0.61198100
H	–4.43741100	–4.11434900	–1.66780600
H	3.03921100	–4.43235900	–1.14222400
H	–2.17186500	1.03216000	3.12711500
H	–6.50020500	–2.17998800	0.76557600
H	–0.26477400	–4.68252400	–2.51403300
H	0.68780000	0.89245600	3.29508100
H	–2.77572600	–2.75659100	0.54777800
H	–6.31705900	–3.71461700	–0.08868000
H	–3.39826600	–0.26640300	3.07966400
H	2.17193200	–1.03217800	3.12705400

H	4.42108500	–1.96234700	3.44649000
H	4.05250700	–3.25311000	2.30167000
H	–4.10564300	–2.40505500	1.66209100
H	–0.45172000	–1.82304300	1.78708300
H	–0.68773500	–0.89251600	3.29508000
H	1.47963500	–3.28121400	1.83922000
H	0.32674800	–5.83385400	–1.30348700
H	–4.03342300	–3.96989300	0.82883100
H	–1.17516700	–4.93800300	–1.02397600
H	–1.88245000	–2.13017200	2.82301800
H	1.54344700	–4.95005400	1.25101600
H	–0.00903100	–4.21568200	1.64797000
N	4.63868200	–0.43239700	0.83229900
N	–4.63866400	0.43239900	0.83240600
O	5.56483900	0.03409800	–1.74185200
O	2.90692600	0.08003600	–1.17156900
O	–5.56487300	–0.03412000	–1.74172600
O	–2.90694900	–0.08004000	–1.17150200
O	1.88927100	0.40453000	1.67739000
O	–1.88923400	–0.40453100	1.67742700
Si	–0.79662300	3.44260700	–0.60691900
Si	4.43539700	0.48731500	–0.60772100
Si	–4.43540600	–0.48732100	–0.60761400
Si	0.79660100	–3.44258200	–0.60693100
Li	1.20728400	–0.07329600	–0.15001800
Li	–1.20728500	0.07330900	–0.14999200

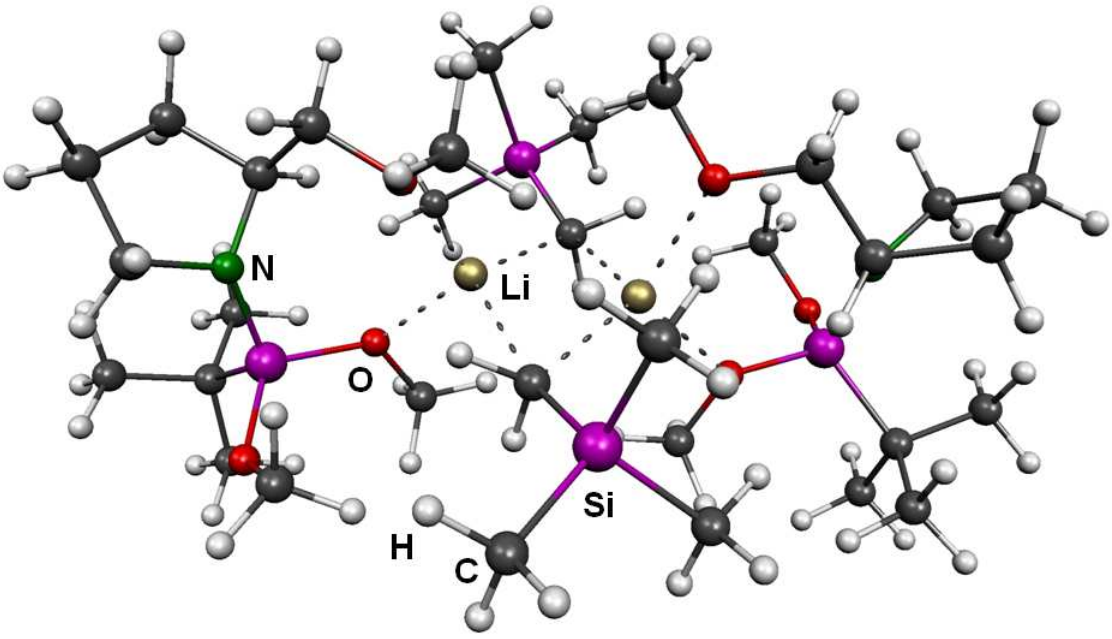

Abbildung 9.2 Molekel-Darstellung von *anti*-[(S_C)-**92**·Me_3SiCH_2Li]$_2$ [M052X/6-31+G(d)].

Tabelle 9.20 Standardorientierung von *anti*-[(S_C)-**92**·Me_3SiCH_2Li]$_2$ [M052X/6-31+G(d)].

Atomsymbol	x	y	z
C	–0.36303800	4.98665200	–0.12938800
C	2.18889900	3.60374700	0.74981000
C	–2.07494500	–0.35981600	2.36761700
C	–3.55934700	3.13320700	0.87547500
C	–0.22457700	1.81819900	0.01636200
C	2.07499500	0.36010600	2.36759500
C	1.26277200	3.46078900	–2.16810600
C	6.50268900	–0.25656400	–2.15696400
C	–5.70055700	1.23356000	–1.25787900
C	5.70029000	1.06426900	–2.13157100
C	5.70052300	–1.23366300	–1.25785600
C	4.33325500	0.66616800	–1.54540400
C	0.22452400	–1.81803800	0.01638500
C	–6.50243200	0.25648300	–2.15729800
C	–4.33320100	–0.66627500	–1.54533500
C	–2.18877800	–3.60360300	0.74994300
C	–1.39955300	0.96979300	–3.03927100
C	–3.40658800	–0.19451200	–2.65787300
C	3.40655300	0.19436300	–2.65784600
C	–5.70026100	–1.06446100	–2.13134500
C	0.36315000	–4.98649300	–0.12948600
C	1.39931500	–0.96956500	–3.03923300

C	–1.26282700	–3.46070700	–2.16806900
H	–0.67461400	5.10210100	0.91348900
H	0.20417400	5.87971600	–0.41125400
H	1.88898100	3.68729900	1.79987200
H	2.74794300	4.50771600	0.49039500
H	–1.26860900	4.95650100	–0.74451900
H	–2.50547200	–1.21312600	2.89269200
H	–2.15923100	0.54051300	2.98094000
H	–4.08040800	4.07088200	1.06579100
H	2.85908000	2.74601600	0.66544300
H	–1.02779100	–0.56666100	2.16167600
H	–2.54632000	3.18672200	1.27274300
H	–0.45626200	1.83099200	1.09538100
H	1.02781300	0.56683800	2.16164200
H	2.50544000	1.21350000	2.89260500
H	1.91646300	4.32345100	–2.32940500
H	7.51366100	–0.10717100	–1.77634200
H	–1.20399900	1.90411300	–0.48205500
H	–3.49915100	2.96032300	–0.20230200
H	–6.32095400	1.71878300	–0.50363100
H	2.15933800	–0.54017300	2.98098600
H	0.42069000	3.55301500	–2.86149100
H	6.17405700	1.78562300	–1.46426400
H	6.59322000	–0.65184300	–3.16988800
H	1.81527200	2.55497000	–2.43193300
H	3.84963700	1.49087600	–1.01644400
H	6.32071600	–1.71917600	–0.50362700
H	–5.25576500	2.03015500	–1.86603400
H	0.45612400	–1.83079600	1.09542700
H	–1.88873200	–3.68730600	1.79995600
H	–0.43815700	1.17969900	–2.57693500
H	–2.85885300	–2.74577400	0.66574000
H	–7.51365600	0.10732600	–1.77725600
H	–1.91769600	1.91179700	–3.24667100
H	5.61716800	1.52661500	–3.11763800
H	–3.84951200	–1.49091400	–1.01632800
H	5.25565800	–2.03004700	–1.86624400
H	–6.59229900	0.65165800	–3.17032400
H	–3.85609600	0.66366400	–3.17396400
H	1.20400100	–1.90384500	–0.48192000
H	–2.74797700	–4.50747100	0.49050600
H	3.25308700	0.99411100	–3.39242300

H	0.67474000	–5.10199800	0.91338000
H	–1.26134700	0.41548300	–3.97340500
H	3.85601700	–0.66382200	–3.17396600
H	–3.25318000	–0.99427800	–3.39244300
H	–5.61723100	–1.52726600	–3.11720300
H	–6.17411600	–1.78542400	–1.46367700
H	0.43796500	–1.17947300	–2.57680200
H	1.26103500	–0.41496400	–3.97318500
H	–1.81543300	–2.55494700	–2.43187300
H	–0.20397600	–5.87958600	–0.41143100
H	1.26872000	–4.95620800	–0.74461500
H	1.91730800	–1.91157100	–3.24699900
H	–1.91641200	–4.32344800	–2.32936900
H	–0.42074600	–3.55282000	–2.86147200
N	–4.65995300	0.41808500	–0.62873800
N	4.66000700	–0.41811700	–0.62871000
O	–2.73210900	–0.17087900	1.10618100
O	2.73218800	0.17114400	1.10619000
O	–2.15495700	0.19523300	–2.11502800
O	2.15497400	–0.19537300	–2.11488900
Si	0.66099500	3.39118700	–0.35976100
Si	–4.26862600	0.50939800	1.04201800
Si	4.26857200	–0.50941000	1.04203700
Si	–0.66097000	–3.39106700	–0.35975400
Li	–1.24105300	–0.16795000	–0.30161200
Li	1.24105600	0.16814500	–0.30156800
C	5.48882500	0.34392900	2.20274100
O	4.28656700	–2.08923700	1.52337100
C	3.55932700	–3.13326100	0.87514300
C	6.89945400	–0.12750800	1.80571300
C	5.41793300	1.86630900	2.02298300
C	5.26082700	–0.02385700	3.67676000
H	2.54634700	–3.18726300	1.27247100
H	3.49898200	–2.96004800	–0.20257100
H	4.08072000	–4.07082400	1.06511700
H	7.00392900	–1.21175200	1.90110100
H	7.14532400	0.15953900	0.77902800
H	7.63943900	0.33982900	2.46631200
H	4.46291100	2.28030100	2.35299400
H	6.20981100	2.34593500	2.61065900
H	5.56128900	2.15678800	0.97698700
H	5.29807700	–1.10525100	3.82347200

H	6.04532600	0.43329100	4.29208600
H	4.30128900	0.33733500	4.05225000
O	–4.28693200	2.08921500	1.52339100
C	–5.48880300	–0.34411500	2.20270900
C	–6.89950100	0.12706700	1.80560500
C	–5.41773000	–1.86650100	2.02309900
C	–5.26091900	0.02383000	3.67671000
H	–7.00414800	1.21130200	1.90091500
H	–7.14530900	–0.16009900	0.77893800
H	–7.63942600	–0.34033200	2.46622900
H	–6.20963400	–2.34614500	2.61072600
H	–5.56094200	–2.15710000	0.97711500
H	–4.46271800	–2.28039200	2.35325000
H	–6.04531200	–0.43347400	4.29205700
H	–4.30129000	–0.33709200	4.05223800
H	–5.29842200	1.10522000	3.82334700

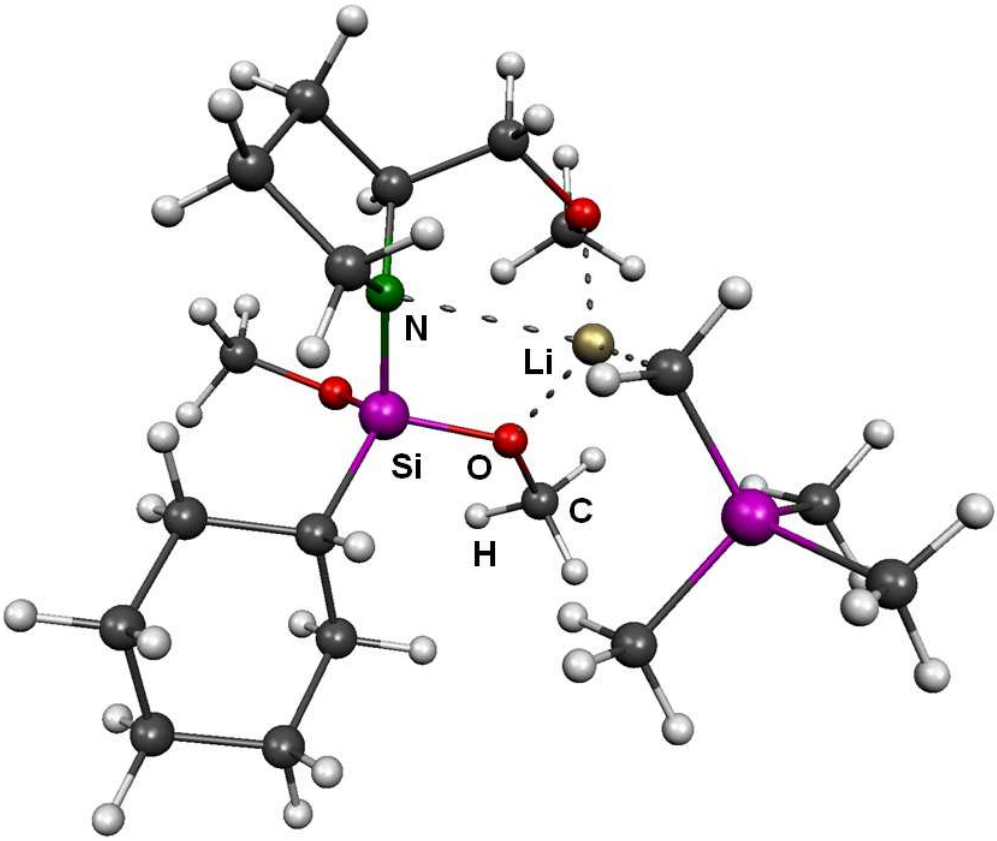

Abbildung 9.3 Molekel-Darstellung von ***syn*-Cy-E** [M052X/6-31+G(d)].

Tabelle 9.21 Standardorientierung von ***syn*-Cy-E** [M052X/6-31+G(d)].

Atomsymbol	x	y	z
C	0.62003100	0.23786900	2.79132800
C	–1.90694500	–1.99302200	–2.64645100
C	–1.76179800	–3.25995000	–1.78248700
C	–0.79510400	–1.08438600	–2.11762900
C	–1.00906700	–2.79020600	–0.50609600
C	2.75126700	–0.35707800	–1.38464500
C	0.34018400	–3.50560000	–0.41276900
C	0.71953100	–3.36166300	1.94368500
H	1.16749200	–0.53129100	3.33629900
H	–0.33537800	0.41441200	3.28637300
H	–2.87667900	–1.52170900	–2.46628000
H	1.21203300	1.15304700	2.77578100
H	–2.72574700	–3.70898200	–1.54186200
H	–1.81787600	–2.19913400	–3.71376400
H	–1.59007300	–2.98517700	0.39815000
H	–0.94666500	–0.02766500	–2.33317300
H	–1.17161100	–4.01704900	–2.30706400
H	0.17949100	–1.36178300	–2.53152300
H	0.19534600	–4.58532400	–0.28271500
H	0.90979400	–3.33248400	–1.32812500
H	1.52651300	–3.10574500	2.62743700
H	–0.18236900	–2.81396900	2.22658200
H	0.53419000	–4.43874800	1.99234000
N	–0.82208700	–1.34374800	–0.67413600
O	0.42008200	–0.21558600	1.45138900
O	1.15939800	–3.00474600	0.63881300
Si	–1.01642000	–0.19393700	0.58942700
Si	3.68439000	0.97037300	–0.54235000
Li	1.59109700	–1.13281600	0.13205700
H	3.40105600	–1.16428800	–1.74911800
H	2.19626100	0.04483600	–2.24312000
O	–2.11218100	–0.75698000	1.70793800
C	–3.45313800	–1.11058800	1.39777500
H	–4.12808200	–0.29834300	1.67271400
H	–3.57437300	–1.32987700	0.33137500
H	–3.71555700	–1.99822500	1.97393300
C	–1.39861700	1.51121900	–0.06354400
C	–2.76333500	1.59708700	–0.77412200
C	–1.32735600	2.57053000	1.05362200

H	–0.60647200	1.74643100	–0.78991700
C	–2.99644100	2.99901900	–1.34512500
H	–3.55997700	1.37660200	–0.05242700
H	–2.84414400	0.85040700	–1.57014400
C	–1.57454300	3.97544800	0.49550700
H	–2.08084000	2.34314200	1.82007900
H	–0.35100700	2.54538800	1.54260700
C	–2.91260300	4.05574500	–0.24229200
H	–3.96850100	3.04602000	–1.84408200
H	–2.23311200	3.20486500	–2.10479900
H	–1.54284100	4.71022900	1.30470900
H	–0.76031400	4.22276100	–0.19575300
H	–3.05367900	5.05464700	–0.66305900
H	–3.72829700	3.89177300	0.47296500
C	4.33809500	0.35869000	1.14851300
C	5.20540600	1.72958400	–1.41329200
C	2.52019000	2.43670000	–0.16930600
H	1.68499400	2.10615900	0.45555000
H	3.03771700	3.24989200	0.34838800
H	2.10212900	2.84123200	–1.09709700
H	5.95670800	0.95929800	–1.61181600
H	4.91622600	2.16290400	–2.37538600
H	5.67508600	2.51491100	–0.81159300
H	4.97712600	–0.52033800	1.01632100
H	4.92542700	1.12600200	1.66221100
H	3.51279200	0.07187600	1.81155700

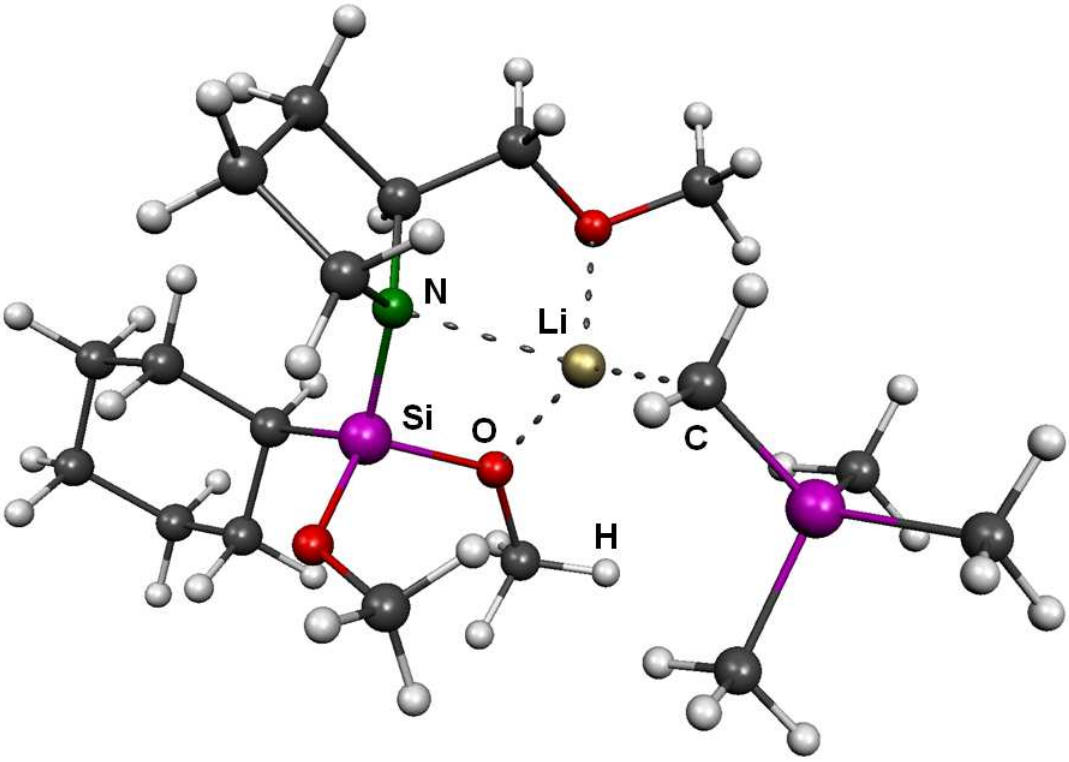

Abbildung 9.4 Molekel-Darstellung von ***anti*-Cy-E** [M052X/6-31+G(d)].

Tabelle 9.22 Standardorientierung von ***anti*-Cy-E** [M052X/6-31+G(d)].

Atomsymbol	x	y	z
C	0.24654300	–2.25070300	–1.45649900
C	–1.43479800	2.71095100	2.06369500
C	–1.48513300	3.34877200	0.66299800
C	–0.32991900	1.65783300	1.93815700
C	–0.80827400	2.31405400	–0.27916800
C	3.17315900	0.55589500	0.77650400
C	0.45067500	2.92275600	–0.88263000
C	2.26902500	2.44982500	–2.31260200
H	1.27220500	–2.38946600	–1.79290300
H	–0.42735200	–2.32193400	–2.31181300
H	–2.38081400	2.21474100	2.29055600
H	0.00099500	–3.02746300	–0.72836000
H	–2.50422000	3.57530800	0.34833200
H	–1.23506400	3.44080100	2.84930800
H	–1.46284700	2.00706400	–1.10023000
H	–0.42465600	0.84939300	2.66126100
H	–0.92542800	4.28835900	0.64538000
H	0.66341400	2.10162800	2.05842900
H	0.19010400	3.79369600	–1.49669500

H	1.13361400	3.24366200	–0.08456900
H	2.69363600	1.63867700	–2.89882200
H	2.01144000	3.28674700	–2.96819300
H	2.99186000	2.76928800	–1.55743400
N	–0.48156000	1.15219200	0.56496900
O	0.14917000	–0.95524000	–0.86632200
O	1.09218400	1.94439600	–1.68711800
Si	–1.04208200	–0.45376300	0.20674700
Si	4.28899400	–0.77728400	0.20335400
Li	1.45738700	0.47602900	–0.38059000
O	–0.98654500	–1.38423300	1.56428300
C	0.23563100	–1.75313000	2.21810100
H	0.09729500	–1.62357000	3.29129600
H	0.44823400	–2.80170000	2.00783600
H	1.07769400	–1.14271600	1.88155100
H	3.61497200	1.54823700	0.59926200
H	2.97687700	0.47935300	1.85499700
C	–2.76101600	–0.59529300	–0.51710200
C	–3.23654000	–2.06267300	–0.55332700
C	–3.76571000	0.26299600	0.27468800
H	–2.72502200	–0.22109200	–1.55101100
C	–4.65124700	–2.17682800	–1.12848900
H	–3.22613900	–2.46221000	0.46669700
H	–2.54936100	–2.67886200	–1.13981400
C	–5.18167500	0.13927500	–0.29512500
H	–3.76770600	–0.06513600	1.32218500
H	–3.45610700	1.31197800	0.27195900
C	–5.63655300	–1.32068600	–0.33135500
H	–4.97016600	–3.22280500	–1.12769900
H	–4.64484600	–1.84305200	–2.17324800
H	–5.87771400	0.74055000	0.29644200
H	–5.19166200	0.54491300	–1.31430800
H	–6.63944100	–1.39509000	–0.75997100
H	–5.69603500	–1.70386800	0.69441300
C	3.62587200	–2.48979700	0.72163200
C	4.39441000	–0.78503000	–1.70562800
C	6.10759300	–0.75309700	0.78676800
H	2.62661800	–2.67575000	0.31684200
H	4.28668900	–3.29009300	0.37530400
H	3.56076700	–2.56034600	1.81243200
H	6.68704200	–1.58208500	0.36682200
H	6.59229000	0.18301200	0.49309400

H	6.15815800	–0.82008900	1.87766500
H	3.40455100	–0.90735900	–2.16080800
H	4.81181500	0.16038800	–2.06803800
H	5.03555400	–1.59198100	–2.07302000

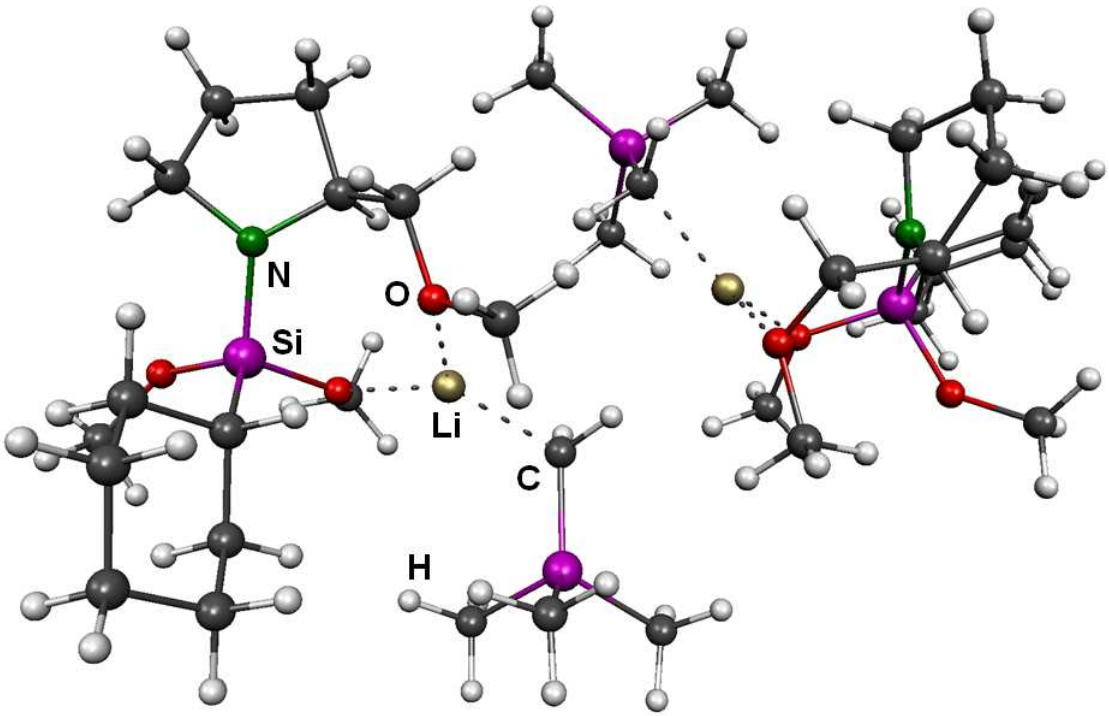

Abbildung 9.5 Molekel-Darstellung von **(*syn*-Cy-E)$_2$** [HF/3-21G].

Tabelle 9.23 Standardorientierung von **(*syn*-Cy-E)$_2$** [HF/3-21G].

Atomsymbol	x	y	z
C	–3.77523700	0.52204500	–2.91658900
C	–0.87173600	–1.54890700	–1.27954800
C	2.97228500	–1.40191200	–1.91973000
C	5.38352300	1.11056900	3.56276600
C	–5.85039200	3.32803300	0.40053500
C	4.69433400	–0.17202600	4.09959300
C	4.74488100	1.32268900	2.17622900
C	4.08790900	–0.86901000	2.83928400
C	1.01981700	1.90103000	0.67829500
C	–4.97936900	4.57479700	0.16631000
C	–3.51089100	2.64939400	0.39187000
C	–1.99391900	–0.33571900	2.10148400
C	–2.82228500	1.86813300	1.49916300
C	2.56100000	–0.86203500	2.93881100

C	–3.63211100	4.14779000	0.77631300
C	1.95981300	–2.77082600	1.49348000
H	–3.15579700	1.40487500	–2.99082600
H	–4.71239000	0.69642800	–3.42390500
H	–3.26220900	–0.32014100	–3.34829400
H	–0.13195200	–1.34494300	–0.50093500
H	1.90545900	–1.53887900	–1.87138400
H	3.46789000	–2.36204700	–1.90150000
H	6.44473900	0.93381100	3.44276100
H	–0.54449800	–1.07182400	–2.20876700
H	–6.68120200	3.26155500	–0.28579100
H	3.22754600	–0.86721200	–2.82167000
H	5.39946400	–0.81812100	4.60435600
H	5.24070300	1.95862600	4.21881400
H	4.44526200	–1.88333200	2.73392200
H	5.38276000	1.88374300	1.51009400
H	–6.22830400	3.32503500	1.41879200
H	–1.92967900	–1.33591200	1.70783900
H	–4.86882000	4.74477000	–0.89778100
H	–2.58027000	–0.32657800	3.01226100
H	3.91064300	0.08181000	4.80451000
H	–2.92982300	2.54480100	–0.51624900
H	3.79762400	1.84098900	2.25291400
H	–5.38490300	5.46402100	0.63037500
H	–3.43565200	1.89152400	2.39121100
H	2.23096300	–1.46843400	3.77647300
H	–1.00018800	0.04353800	2.28517600
H	2.20169800	0.14737000	3.06032700
H	–1.84591600	2.28530900	1.70289200
H	–3.67962000	4.24736000	1.85631300
H	–2.79189600	4.72099100	0.41257800
H	1.26148100	–2.96287400	0.69782400
H	2.94929800	–3.08600500	1.19966400
H	1.64322600	–3.29486800	2.38779000
N	–4.90558800	2.21139300	0.17243800
N	4.54600000	–0.05938200	1.69707500
O	–4.02003800	0.21677300	–1.51468700
O	3.37297300	–0.61623900	–0.75907700
O	–2.65143600	0.47979700	1.09032600
O	1.93068000	–1.33833000	1.72593000
Si	–1.27790500	–3.35004200	–1.49319900
Si	–5.33508300	0.71524900	–0.57650600

Si	4.81874300	–0.66000200	0.10196800
Si	1.43212700	3.15496500	–0.63333800
Li	–2.45100300	–0.31415600	–0.64519900
Li	1.98632000	0.04936700	0.38354500
H	0.00114400	1.51615800	0.57119500
H	1.14604900	2.28691800	1.69588100
O	5.15282300	–2.28991700	0.18812200
C	6.26388600	–3.11796200	0.53968500
H	7.00867100	–3.11437600	–0.24564300
H	6.72924600	–2.78997600	1.46230200
H	5.89876300	–4.12563300	0.66902400
O	–6.58230200	1.06508500	–1.61477900
C	–7.67382000	0.41716900	–2.26485300
H	–8.15651600	1.14202300	–2.90342000
H	–7.33620800	–0.41443500	–2.87230700
H	–8.39584600	0.04920300	–1.54642300
C	6.17247200	0.32216500	–0.78253000
C	7.51717300	0.29613500	–0.01284400
C	6.39329900	–0.16007900	–2.23787200
H	5.84132200	1.35730600	–0.83610000
C	8.57192000	1.16603600	–0.72130300
H	7.88678900	–0.72439600	0.03788700
H	7.37747800	0.63927000	1.00597300
C	7.45983900	0.69654700	–2.94604500
H	6.71049400	–1.19995800	–2.23347200
H	5.46422800	–0.10363500	–2.79252100
C	8.78742700	0.68556800	–2.16768200
H	9.50833400	1.13270700	–0.17311900
H	8.23288700	2.19780400	–0.73132600
H	7.61609800	0.32904600	–3.95530000
H	7.09649200	1.71719700	–3.02116300
H	9.51593400	1.31676500	–2.66581000
H	9.18692600	–0.32511000	–2.15297800
C	–5.76716400	–0.69180800	0.60522400
C	–6.92359100	–0.29037400	1.55327700
C	–6.08597300	–2.03263700	–0.09513500
H	–4.88335200	–0.84489300	1.21785800
C	–7.19748800	–1.40048800	2.58466300
H	–7.82666500	–0.11261200	0.97445200
H	–6.67571400	0.63513200	2.06324100
C	–6.35822300	–3.13803600	0.94248500
H	–6.96432900	–1.92188800	–0.72457600

H	–5.26058100	–2.32490900	–0.73437200
C	–7.50841600	–2.73549800	1.88332800
H	–8.02410200	–1.11462600	3.22782000
H	–6.31930800	–1.52263900	3.21260900
H	–6.59648600	–4.06858700	0.43748900
H	–5.45715300	–3.30487600	1.52542900
H	–7.67633100	–3.51326400	2.62129100
H	–8.42337100	–2.63116500	1.30591300
C	3.24630400	3.81165000	–0.46448400
C	1.30951400	2.39175100	–2.40646900
C	0.34874700	4.76859600	–0.72509000
C	–2.65163700	–3.61254300	–2.82761900
C	0.15130700	–4.55488200	–2.03188500
C	–1.96255000	–4.11949000	0.14901800
H	–1.25531300	–4.00218800	0.96793100
H	–2.89183100	–3.63561700	0.44064700
H	–2.16119200	–5.18189900	0.03153700
H	–2.33177500	–3.22336900	–3.79198400
H	–2.88319100	–4.66731000	–2.95353300
H	–3.56558500	–3.09582700	–2.54635500
H	0.97447800	–4.53998100	–1.32025100
H	–0.20324600	–5.58053400	–2.11112600
H	0.54883700	–4.26211100	–3.00139800
H	3.95558600	2.99643000	–0.57792700
H	3.46350700	4.55648600	–1.22622200
H	3.41138100	4.26861100	0.50864300
H	2.06376300	1.62085300	–2.53921600
H	0.33813400	1.92890900	–2.56669400
H	1.45600100	3.14781400	–3.17416600
H	0.70704100	5.44628600	–1.49734800
H	–0.68647700	4.52141000	–0.95262500
H	0.36469500	5.29945900	0.22442500

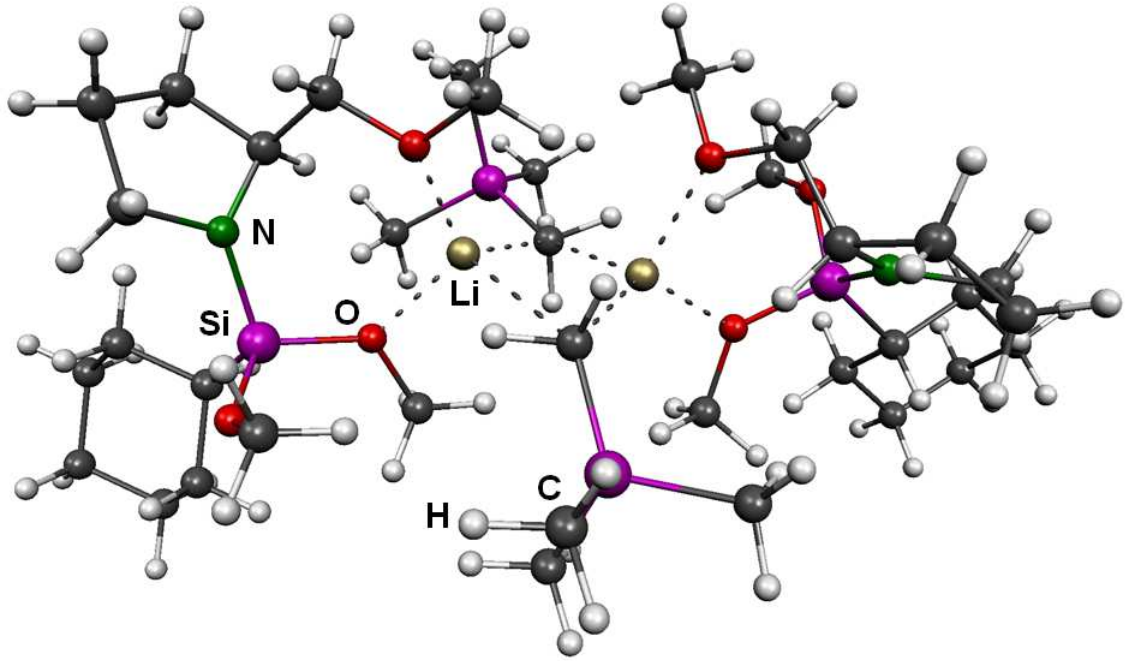

Abbildung 9.6 Molekel-Darstellung von **(*anti*-Cy-E)$_2$** [HF/3-21G].

Tabelle 9.24 Standardorientierung von **(*anti*-Cy-E)$_2$** [HF/3-21G].

Atomsymbol	x	y	z
C	2.51555800	–0.00508500	2.05227500
C	0.09746000	–1.79305800	–0.24681200
C	–2.07148900	–0.07548800	1.91876900
C	–6.31554700	0.25364400	–3.05624600
C	6.12959700	1.81429400	–0.81103700
C	–5.49359500	–1.05219800	–2.94020600
C	–5.84493200	1.12816800	–1.85123200
C	–4.22763600	–0.62105000	–2.16857200
C	0.18218800	2.13527100	–0.17717700
C	5.77769700	3.29904400	–1.00273000
C	3.80503500	1.97766800	–1.50812400
C	2.09456600	–0.85373800	–3.17455500
C	3.19766500	1.25435100	–2.69746200
C	–3.22058800	0.00119200	–3.12858300
C	4.59246700	3.22616900	–1.97727400
C	–1.00892700	0.94684600	–3.30280000
H	3.32229600	0.40403500	2.64632600
H	2.19875700	–0.95009900	2.46542200
H	1.69314500	0.68655700	2.05297000
H	0.16834900	–1.77525100	0.84857400
H	–1.01955700	0.08405900	1.77280100

H	–2.24821700	–1.07589100	2.28379800
H	–7.37842300	0.05995600	–3.01285500
H	1.12479300	–1.87676900	–0.61338500
H	6.66258800	1.64898700	0.11392100
H	–2.44751400	0.65150800	2.62376000
H	–6.03163500	–1.77607100	–2.34287700
H	–6.10559700	0.75694100	–3.99128700
H	–3.76242500	–1.45452000	–1.66484300
H	–6.65142400	1.29855600	–1.15169500
H	6.74947000	1.46867000	–1.63383600
H	1.33259800	–1.49240800	–2.76693700
H	5.45424200	3.71941400	–0.05910800
H	3.02180700	–1.39084700	–3.29419100
H	–5.27399800	–1.49413700	–3.90351700
H	3.01186300	2.26206400	–0.83545100
H	–5.49653700	2.09279100	–2.19957600
H	6.60687400	3.87650000	–1.38958100
H	3.98998400	0.79479200	–3.27348100
H	–3.00508100	–0.68847700	–3.93642800
H	1.76615300	–0.45519400	–4.12741100
H	–3.62134800	0.91672500	–3.54417200
H	2.64154300	1.94297300	–3.32313600
H	4.96425700	3.07233700	–2.98608800
H	3.97408700	4.11320000	–1.96616600
H	–0.08947600	1.01082200	–2.75196600
H	–0.86479500	0.35804800	–4.20092900
H	–1.35534500	1.93791900	–3.56561100
N	4.81093300	1.14567000	–0.80102100
N	–4.75184900	0.35666700	–1.21105100
O	2.92186300	–0.19194800	0.67468000
O	–2.72115800	0.09115300	0.61990500
O	2.28872800	0.22519500	–2.22388300
O	–1.98094400	0.29729200	–2.44238700
Si	–0.83426300	–3.34134600	–0.76244300
Si	4.44916800	–0.35703900	–0.02588700
Si	–4.34665100	0.53718600	0.46172300
Si	0.53899200	3.43282800	1.13713000
Li	1.36031500	0.25224700	–0.42814500
Li	–1.30952200	–0.11803900	–0.66268500
O	–4.53981700	2.11764200	0.91541900
O	4.38484200	–1.61710300	–1.11214100
C	–3.95397300	3.34729200	0.45968900

C	4.02658900	–3.00230600	–0.99885800
H	4.82497700	–3.56623000	–0.53332700
H	3.11756500	–3.13037500	–0.42740800
H	3.86728700	–3.38646400	–1.99493200
H	–2.87523900	3.29594600	0.48730400
H	–4.26655300	3.56902900	–0.55350800
H	–4.29161800	4.13441200	1.11615300
H	0.51217900	2.52732400	–1.14956700
H	–0.90725200	2.02345600	–0.25021700
C	–5.39629000	–0.50994400	1.64719100
C	–5.56883700	0.13981200	3.04251600
C	–6.78931100	–0.82327200	1.04791100
H	–4.88228400	–1.46170200	1.77950200
C	–6.38411100	–0.77212000	3.97861900
H	–6.07085400	1.09355300	2.92719000
H	–4.60332400	0.34258100	3.49191500
C	–7.59880200	–1.73983700	1.98221300
H	–7.33755500	0.10463900	0.90507100
H	–6.67821200	–1.29075600	0.07682300
C	–7.76034200	–1.09695900	3.37121600
H	–6.50800700	–0.29109800	4.94402800
H	–5.83775100	–1.69720700	4.14100700
H	–8.57364800	–1.94226400	1.54890300
H	–7.08072800	–2.68936400	2.08342000
H	–8.31214500	–1.76113600	4.02862800
H	–8.33442600	–0.17928700	3.27571700
C	5.77504200	–0.78220800	1.27742700
C	5.35296200	–1.89460300	2.27451100
C	7.09684200	–1.22887100	0.59098000
H	5.98364900	0.11582200	1.85750300
C	6.45542600	–2.14352100	3.32253700
H	5.17049600	–2.81692200	1.73193100
H	4.43432000	–1.63684800	2.78310400
C	8.20826700	–1.47460700	1.62810100
H	6.91085900	–2.14430300	0.03881300
H	7.43079100	–0.49110400	–0.12794900
C	7.77839700	–2.54364600	2.64739200
H	6.13830500	–2.92061000	4.01104200
H	6.60612500	–1.23547400	3.89966400
H	9.11892300	–1.78467700	1.12489200
H	8.42152000	–0.54538400	2.14922100
H	8.55281300	–2.68257200	3.39473100

H	7.64504600	–3.49230800	2.13457300
C	–0.15853800	5.21179400	0.79092300
C	–0.19346600	2.97834300	2.87084300
C	2.42403500	3.76276400	1.43772400
H	0.12033100	5.90390800	1.58297200
H	0.23295700	5.59963600	–0.14706500
H	–1.24320400	5.20731000	0.71817800
H	–1.27769600	2.91029100	2.83213800
H	0.18604600	2.03182700	3.24563700
H	0.06151600	3.74894000	3.59445300
H	2.55531100	4.35455700	2.34080200
H	2.99522100	2.84685400	1.54587400
H	2.85247900	4.32789300	0.61340700
C	–1.22850800	–3.35599300	–2.65884300
C	0.05939000	–5.03424500	–0.45347300
C	–2.51550600	–3.50589700	0.18188400
H	–3.16168800	–4.24433600	–0.28675900
H	–2.33721300	–3.82518600	1.20654700
H	–3.04094800	–2.55869100	0.22030200
H	–1.63324400	–2.40088900	–2.97396000
H	–0.32593800	–3.54089300	–3.23815300
H	–1.94242800	–4.13774900	–2.90723900
H	–0.55763800	–5.87196400	–0.77192300
H	0.99829100	–5.08458400	–1.00089200
H	0.28291900	–5.16246200	0.60292900

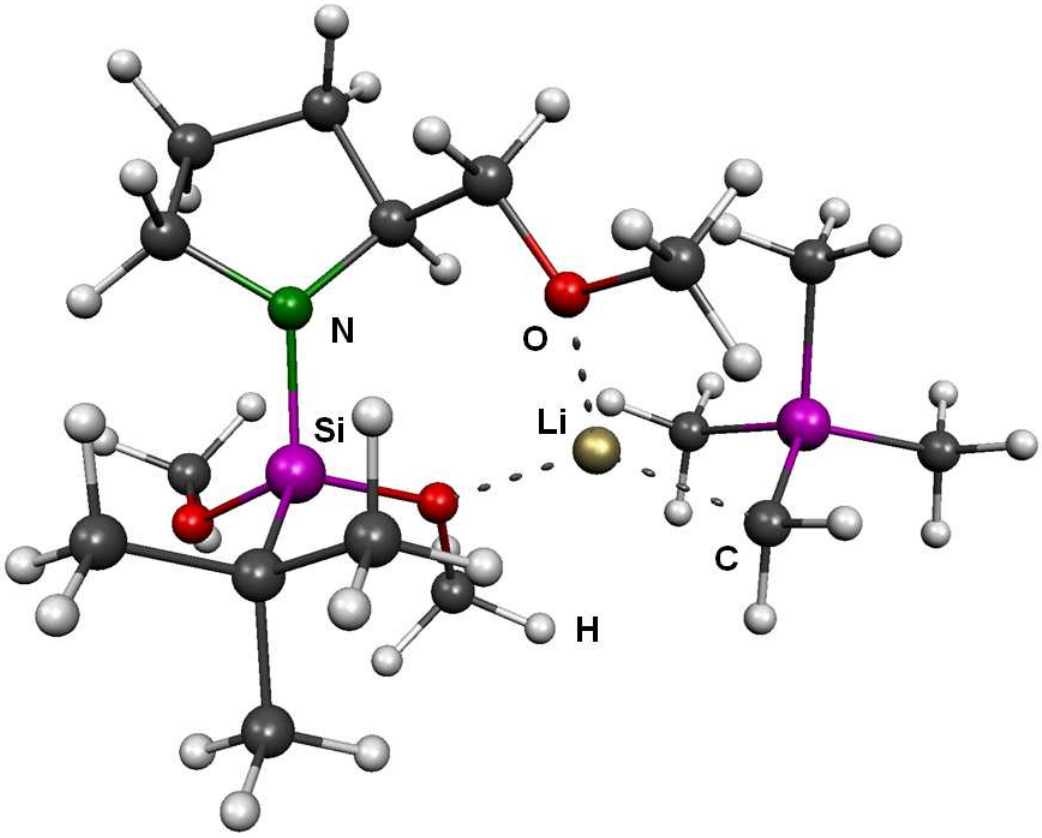

Abbildung 9.7 Molekel-Darstellung von ***syn-t*Bu-E** [M052X/6-31+G(d)].

Tabelle 9.25 Standardorientierung von ***syn-t*Bu-E** [M052X/6-31+G(d)].

Atomsymbol	x	y	z
C	–2.60145300	–0.45985200	–2.89140100
C	0.19570400	–2.01479300	–1.59678400
C	–2.61532200	3.03634300	–1.11734200
C	–1.20744000	3.35379600	–0.60428700
C	–3.02577300	1.87039500	–0.21715400
C	–0.63897800	1.98848000	–0.14070800
C	–2.37325000	–3.12382300	0.78827000
C	3.10757900	–1.44496900	0.71210200
C	3.52166400	–0.25261300	–2.08468100
C	–2.44253000	–1.62674000	1.12714300
C	0.02103400	2.14422100	1.21860100
C	–3.90353600	–1.22986400	1.39160200
C	–1.60823700	–1.35150100	2.38586600
C	6.02799400	–0.71589700	–0.42687100
C	1.28596100	1.00183900	2.86284100
C	4.06300800	1.45550200	0.38438300
H	–3.55536400	–0.00877700	–3.16926800

H	–1.82773600	0.31457700	–2.89870900
H	–2.34432700	–1.22758200	–3.62250100
H	0.40005900	–1.53703100	–2.55509400
H	–0.60016400	–2.75077600	–1.71289200
H	–2.57750400	2.69866100	–2.15573600
H	1.10154800	–2.49175900	–1.22778100
H	–0.57036600	3.82482900	–1.35241500
H	–3.29269900	3.88892600	–1.05291800
H	0.11168400	1.61450100	–0.84380400
H	–3.83636900	1.26764000	–0.63313700
H	–2.95010600	–3.35941400	–0.10919900
H	3.12728000	–2.47328600	0.32683900
H	3.49444900	–1.25239300	–2.53008500
H	2.50500500	0.15651500	–2.12320200
H	–1.34101300	–3.45320100	0.63676000
H	–1.27234700	4.03456400	0.25099200
H	–4.53108000	–1.40190100	0.51333400
H	–3.35294700	2.24483000	0.76204000
H	3.44299100	–1.48261500	1.75763000
H	–2.78420100	–3.70835400	1.61976700
H	4.15845400	0.37661900	–2.71343600
H	0.77219500	2.94406700	1.18752500
H	–3.98924200	–0.17772900	1.67986600
H	6.18163100	–1.70437900	–0.86973200
H	–0.56769200	–1.66761000	2.26216800
H	–4.30413300	–1.83040900	2.21669100
H	–0.73980700	2.39645700	1.96885700
H	–1.61186500	–0.28946600	2.64600600
H	1.79625500	0.05469600	3.02135100
H	2.01732300	1.81402700	2.87031600
H	3.03873500	1.83948700	0.31735100
H	6.55603100	0.01975800	–1.04257900
H	–2.02484600	–1.91238100	3.23064300
H	6.49019400	–0.72526500	0.56471200
H	0.53257200	1.16552100	3.63863400
H	4.71487900	2.13370400	–0.17412000
H	4.36601800	1.48955600	1.43599900
N	–1.79383600	1.08369300	–0.10857000
O	–2.72864300	–1.06333200	–1.60958200
O	–0.18289500	–1.00416000	–0.64056400
O	0.65583000	0.92835700	1.58519300
Si	–1.78917900	–0.62462100	–0.31355100

Si	4.16398000	–0.33118200	–0.28668400
Li	1.26108700	–0.56642500	0.53752200

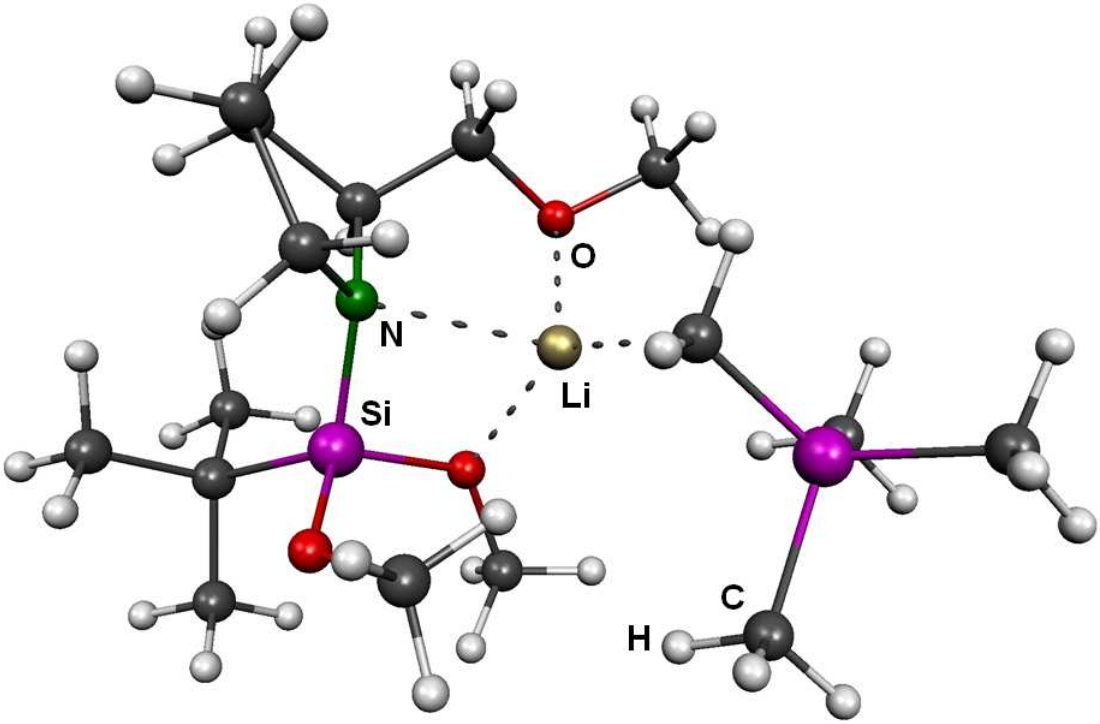

Abbildung 9.8 Molekel-Darstellung von ***anti-t*Bu-E** [M052X/6-31+G(d)].

Tabelle 9.26 Standardorientierung von ***anti-t*Bu-E** [M052X/6-31+G(d)].

Atomsymbol	x	y	z
C	0.13748300	–2.15785300	–1.74900800
C	–1.99897400	2.56934200	2.04016800
C	–2.57618400	2.75686200	0.62869400
C	–1.25475500	1.21464000	1.98636000
C	–1.57333900	2.01068200	–0.25787500
C	2.56133000	0.66903000	0.91048800
C	–0.37326400	2.89041500	–0.58750800
C	1.64393400	2.89467300	–1.82064000
H	1.19112800	–2.07628900	–2.00922000
H	–0.44965400	–2.29354800	–2.65820100
H	–2.77554400	2.57521600	2.80528500
H	–0.00214400	–3.01595200	–1.08755800
H	–3.55289700	2.27536000	0.54475800
H	–1.30247400	3.37538400	2.27695500
H	–2.00427200	1.68849500	–1.20771800
H	–1.78433300	0.44364900	2.54942900

H	–2.69183500	3.80733400	0.35342000
H	–0.24572400	1.29798800	2.39631000
H	–0.70135300	3.78541900	–1.12972300
H	0.15292800	3.19675900	0.32569200
H	2.26383300	2.23840600	–2.42594300
H	1.32008300	3.75405100	–2.41490200
H	2.21204800	3.22986300	–0.94971000
N	–1.19174000	0.84157600	0.55138900
O	–0.25087400	–0.94618600	–1.09832600
O	0.50840800	2.13843600	–1.40991400
Si	–1.45803500	–0.80601900	0.06115500
Si	3.88800800	–0.41442700	0.25918800
Li	0.90263600	0.54010000	–0.33216500
O	–1.16344100	–1.81094200	1.33019800
C	0.07747400	–1.91666100	2.03942900
H	–0.09665100	–1.65387300	3.08345800
H	0.41942900	–2.95000400	1.97992900
H	0.84134000	–1.25635400	1.62268100
H	2.86133600	1.72642300	0.84504900
H	2.36451500	0.46271100	1.97163300
C	–3.17062500	–1.29599700	–0.54635800
C	–3.18122400	–2.79374100	–0.89795800
C	–4.15549900	–1.05653100	0.61063500
H	–2.82381600	–3.40501500	–0.06662400
H	–2.56940400	–3.01045300	–1.77688800
H	–3.89964100	–1.66510100	1.48070500
H	–4.17071900	–0.00670500	0.91929200
C	3.48286700	–2.25550200	0.55424800
C	4.06721500	–0.18499000	–1.63044000
C	5.65642100	–0.18522900	0.94278800
H	2.54095800	–2.54765600	0.08066100
H	4.27468600	–2.89806600	0.15773800
H	3.39301400	–2.46224100	1.62568600
H	6.37222800	–0.86685600	0.47138000
H	6.00351200	0.83919800	0.77700500
H	5.67338900	–0.36654200	2.02159500
H	3.12086600	–0.37026400	–2.15179600
H	4.37821800	0.83940000	–1.86129100
H	4.81958900	–0.85966500	–2.04983900
C	–3.61795800	–0.49221700	–1.77516200
H	–5.17003000	–1.32430700	0.29282900
H	–4.20709700	–3.10255700	–1.13088700

H	–2.88177800	–0.53327700	–2.58364600
H	–4.55860700	–0.90475800	–2.15789300
H	–3.80264600	0.55674100	–1.53052100

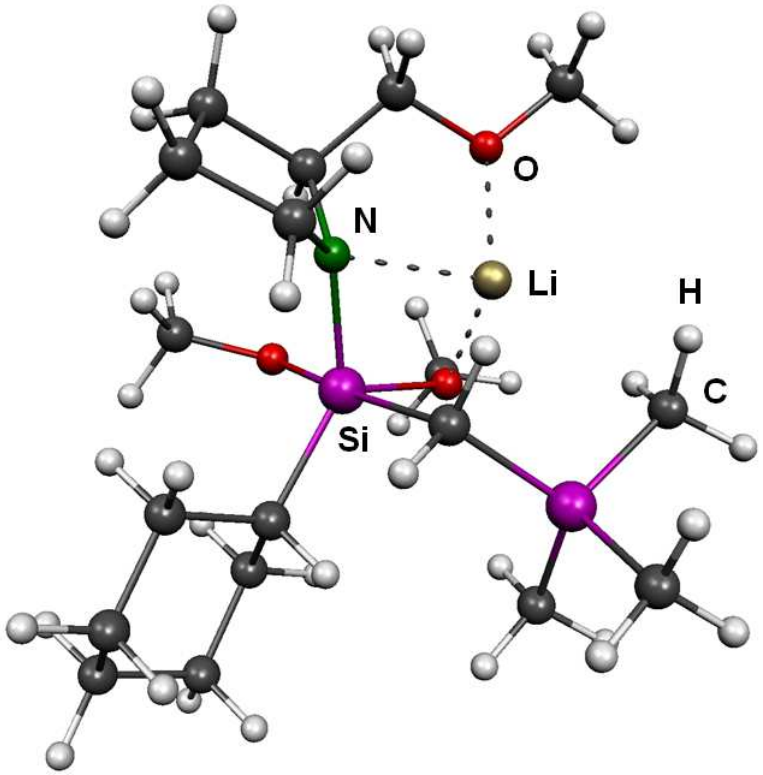

Abbildung 9.9 Molekel-Darstellung von **I1** [M052X/6-31+G(d)].

Tabelle 9.27 Standardorientierung von **I1** [M052X/6-31+G(d)].

Atomsymbol	x	y	z
C	0.74901100	0.75376700	2.73129100
C	1.46582600	–2.85823700	–2.03196600
C	2.37634200	–3.14314900	–0.81924300
C	1.32946200	–1.32892100	–2.03059100
C	2.31484800	–1.83312500	0.01688700
C	–0.08864600	1.24897300	–1.19321800
C	3.68760200	–1.15710700	–0.03131300
C	4.85997900	0.78223500	0.69157400
H	1.06662900	1.72092300	3.13011700
H	1.51796200	0.00425500	2.92520100
H	0.47930200	–3.30143300	–1.87802400
H	–0.16934200	0.43839100	3.22473700
H	2.03693400	–4.00429700	–0.24373900
H	1.87045400	–3.24930700	–2.96719900

H	2.04757700	–1.99955600	1.05969400
H	0.43031700	–0.98246200	–2.53670200
H	3.40239800	–3.35284600	–1.13915700
H	2.18983100	–0.87946800	–2.55084100
H	4.41354000	–1.72392900	0.56236100
H	4.05679000	–1.08841600	–1.06213800
H	4.68649700	1.78723000	1.07154200
H	5.44425800	0.21388500	1.41938300
H	5.40663800	0.83397300	–0.25481500
N	1.31356200	–0.97086800	–0.60950400
O	0.53764500	0.92301700	1.33439400
O	3.59030800	0.17293500	0.50056600
Si	–0.16356700	–0.24629600	0.24337900
Si	–0.37748500	3.00921200	–0.60214300
Li	1.90882500	0.97415400	0.01306800
H	0.84142300	1.29744600	–1.79444200
H	–0.84880500	1.00837700	–1.94733900
O	–0.10208400	–1.45239100	1.54038600
C	–0.33814900	–2.82012000	1.36998800
H	–1.37780900	–3.08613900	1.59547400
H	–0.12697200	–3.15959700	0.34745900
H	0.30512400	–3.39034400	2.05123700
C	–2.07579700	–0.38368700	–0.00363600
C	–2.46800400	–1.48489400	–1.00689400
C	–2.88431300	–0.52081700	1.29478600
H	–2.38056100	0.56781300	–0.45797600
C	–3.97629100	–1.47944100	–1.28079600
H	–2.18782900	–2.46783800	–0.61107000
H	–1.92227100	–1.35675900	–1.94974800
C	–4.39037400	–0.50624300	1.01026900
H	–2.62383900	–1.44939200	1.80851600
H	–2.62630700	0.29283200	1.98094800
C	–4.76831100	–1.61263600	0.02216000
H	–4.24260500	–2.28571200	–1.97168200
H	–4.24501800	–0.53432800	–1.76875600
H	–4.95545400	–0.62053100	1.94063200
H	–4.66840100	0.46578400	0.58308300
H	–5.84271900	–1.59203400	–0.18332700
H	–4.54812200	–2.58716400	0.47660700
C	1.27722100	3.69428900	0.06626600
C	–0.85913500	4.13804700	–2.05042300
C	–1.71091100	3.20004900	0.72375000

H	–1.46766600	2.61017100	1.60894100
H	–1.80191600	4.24996200	1.01783700
H	–2.68660900	2.87322300	0.35333400
H	–0.09857900	4.11672200	–2.83635900
H	–1.80419500	3.81303300	–2.49501000
H	–0.98090300	5.17540100	–1.72451100
H	2.09657500	3.50912000	–0.64196900
H	1.22272600	4.77907200	0.19353500
H	1.53515600	3.26433800	1.03806500

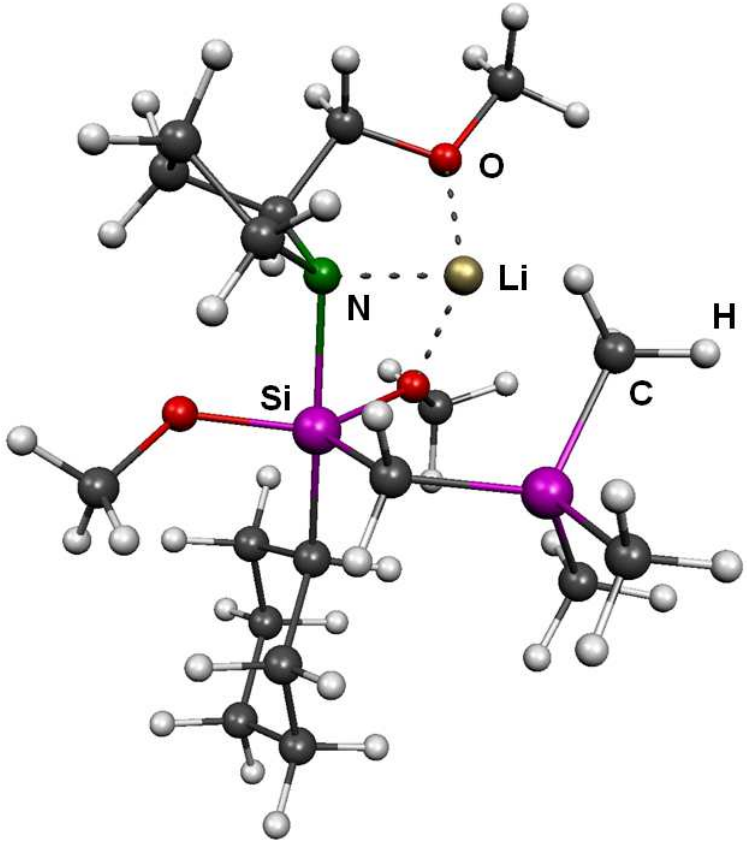

Abbildung 9.10 Molekel-Darstellung von **I2** [M052X/6-31+G(d)].

Tabelle 9.28 Standardorientierung von **I2** [M052X/6-31+G(d)].

Atomsymbol	x	y	z
C	–0.12201500	0.03613700	2.59777400
C	3.11197800	–1.77266400	–2.10633300
C	2.71359800	–2.62658000	–0.89906000
C	2.15936900	–0.56736700	–2.01389700
C	2.34188700	–1.56261300	0.14285100
C	–0.38227100	1.21474900	–1.47543300

C	3.61523400	–1.13406300	0.87825300
C	4.50071100	0.47011500	2.38778100
H	0.32192600	0.82914900	3.20874100
H	0.21370200	–0.92711500	2.99470900
H	3.00682800	–2.30615500	–3.05239200
H	–1.20718900	0.09551000	2.70123700
H	1.82424500	–3.21204900	–1.12654300
H	4.15490600	–1.45310700	–2.02728500
H	1.64364200	–1.95598700	0.88766500
H	1.29556600	–0.74310200	–2.66061000
H	3.51058500	–3.29730100	–0.56333200
H	2.64993100	0.34908500	–2.36047900
H	3.96817200	–1.93499900	1.53823800
H	4.40809500	–0.88655100	0.16220600
H	4.21694600	1.35383000	2.95592200
H	4.83930100	–0.31063500	3.07419500
H	5.31054000	0.72026900	1.69526800
N	1.72539800	–0.44346200	–0.60453600
O	0.31034200	0.20179800	1.26724500
O	3.35584400	0.03220600	1.67558800
Si	–0.23946700	–0.34558200	–0.38121400
Si	–0.35176300	2.85814100	–0.56527100
Li	1.92874300	0.89259100	0.75780000
H	0.42557000	1.26279100	–2.21178800
H	–1.31698300	1.18625200	–2.04549900
O	–0.24029000	–1.86462700	–1.21711900
C	–1.15680700	–2.30083700	–2.19050000
H	–1.53332500	–1.47055900	–2.79899100
H	–0.63862300	–3.00028600	–2.85440200
H	–2.01333200	–2.82151400	–1.75109800
C	–2.08168500	–0.49573200	0.29186000
C	–3.27020400	–0.26049000	–0.66036300
C	–2.30604200	–1.82004600	1.04770500
H	–2.17408200	0.31568700	1.02657000
C	–4.59944600	–0.25149000	0.10685400
H	–3.32257700	–1.03839100	–1.42771600
H	–3.16264500	0.69228700	–1.18752000
C	–3.63027800	–1.82805200	1.81877000
H	–2.31235800	–2.64683200	0.32927000
H	–1.47725900	–2.03340900	1.73116400
C	–4.80462400	–1.55824500	0.87590500
H	–5.43536800	–0.08215400	–0.57988400

H	–4.59298500	0.58474100	0.81817400
H	–3.77154800	–2.78364300	2.33443100
H	–3.60346600	–1.04731300	2.59055800
H	–5.74606500	–1.53047000	1.43290600
H	–4.88162800	–2.38524700	0.15857200
C	–0.59405700	4.25872800	–1.81609400
C	–1.66463200	3.03453800	0.77949900
C	1.34748300	3.17746500	0.26286100
H	0.18406200	4.23952800	–2.58434500
H	–1.55962000	4.16060000	–2.31972000
H	–0.56684900	5.23743600	–1.32846400
H	2.18140200	2.75974100	–0.31530900
H	1.52751500	4.25387600	0.32112400
H	1.37161700	2.81547000	1.29801600
H	–2.65651700	2.76589800	0.40634600
H	–1.44085900	2.38930700	1.63148600
H	–1.70442300	4.06967300	1.13141400

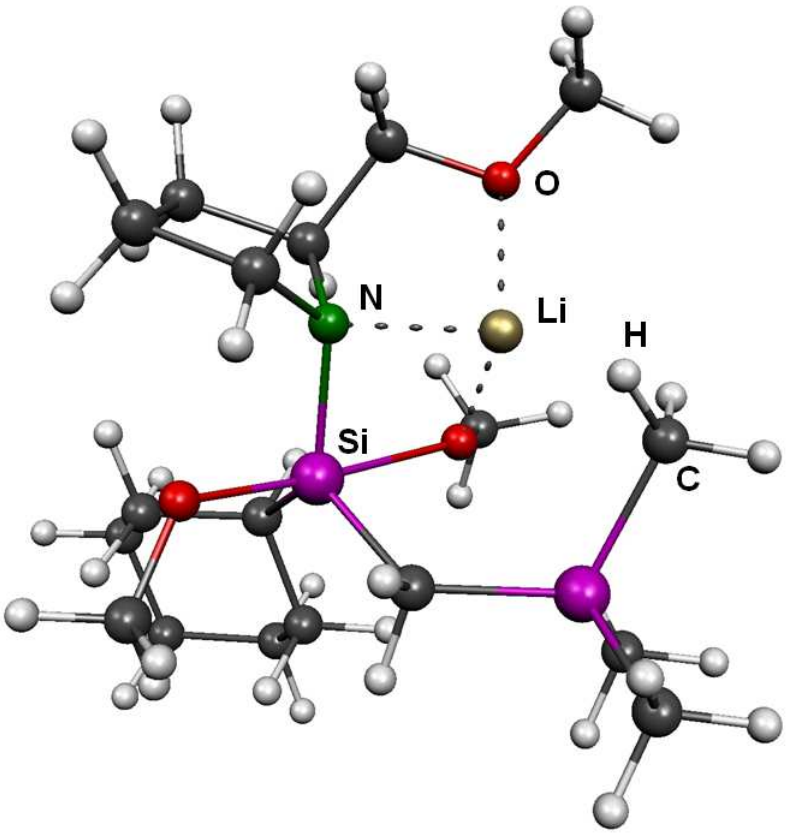

Abbildung 9.11 Molekel-Darstellung von **I3** [M052X/6-31+G(d)].

Tabelle 9.29 Standardorientierung von **I3** [M052X/6-31+G(d)].

Atomsymbol	x	y	z
C	–0.23833300	0.42123600	–2.50367400
C	–0.41522500	–3.18693200	1.95741700
C	–0.21812200	–3.55287400	0.46718100
C	–1.26398800	–1.90453400	1.92398700
C	–0.84688800	–2.37119600	–0.31340200
C	–0.22074200	1.70794900	1.24204100
C	–2.22428700	–2.79196300	–0.82414000
C	–4.18223500	–1.95805000	–1.88008600
H	0.68820500	0.95012400	–2.75772600
H	–1.04336400	0.86235200	–3.10721900
H	0.54431100	–2.95170500	2.41528000
H	–0.12274400	–0.62219600	–2.83320500
H	0.83930500	–3.64603200	0.22120700
H	–0.89323300	–3.98785700	2.52483800
H	–0.24497700	–2.07465600	–1.17343100
H	–1.04029000	–1.23820000	2.75269500
H	–0.69823900	–4.50057700	0.20408200
H	–2.33322600	–2.15094100	1.95359900
H	–2.12129100	–3.54249000	–1.61538100
H	–2.82944800	–3.21710600	–0.01429800
H	–4.62357300	–1.02967500	–2.23644100
H	–4.08509900	–2.65984000	–2.71254100
H	–4.81876100	–2.39607100	–1.10547200
N	–0.94842500	–1.25438400	0.64320100
O	–0.55672600	0.53120900	–1.14434900
O	–2.90303500	–1.64671700	–1.35085600
Si	0.37293600	0.02151400	0.56932800
Si	–1.43533900	2.83437000	0.36223300
Li	–2.11790500	–0.11982300	–0.51151300
H	–0.59516700	1.52446000	2.25831900
H	0.68250500	2.31844600	1.39543900
O	1.05108300	–0.51817700	2.10699600
C	1.87667100	0.26290200	2.92622000
H	2.54158200	0.92527900	2.35572400
H	1.28910100	0.89316200	3.60631500
H	2.50619000	–0.39601700	3.53217400
C	1.97575100	–0.18782800	–0.46130800
C	2.58557700	1.19912000	–0.75468500
C	3.05976300	–1.11392500	0.10798100

H	1.68879200	–0.61181600	–1.43214300
C	3.76604500	1.09417200	–1.72491600
H	2.94286100	1.64369500	0.18367200
H	1.82540500	1.88127300	–1.14785100
C	4.23829600	–1.23399000	–0.86508000
H	3.42535200	–0.72485100	1.06277000
H	2.64472500	–2.10278500	0.32464100
C	4.83335000	0.14089600	–1.18100000
H	4.19923100	2.08186100	–1.91144500
H	3.40152100	0.71487000	–2.68826400
H	5.00961200	–1.89065700	–0.45032200
H	3.89163600	–1.69703300	–1.79799200
H	5.65781800	0.04584500	–1.89393000
H	5.25341100	0.56623200	–0.26093800
C	–1.94899200	4.17189400	1.60922200
C	–0.71936700	3.73152600	–1.13206500
C	–3.09266000	1.99962100	–0.12799500
H	–2.46225800	3.73433600	2.47077400
H	–1.07287300	4.70766100	1.98566500
H	–2.62050900	4.90581800	1.15363200
H	–3.39266600	1.20770300	0.57245800
H	–3.89103600	2.74469400	–0.08184200
H	–3.08634700	1.62124300	–1.15652300
H	0.18266400	4.27922600	–0.84353100
H	–0.45479000	3.03322300	–1.92573900
H	–1.43628000	4.45812500	–1.52529700

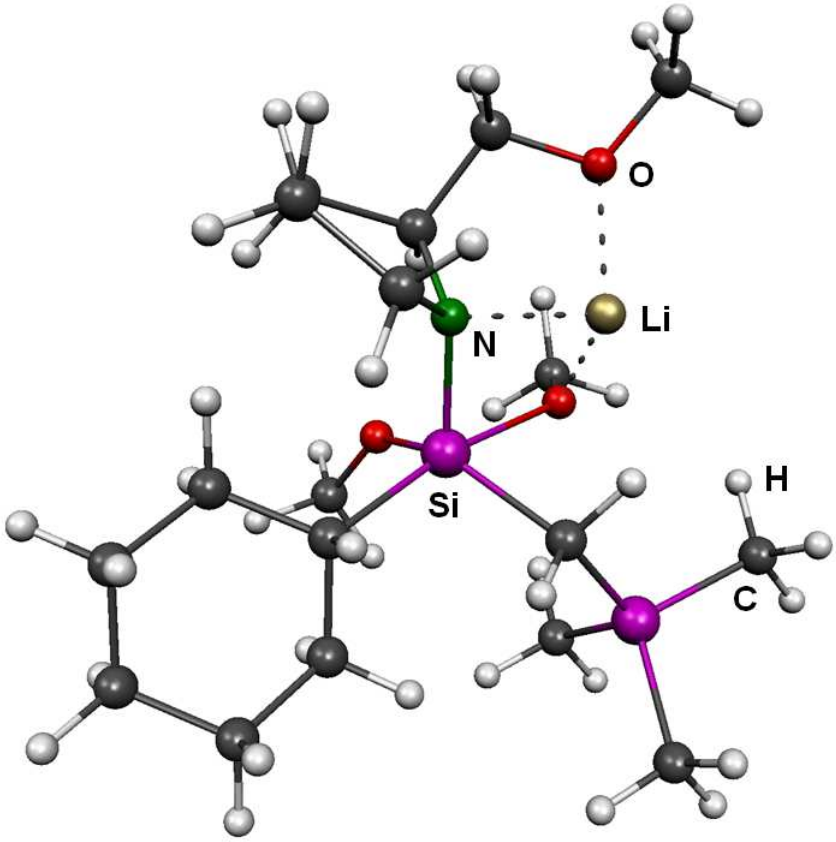

Abbildung 9.12 Molekel-Darstellung von **I4** [M052X/6-31+G(d)].

Tabelle 9.30 Standardorientierung von **I4** [M052X/6-31+G(d)].

Atomsymbol	x	y	z
C	1.56092900	1.76662600	1.96437300
C	1.86256700	–3.18527600	–1.02082400
C	2.17431700	–2.84952500	0.44848700
C	1.33343000	–1.85247800	–1.62191100
C	2.38120300	–1.32950300	0.42205100
C	–0.60648600	1.35153400	–1.18541200
C	3.81613700	–1.02967100	–0.01560400
C	5.28090200	0.74101000	–0.62255400
H	1.67624200	2.85456800	2.04886500
H	2.53696300	1.30846400	2.18329200
H	1.13457200	–3.99206600	–1.10833400
H	0.86021100	1.43188300	2.73204500
H	1.31899200	–3.06302800	1.09059700
H	2.76251000	–3.51226500	–1.54656800
H	2.19780300	–0.87104200	1.39359000
H	0.31598700	–1.94577300	–1.99651500
H	3.03950400	–3.39646400	0.83383000

H	1.95999500	–1.55574700	–2.47085700
H	4.51458700	–1.27567200	0.79164900
H	4.08927600	–1.60839700	–0.90605900
H	5.27961700	1.80441300	–0.85163100
H	5.92196200	0.55594000	0.24309900
H	5.65581100	0.17786800	–1.48232300
N	1.39763200	–0.83630300	–0.55451500
O	1.10611600	1.44250500	0.67576400
O	3.94456800	0.36325100	–0.32944500
Si	–0.10716900	–0.01022400	0.11035500
Si	–1.22356700	3.00543700	–0.51246400
Li	2.19986800	1.01571300	–0.67738400
H	0.29384300	1.61267700	–1.76444900
H	–1.31817400	0.95003700	–1.91248500
O	–0.17030700	–0.39133000	1.77689600
C	–1.12786800	–0.39404300	2.80298600
H	–1.72353900	0.52249000	2.81229300
H	–1.81016700	–1.24599100	2.72772100
H	–0.59861800	–0.46621800	3.75782200
C	–1.58264800	–1.19937100	–0.41207300
C	–1.53701000	–2.63570500	0.12632700
C	–2.95043500	–0.56867900	–0.07708200
H	–1.56083000	–1.26694100	–1.51250800
C	–2.70692800	–3.48733000	–0.38132900
H	–1.55597000	–2.62358600	1.22105500
H	–0.59644700	–3.11560600	–0.15180700
C	–4.11928900	–1.41586200	–0.59312400
H	–3.06066700	–0.45943600	1.00808600
H	–3.02288700	0.43944200	–0.49822400
C	–4.04862600	–2.83891800	–0.03684500
H	–2.65548400	–4.49783600	0.03747300
H	–2.62981600	–3.58758600	–1.47180000
H	–5.07452700	–0.95109100	–0.32825100
H	–4.07334000	–1.45667400	–1.68871400
H	–4.87650000	–3.44259800	–0.42083100
H	–4.15873200	–2.80201700	1.05475300
C	0.13226600	4.32122800	–0.61652500
C	–2.67484900	3.59225600	–1.58510600
C	–1.85146300	2.91674400	1.26780000
H	–1.04930900	2.64157700	1.95479000
H	–2.24719200	3.88943400	1.57488800
H	–2.65746200	2.18427700	1.36462500

H	–2.36968800	3.69667500	–2.63030200
H	–3.50230600	2.87736400	–1.55018300
H	–3.05416500	4.56024300	–1.24531800
H	0.47300700	4.44536200	–1.64924500
H	–0.23385900	5.29110800	–0.26807600
H	0.98617300	4.03257400	–0.00024500

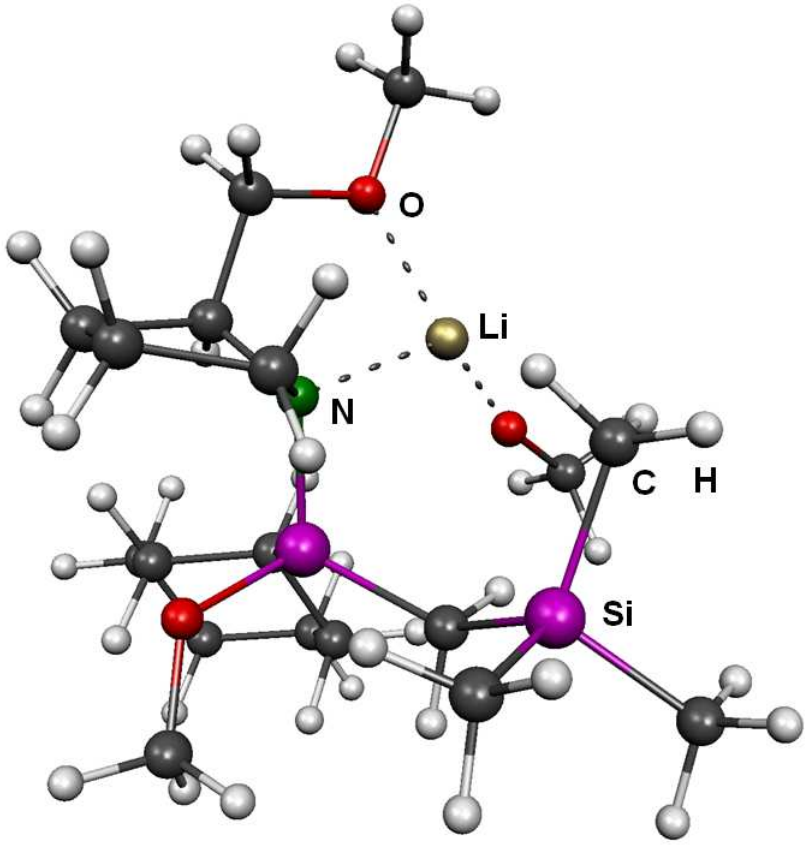

Abbildung 9.13 Molekel-Darstellung von **P1** [M052X/6-31+G(d)].

Tabelle 9.31 Standardorientierung von **P1** [M052X/6-31+G(d)].

Atomsymbol	x	y	z
C	0.22273600	–0.70459200	3.63092900
C	–0.82848800	2.22829200	–2.63258600
C	0.63170600	2.50983000	–2.21204800
C	–1.48698600	1.59453000	–1.38263300
C	0.62371400	2.28279200	–0.69086600
C	–1.04110100	–1.66724800	0.22605700
C	0.22558100	3.57655300	0.01638200
C	–0.29627900	4.43702700	2.16787600
H	–0.15436200	–1.73983800	3.49882100

H	–0.17757800	–0.35914600	4.59968500
H	–0.85472800	1.53300800	–3.46973900
H	1.31736600	–0.79315100	3.75947000
H	1.30111200	1.78960600	–2.68199500
H	–1.35266800	3.13895800	–2.92828900
H	1.58888200	1.96415800	–0.29577300
H	–2.08172000	0.71778800	–1.63057700
H	0.96678000	3.51519300	–2.48072700
H	–2.15262700	2.31338200	–0.89435900
H	1.06072700	4.28486300	–0.02160800
H	–0.64385800	4.04309900	–0.46335500
H	–0.52854000	4.09603100	3.17386700
H	0.60964100	5.04852100	2.18840900
H	–1.12862000	5.02800700	1.77364700
N	–0.38482700	1.22964100	–0.46458900
O	–0.12158000	0.11942800	2.58631100
O	–0.08877400	3.28134000	1.37107300
Si	0.13789600	–0.47377400	–0.58642900
Si	–2.91898400	–1.55089700	0.21134000
Li	–0.56569400	1.41230700	1.63174700
H	–0.76010600	–2.67646200	–0.10471800
H	–0.77905800	–1.58429000	1.28833700
O	0.13396500	–0.73837400	–2.25446700
C	0.14301000	–2.03923100	–2.81747100
H	0.92027800	–2.66916100	–2.37131700
H	–0.82618100	–2.52809800	–2.68327100
H	0.34524700	–1.94566800	–3.88464100
C	1.90270200	–0.64834000	0.07876700
C	2.13096000	–2.01676700	0.74968400
C	2.98086700	–0.41110100	–0.99525500
H	2.00521300	0.10215700	0.87492600
C	3.54169700	–2.11838600	1.33582200
H	1.99276100	–2.82162600	0.01352600
H	1.39442800	–2.17114000	1.53926300
C	4.39142300	–0.51163500	–0.40577400
H	2.87183700	–1.16103600	–1.78837800
H	2.85233400	0.56033300	–1.48165400
C	4.60801300	–1.86737500	0.26854500
H	3.68740600	–3.09985600	1.79644100
H	3.64244100	–1.37163300	2.13253100
H	5.13939700	–0.35182800	–1.18832200
H	4.52646400	0.28421000	0.33704700

H	5.60845100	–1.91873600	0.70753500
H	4.55010900	–2.65785200	–0.49051800
C	–3.64800900	–1.70615400	–1.53103500
C	–3.57622700	–3.00476100	1.22399600
C	–3.47489300	0.03014800	1.08397800
H	–3.20660600	–1.01554100	–2.25275000
H	–3.48602700	–2.72129300	–1.90585600
H	–4.72739600	–1.53166300	–1.51123900
H	–3.24624900	0.93581400	0.51944000
H	–4.55256100	0.01301600	1.26883900
H	–2.95957900	0.08377400	2.04825400
H	–3.25706000	–3.95938000	0.79663600
H	–3.20140400	–2.95379200	2.24981800
H	–4.66927300	–3.00039800	1.26118500

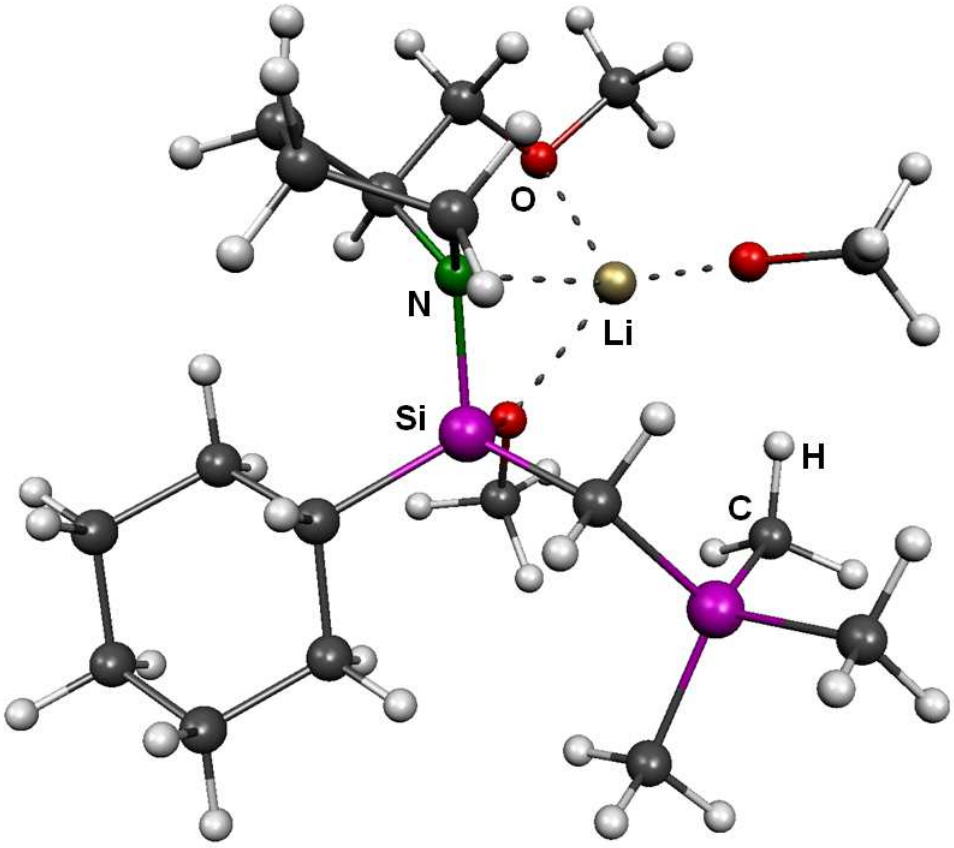

Abbildung 9.14 Molekel-Darstellung von **P2** [M052X/6-31+G(d)].

Tabelle 9.32 Standardorientierung von **P2** [M052X/6-31+G(d)].

Atomsymbol	x	y	z
C	4.19489200	1.16077500	–0.72453200
C	–0.07908500	–2.84402900	–2.39246200
C	0.06406800	–3.69852700	–1.11956600
C	0.79544800	–1.61975000	–2.09298500
C	0.56680500	–2.70807900	–0.03004700
C	0.19764800	1.48252400	–1.08989400
C	1.97557900	–3.11122000	0.39513600
C	3.82306200	–2.40173800	1.68446500
H	4.23105900	2.22292900	–0.40878800
H	3.95640300	1.17289900	–1.80677600
H	–1.11639800	–2.52083000	–2.51557500
H	5.23212900	0.78706900	–0.64459000
H	–0.87414300	–4.17568300	–0.83416100
H	0.22135700	–3.37661200	–3.29608700
H	–0.06385900	–2.69798300	0.86111100
H	0.52941700	–0.74587200	–2.68809000
H	0.79787900	–4.49590500	–1.26962900
H	1.85364600	–1.83234300	–2.28033900
H	1.97803100	–4.14546600	0.76122700
H	2.65588000	–3.03882400	–0.46293000
H	4.06466100	–1.75772900	2.52650500
H	4.04195000	–3.44303300	1.93871700
H	4.39760200	–2.08187400	0.81251600
N	0.57369000	–1.38018900	–0.66389800
O	3.30371700	0.41708200	0.00599000
O	2.42747900	–2.24769900	1.42778700
Si	–0.38113900	–0.01031900	–0.13834200
Si	0.53277700	3.17452400	–0.28443900
Li	2.10148300	–0.42159900	0.81631000
H	1.19273400	1.20196000	–1.46259300
H	–0.45242400	1.65244200	–1.95776000
O	0.15481700	0.01292900	1.46231600
C	–0.48268300	0.64154900	2.56562500
H	–1.34137400	0.05126700	2.89223900
H	0.23830700	0.70461600	3.37933300
H	–0.81630900	1.65021700	2.31237900
C	–2.24777300	–0.26226500	–0.27797900
C	–2.76364200	–1.52372800	0.43441300
C	–3.08078500	0.96944200	0.11867800

H	–2.39820900	–0.41411600	–1.36132000
C	–4.26134500	–1.73677600	0.19094800
H	–2.58582600	–1.43536200	1.51397400
H	–2.21070400	–2.40340300	0.09411100
C	–4.57378100	0.74123500	–0.13598500
H	–2.93833800	1.18422600	1.18521500
H	–2.73767500	1.85127700	–0.42863200
C	–5.07019800	–0.50451900	0.60012600
H	–4.60929900	–2.61944000	0.73515800
H	–4.42224100	–1.93285900	–0.87630300
H	–5.14675100	1.62017500	0.17227900
H	–4.73655600	0.61217000	–1.21298300
H	–6.13321900	–0.66557500	0.40208800
H	–4.96616300	–0.34836900	1.68111500
C	1.37659100	4.20666000	–1.62221400
C	–1.06593000	4.06350800	0.20957900
C	1.68731900	3.05167100	1.19699900
H	2.43158500	2.26859400	1.01838000
H	2.20330100	4.00708300	1.33184700
H	1.15982800	2.82814200	2.12643200
H	–1.74368900	4.17547300	–0.64147700
H	–1.60967000	3.55149000	1.00747400
H	–0.81873700	5.06646000	0.57002700
H	0.76500900	4.26795300	–2.52666100
H	1.56507800	5.22477500	–1.27045100
H	2.33727100	3.75842100	–1.89026700

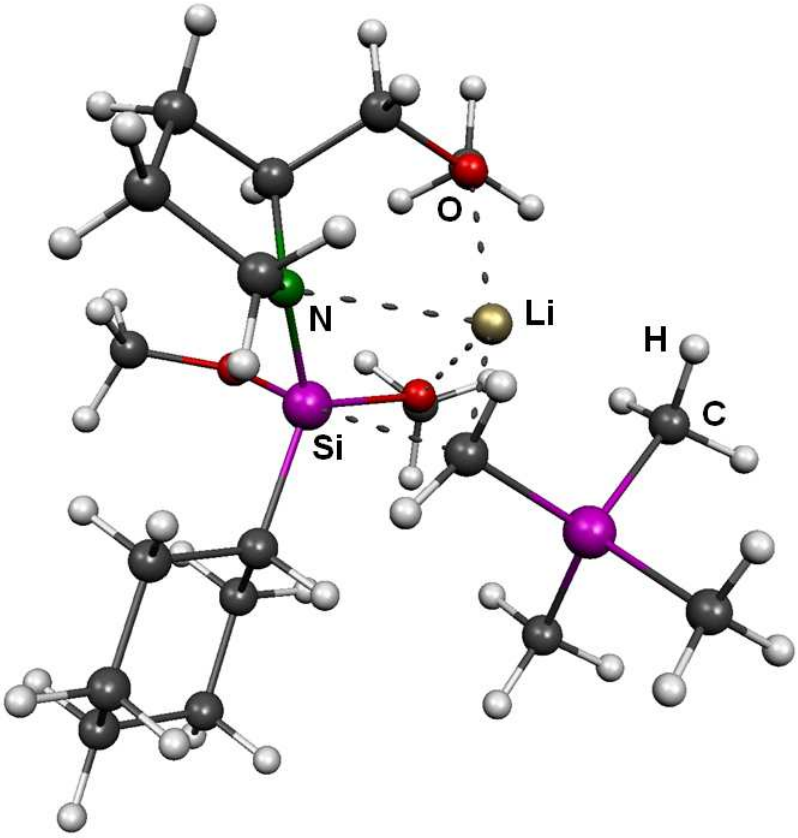

Abbildung 9.15 Molekel-Darstellung von **[TS1]**‡ [M052X/6-31+G(d)].

Tabelle 9.33 Standardorientierung von **[TS1]**‡ [M052X/6-31+G(d)].

Atomsymbol	x	y	z
C	0.33564800	0.76296700	2.84273400
C	2.01564700	–2.43205500	–2.37797200
C	3.05315700	–2.55684600	–1.23897800
C	1.35162300	–1.07053500	–2.12805300
C	2.65228500	–1.44465900	–0.23095000
C	–0.12702900	1.53171000	–1.35043900
C	3.68322400	–0.30954600	–0.32431000
C	3.56474600	0.77256500	1.79212900
H	0.85979800	1.64590500	3.21206900
H	0.77053500	–0.14170500	3.26468500
H	1.26209300	–3.21751800	–2.28581000
H	–0.71088900	0.82778500	3.14538000
H	3.02601500	–3.54243200	–0.77351300
H	2.46517000	–2.50779700	–3.36938900
H	2.59013600	–1.81162600	0.79454500
H	0.34853100	–0.99712500	–2.53686400
H	4.07238700	–2.40111700	–1.60599300

H	1.93891300	–0.26505700	–2.58871100
H	4.66416900	–0.64053100	0.03575100
H	3.78898700	0.00662300	–1.36304400
H	3.25838400	1.71491000	2.24238900
H	3.00204300	–0.04600900	2.24469300
H	4.63654000	0.62675300	1.95028100
N	1.34673400	–0.97263000	–0.67361600
O	0.43533100	0.76335600	1.42106400
O	3.29515500	0.86601200	0.39525800
Si	0.02945600	–0.54336100	0.39657900
Si	–0.74411300	3.13145700	–0.67202800
Li	1.46464800	1.51492200	0.00087700
H	0.68942600	1.75027800	–2.06723000
H	–0.88244900	1.00483200	–1.94033400
O	0.29328400	–1.72979400	1.61057700
C	0.26548800	–3.11491900	1.35547700
H	–0.75418700	–3.50966900	1.41540200
H	0.66744100	–3.35285000	0.36289300
H	0.87269100	–3.62265200	2.10905600
C	–1.80854800	–0.74749700	–0.00993700
C	–2.09538800	–1.83118000	–1.06562900
C	–2.61723300	–1.02137500	1.27354800
H	–2.15395400	0.20837900	–0.41144800
C	–3.59689200	–1.95182900	–1.34854700
H	–1.71806600	–2.80171900	–0.72034100
H	–1.57260300	–1.60261400	–1.99765100
C	–4.11471800	–1.12553700	0.97016800
H	–2.27896400	–1.95061000	1.74197900
H	–2.44494900	–0.22501500	2.00356500
C	–4.38392400	–2.21906100	–0.06476000
H	–3.77893700	–2.74397600	–2.08087600
H	–3.94790400	–1.01339700	–1.79449900
H	–4.67177200	–1.32580300	1.89020900
H	–4.47042400	–0.16392800	0.58078100
H	–5.45370900	–2.28628900	–0.28184200
H	–4.07870100	–3.18843400	0.34956000
C	0.70617400	3.90946100	0.32534900
C	–1.26175400	4.47497000	–1.91588200
C	–2.19367400	2.91847600	0.53318100
H	–1.92821900	2.23293600	1.34162900
H	–2.47599200	3.87903600	0.97420400
H	–3.07491000	2.51606500	0.02434900

H	–0.43586400	4.71361300	–2.59223700
H	–2.09841400	4.12661500	–2.52821200
H	–1.56924700	5.39818200	–1.41422100
H	1.63316000	3.95339800	–0.26266100
H	0.47128600	4.94119000	0.60051400
H	0.90341600	3.37440500	1.26195100

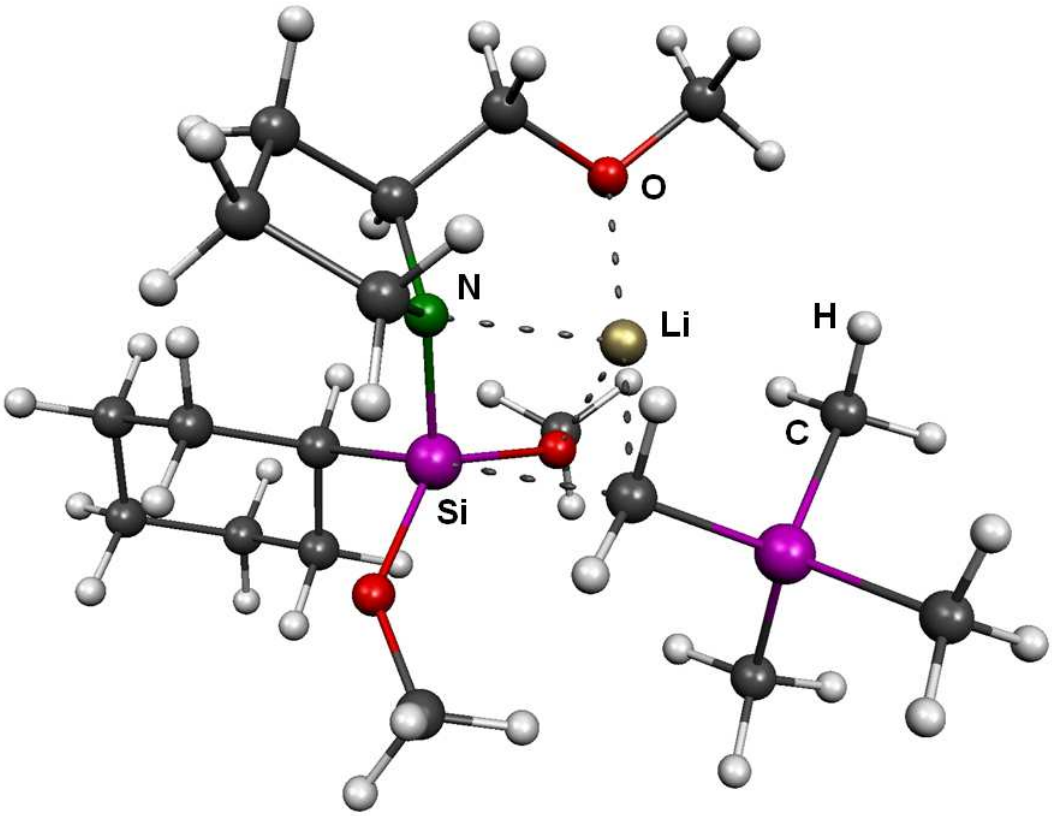

Abbildung 9.16 Molekel-Darstellung von **[TS2]**‡ [M052X/6-31+G(d)].

Tabelle 9.34 Standardorientierung von **[TS2]**‡ [M052X/6-31+G(d)].

Atomsymbol	x	y	z
C	0.14923200	–0.76156200	–2.52213800
C	–1.34065000	2.50970500	2.40398300
C	–1.66433400	3.19494300	1.05981300
C	–0.07341400	1.69569100	2.10979900
C	–0.84945700	2.39263000	0.00560500
C	2.07993600	–0.39317500	1.20521000
C	0.23563700	3.29915600	–0.57798700
C	2.07714000	3.32103800	–2.07086700
H	0.86876200	–0.21899200	–3.13906600
H	–0.84636600	–0.36292400	–2.71694100

H	–2.14599900	1.82971300	2.68589000
H	0.17601100	–1.81661900	–2.80042000
H	–2.73175100	3.18077600	0.83887300
H	–1.20150700	3.22553200	3.21581300
H	–1.47177300	2.02771300	–0.81426300
H	0.04718500	0.83012100	2.75972900
H	–1.35208700	4.24403000	1.06677900
H	0.81996000	2.32317500	2.23342500
H	–0.21007000	4.07074300	–1.21641900
H	0.79448100	3.79192800	0.22771200
H	2.72950000	2.64973100	–2.62495200
H	1.54635100	3.97572900	–2.76683900
H	2.67263400	3.92729600	–1.38141200
N	–0.23368200	1.27543400	0.71576900
O	0.53827200	–0.61420900	–1.16360200
O	1.14968700	2.51660900	–1.35262500
Si	–0.41838700	–0.43509500	0.25245800
Si	3.43906900	–1.18628700	0.23407500
Li	1.57282500	0.83673300	–0.39243500
O	–0.67478200	–1.58570900	1.41752800
C	0.09711000	–2.53974700	2.11371900
H	0.41212900	–2.14490200	3.08163700
H	–0.53644900	–3.41354100	2.27794400
H	0.97761800	–2.83348000	1.54403600
H	2.42316500	0.62814300	1.47674000
H	1.93816700	–0.87593500	2.17299600
C	–2.19139900	–0.56846500	–0.47751200
C	–2.50416700	–2.00975800	–0.92415000
C	–3.26636900	–0.12114800	0.52693500
H	–2.30056900	0.07919600	–1.36026100
C	–3.90538200	–2.12826800	–1.53197100
H	–2.43786900	–2.66103500	–0.04570600
H	–1.76044900	–2.37639800	–1.63816200
C	–4.67735700	–0.23389700	–0.06122900
H	–3.19359500	–0.74502400	1.42559700
H	–3.08891800	0.90998600	0.84241000
C	–4.96839400	–1.65836000	–0.53724400
H	–4.10208200	–3.16107900	–1.83602500
H	–3.96079900	–1.51085400	–2.43797100
H	–5.42330300	0.07831300	0.67657600
H	–4.76298500	0.45224300	–0.91412300
H	–5.96485600	–1.71488700	–0.98531300

H	–4.96696900	–2.33140800	0.32878300
C	2.98821900	–2.89068800	–0.46245500
C	3.81697200	–0.03722100	–1.26218400
C	5.11908600	–1.38851300	1.10681500
H	2.01768800	–2.85753600	–0.96327900
H	3.74106800	–3.22476600	–1.18281900
H	2.94002500	–3.64250300	0.33089600
H	5.86886200	–1.83640200	0.44660300
H	5.49770500	–0.42012200	1.44635800
H	5.01911600	–2.02939700	1.98763400
H	3.00268900	0.00625700	–1.99458400
H	4.05497500	0.98206200	–0.93007100
H	4.69816800	–0.40145600	–1.79761500

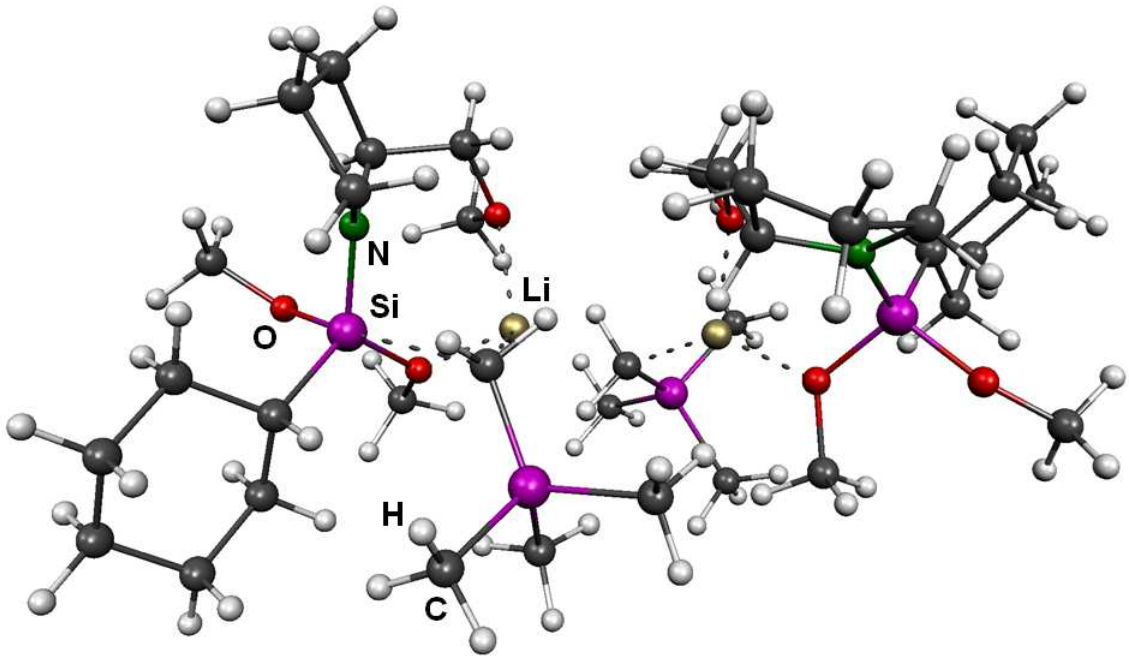

Abbildung 9.17 Molekel-Darstellung von **dim-[TS1]‡** [HF/3-21G].

Tabelle 9.35 Standardorientierung von **dim-[TS1]‡** [HF/3-21G].

Atomsymbol	x	y	z
C	3.13430600	–0.06479900	–2.77834000
C	0.57881800	2.32535300	–0.53965700
C	–3.41139500	2.94441800	–0.59284000
C	–4.16005300	–2.11824000	3.52421700
C	3.93989100	–3.84198300	0.42366100
C	–3.68391200	–0.86458500	4.30084100

C	–3.53908300	–1.92441100	2.12719100
C	–3.32410800	0.17349400	3.18678100
C	–1.95129600	–1.08121800	–0.49554100
C	2.63351700	–4.65454800	0.38569600
C	2.06394200	–2.33017300	0.77039300
C	2.14615300	1.01625000	2.45976300
C	1.90900100	–1.34945900	1.91826300
C	–1.82273300	0.46442500	3.23608300
C	1.67551000	–3.76673800	1.20028000
C	–1.81918200	2.77734200	2.46154700
H	3.13878100	–1.03357700	–3.25093700
H	3.97386600	0.51829500	–3.12775600
H	2.21916000	0.45355600	–3.00321600
H	0.17449300	2.52052200	0.45924900
H	–2.50973600	3.45678600	–0.89168700
H	–3.88738600	3.45552900	0.22513800
H	–5.23842700	–2.10795100	3.43438400
H	–0.25350800	2.19155000	–1.23848500
H	4.59849000	–4.07188100	–0.39970500
H	–4.09434700	2.91266500	–1.42873900
H	–4.45162100	–0.48363700	4.96046700
H	–3.85223800	–3.04085900	3.99921800
H	–3.88169500	1.08841000	3.30548600
H	–4.05711500	–2.48337200	1.36456100
H	4.46198000	–4.01931800	1.35914200
H	2.55960800	1.91632000	2.03852100
H	2.28453900	–4.73195600	–0.63646300
H	2.71215000	0.72212600	3.33503600
H	–2.81222300	–1.09806400	4.90359800
H	1.42833500	–2.01347700	–0.04345900
H	–2.50098800	–2.24241300	2.12866400
H	2.74409200	–5.64585900	0.80457300
H	2.58225600	–1.61416100	2.72347600
H	–1.53503200	0.86089500	4.20542500
H	1.10876200	1.17689400	2.70606100
H	–1.27179900	–0.44123300	3.04135500
H	0.88759100	–1.34229700	2.27826900
H	1.86871900	–3.90411800	2.25992700
H	0.63161500	–3.96870000	1.00403000
H	–1.31421400	3.39628300	1.74115900
H	–2.88550300	2.87147100	2.33958500
H	–1.52621700	3.06919600	3.46321000

N	3.46880400	–2.43843300	0.32875900
N	–3.67534800	–0.47770800	1.92253400
O	3.20731500	–0.21295500	–1.32652400
O	–3.02394200	1.60180300	–0.21414500
O	2.25040500	–0.01890700	1.44117700
O	–1.39832700	1.40633200	2.21121900
Si	1.55625800	3.84334000	–1.06675200
Si	4.33021800	–1.21024000	–0.53133900
Si	–4.02743200	0.36111900	0.42054200
Si	–1.56674800	–1.29222600	–2.33966200
Li	1.91266800	0.68712900	–0.32191900
Li	–1.37415500	0.96300100	0.21209800
H	–1.00487900	–1.10565100	0.07816500
H	–2.47171100	–1.98541200	–0.18268000
O	–5.10107500	1.54313300	1.07622500
C	–6.17877500	1.47750700	1.99767300
H	–7.12774600	1.60423700	1.48864000
H	–6.20624000	0.53536100	2.53589400
H	–6.08347400	2.27947300	2.72280100
O	5.17566500	–1.99617200	–1.71996900
C	6.35230200	–1.90891000	–2.51661900
H	6.40697200	–2.79720800	–3.12819900
H	6.32563400	–1.04107300	–3.16510000
H	7.24248100	–1.85302900	–1.90204100
C	–5.13900700	–0.59429400	–0.79903700
C	–6.38940800	–1.20059800	–0.11436500
C	–5.59764000	0.35380500	–1.93803800
H	–4.57372600	–1.40230200	–1.23928500
C	–7.26683100	–1.95209800	–1.13378500
H	–6.98064800	–0.40772400	0.32675100
H	–6.10136500	–1.87368100	0.68545800
C	–6.51708000	–0.36209800	–2.94676500
H	–6.12602000	1.19497600	–1.49903200
H	–4.73206100	0.74554600	–2.46076300
C	–7.73108600	–0.99565600	–2.24607200
H	–8.12666000	–2.38796000	–0.63296000
H	–6.69372600	–2.76403800	–1.57234400
H	–6.84868200	0.34166400	–3.70469000
H	–5.95287800	–1.14086600	–3.44877400
H	–8.34410600	–1.52627900	–2.96807700
H	–8.34414500	–0.21201200	–1.80852700
C	5.46344800	–0.11803400	0.51384300

C	6.49523700	–0.96001600	1.30240900
C	6.17946600	0.98422000	–0.30107900
H	4.82289700	0.37539800	1.23858600
C	7.35001900	–0.06358900	2.21742700
H	7.14775300	–1.48389600	0.60847300
H	5.98100400	–1.71012400	1.89484400
C	7.03167700	1.87778200	0.61961200
H	6.82738000	0.53224200	–1.04655500
H	5.45051100	1.59199900	–0.82668900
C	8.05564400	1.03652500	1.40327800
H	8.08286400	–0.66422300	2.74711500
H	6.70563400	0.39891300	2.95997300
H	7.54126900	2.63507400	0.03267400
H	6.37666000	2.39130100	1.31743300
H	8.63468000	1.67428200	2.06313400
H	8.74915700	0.57518600	0.70508500
C	–2.87796600	–2.39116400	–3.24024100
C	–1.46130200	0.33524700	–3.37297700
C	0.10480400	–2.21634800	–2.69256100
C	2.32758100	3.66086600	–2.82644600
C	0.55230900	5.49875300	–1.10963600
C	3.03064100	4.18498600	0.14034600
H	2.67426100	4.37332900	1.15114000
H	3.71821700	3.34297900	0.17606500
H	3.59372600	5.05869000	–0.17779400
H	1.59121500	3.30441900	–3.54240300
H	2.70373500	4.61697500	–3.18121100
H	3.15652400	2.95898000	–2.81998200
H	0.12275100	5.71657900	–0.13408800
H	1.18128300	6.33932100	–1.39439400
H	–0.26454800	5.43332800	–1.82469100
H	–3.81285700	–1.86699900	–3.39956200
H	–2.49641800	–2.68795800	–4.21444700
H	–3.08797000	–3.29559000	–2.67461400
H	–2.33281800	0.95951100	–3.20191700
H	–0.58401400	0.92015200	–3.11508900
H	–1.41088800	0.10280400	–4.43439100
H	0.29715200	–2.26876500	–3.76233000
H	0.95122300	–1.72522200	–2.22432500
H	0.05753400	–3.23357800	–2.30970300

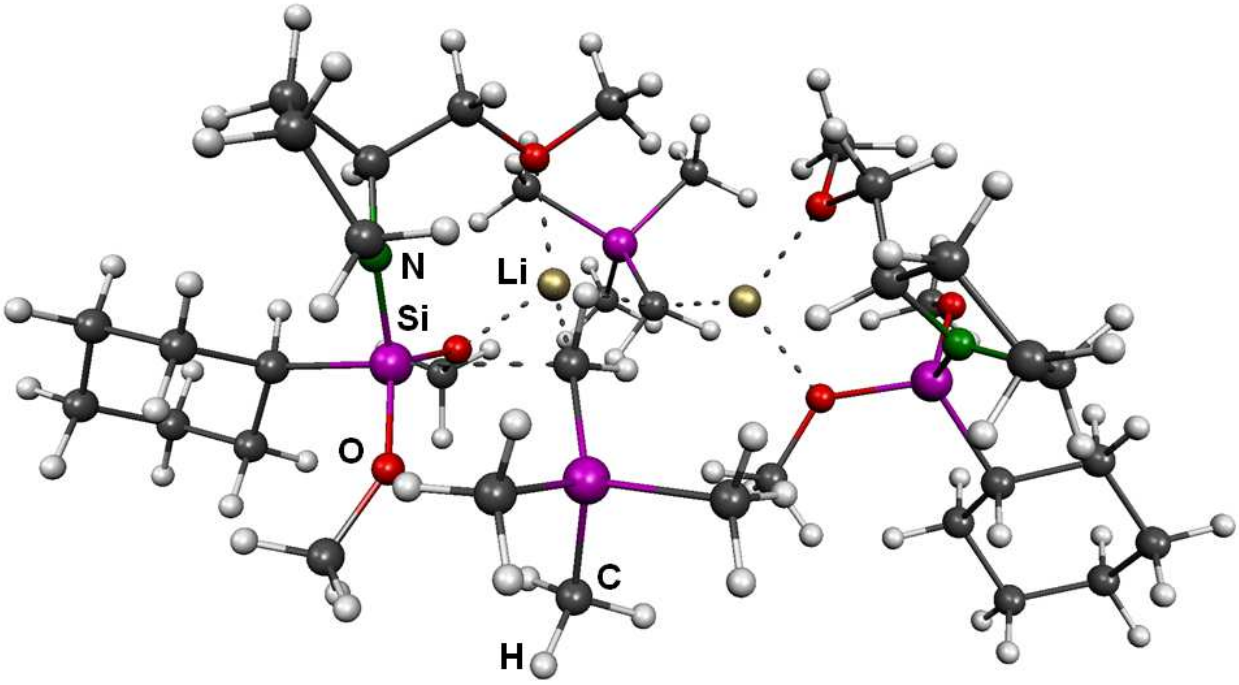

Abbildung 9.18 Molekel-Darstellung von **dim-[TS2]‡** [HF/3-21G].

Tabelle 9.36 Standardorientierung von **dim-[TS2]‡** [HF/3-21G].

Atomsymbol	x	y	z
C	2.32504100	–0.38780600	–1.84298100
C	0.36484300	2.46972800	–0.60662700
C	–2.97047100	1.77969200	–2.00715400
C	–4.83588800	–1.58930800	3.21797300
C	5.18232800	–2.28547700	1.67261200
C	–5.22771800	–0.09422100	3.05899700
C	–3.86503300	–1.88825700	2.02829700
C	–4.16577900	0.46891400	2.07909900
C	–1.03329000	–1.23728800	0.23060600
C	4.29622800	–3.36401400	2.31719000
C	3.01160100	–1.30545100	2.17018500
C	2.75644300	2.35880400	2.66032500
C	2.80980800	–0.05207800	3.00441200
C	–2.96183400	0.91698100	2.90904800
C	3.27054100	–2.52359400	3.09342800
C	–0.86214900	2.08926400	2.89844600
H	2.91895000	–1.21889200	–2.19683900
H	2.25990300	0.37300500	–2.60409300
H	1.34060900	–0.74155700	–1.59933900
H	–0.16687000	1.98356300	–1.43274100

H	–2.25346500	2.57210200	–1.89686300
H	–3.96544000	2.19115100	–1.93402300
H	–5.71116500	–2.22325600	3.17386200
H	1.40188000	2.56197600	–0.97693700
H	5.69230500	–2.66096800	0.79747800
H	–2.83749700	1.32468600	–2.97869800
H	–6.20520400	–0.00841900	2.60660200
H	–4.34415000	–1.76645500	4.16628200
H	–4.53619000	1.31351100	1.51369900
H	–4.19690600	–2.73634500	1.44828000
H	5.92503700	–1.93450700	2.38335400
H	2.43265200	3.07992300	1.93091300
H	3.79540500	–3.93272700	1.54546000
H	3.82523000	2.41473800	2.78991000
H	–5.24645800	0.42978400	4.00734200
H	2.13170700	–1.47673500	1.56703600
H	–2.87066800	–2.10910800	2.39565800
H	4.85690900	–4.03431300	2.95489200
H	3.74375700	0.20555000	3.48498000
H	–3.28227100	1.67788000	3.61305300
H	2.24902000	2.53639300	3.59981600
H	–2.55746400	0.07835900	3.46094300
H	2.04018200	–0.20406700	3.75117300
H	3.70882900	–2.19191200	4.03008800
H	2.35653300	–3.05963800	3.30597700
H	–0.14828800	2.50347600	2.21252500
H	–1.28067700	2.86816800	3.52429200
H	–0.39045700	1.33669800	3.51846700
N	4.22217100	–1.21628200	1.31692100
N	–3.88777800	–0.66842400	1.21182100
O	2.91200200	0.19427600	–0.64321400
O	–2.71801400	0.82013800	–0.96053600
O	2.40522000	1.04818200	2.14286600
O	–1.90630800	1.48894800	2.09364100
Si	–0.22417100	4.25467300	–0.39921800
Si	4.43580600	–0.06282200	0.04916100
Si	–3.56048200	–0.60372100	–0.50884900
Si	–0.69627600	–2.95678100	–0.46797000
Li	1.58716500	1.02433500	0.42681000
Li	–1.36977300	1.00701600	0.28511200
O	–3.33917400	–2.06731000	–1.29269000
O	4.93573200	1.42100700	0.62366500

C	–3.99950500	–2.85635900	–2.28535600
C	5.05642200	2.71172200	0.00814400
H	5.92921200	2.75351600	–0.63032200
H	4.17807100	2.95257400	–0.57875600
H	5.16470600	3.44609500	0.79116300
H	–3.54175600	–3.83311600	–2.27197600
H	–5.05536200	–2.96241700	–2.08421700
H	–3.87128400	–2.42800900	–3.27040000
H	–0.20844800	–0.59084700	–0.12184200
H	–0.98271600	–1.25045400	1.32677100
C	–5.35404800	–0.07478500	–1.13302600
C	–5.66909300	0.00369300	–2.65107100
C	–6.48024100	–0.91289500	–0.47379600
H	–5.47870600	0.93895600	–0.74305800
C	–7.03505700	0.67881600	–2.89687900
H	–5.71185500	–0.99606600	–3.06555500
H	–4.90445400	0.53596000	–3.20055000
C	–7.86421700	–0.27221400	–0.70042100
H	–6.48830900	–1.91438200	–0.89473700
H	–6.28878000	–1.01162900	0.58349600
C	–8.16026800	–0.10941400	–2.20233500
H	–7.23380100	0.74543400	–3.96302500
H	–7.00892400	1.69185700	–2.50412500
H	–8.63832000	–0.87588800	–0.23430800
H	–7.88139600	0.70548200	–0.22550600
H	–9.11399700	0.38930300	–2.34642600
H	–8.23492600	–1.09346800	–2.65811800
C	5.70293100	–0.65933000	–1.23801600
C	5.64253700	0.11353400	–2.58310800
C	7.15007100	–0.54606700	–0.68001800
H	5.50591600	–1.70865700	–1.45190700
C	6.65967100	–0.45668000	–3.59063200
H	5.87175100	1.16028800	–2.40901100
H	4.65228000	0.07111200	–3.01616400
C	8.17550300	–1.11649700	–1.67713500
H	7.37124200	0.49979400	–0.49294600
H	7.24301100	–1.06209500	0.26790900
C	8.08993400	–0.38660400	–3.02866400
H	6.59831700	0.09344500	–4.52426000
H	6.40575300	–1.49138600	–3.80244900
H	9.17637700	–1.02490000	–1.26704900
H	7.97745200	–2.17424800	–1.82591200

H	8.79022700	–0.82143200	–3.73411300
H	8.36917900	0.65440000	–2.89061600
C	–1.84364300	–4.36566000	0.17781600
C	–0.60334000	–2.96985600	–2.40212900
C	1.04959000	–3.69556800	0.01541200
H	–2.88344400	–4.15573700	–0.02270800
H	–1.57583500	–5.31006600	–0.29160800
H	–1.71738400	–4.48790700	1.25161400
H	–1.23582100	–2.19585600	–2.81738200
H	0.41715000	–2.81004800	–2.74264900
H	–0.92797200	–3.92811300	–2.80140300
H	1.10633000	–3.87350400	1.08746700
H	1.20392500	–4.64947400	–0.48682100
H	1.87070300	–3.03759300	–0.25979000
C	0.96050800	5.23252700	0.77818600
C	–0.24500100	5.27881300	–2.04138400
C	–1.99457700	4.47385700	0.35064000
H	–2.06837400	5.44237600	0.84050200
H	–2.75868800	4.44314600	–0.42116700
H	–2.22653400	3.70316300	1.07508800
H	0.86810500	4.90078900	1.80921400
H	1.99999900	5.12264400	0.47589300
H	0.72077500	6.29245500	0.75210200
H	–0.59231800	6.29514900	–1.86864500
H	0.75044100	5.33146900	–2.47613200
H	–0.90122400	4.82234800	–2.77916300

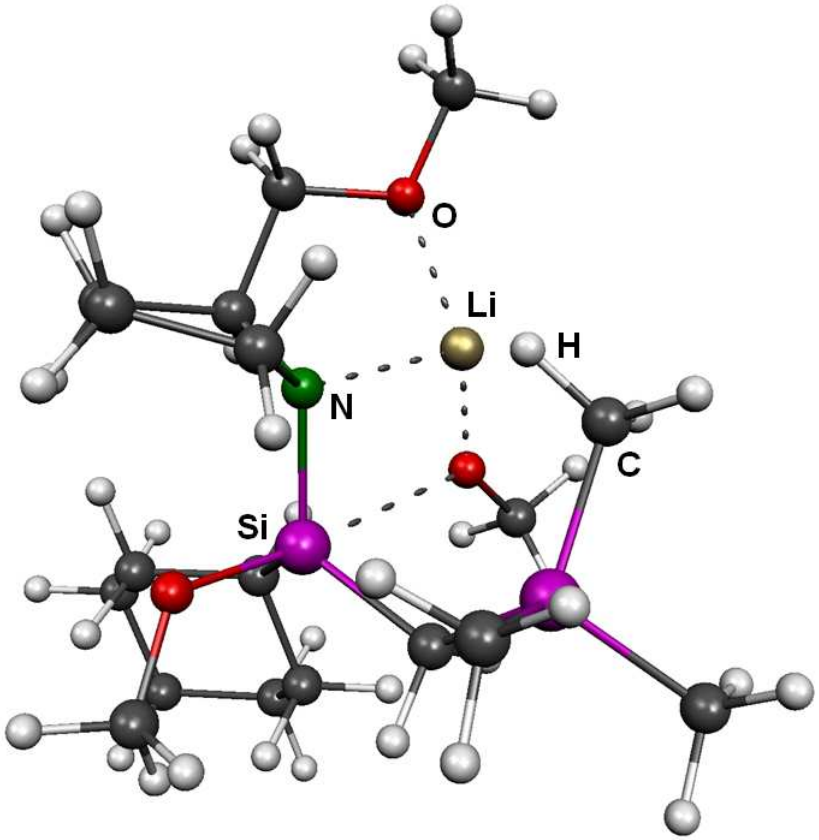

Abbildung 9.19 Molekel-Darstellung von **[TS3]**‡ [M052X/6-31+G(d)].

Tabelle 9.37 Standardorientierung von **[TS3]**‡ [M052X/6-31+G(d)].

Atomsymbol	x	y	z
C	–0.38323600	–0.55861800	–3.16143800
C	0.97452700	2.03975900	2.65079200
C	–0.14414000	2.75394700	1.85992400
C	1.64497500	1.09627600	1.62373200
C	0.14559700	2.37703700	0.39326300
C	0.44212100	–2.03941400	–0.07663500
C	1.12934400	3.40474100	–0.17236200
C	2.57264100	3.84886300	–1.99903800
H	–0.32935800	–1.66384500	–3.18146800
H	0.09495100	–0.20964700	–4.09101100
H	0.54907200	1.46270900	3.46945500
H	–1.45305200	–0.29748400	–3.24241800
H	–1.11631800	2.36617900	2.15729000
H	1.69770300	2.74466800	3.06618800
H	–0.74313600	2.35436600	–0.24015600
H	1.80594600	0.10093800	2.02940600
H	–0.14934400	3.83692800	2.01374400

H	2.62107900	1.49607200	1.32319200
H	0.60124000	4.33972600	–0.38918300
H	1.92716700	3.61752800	0.54999900
H	2.97419000	3.38037600	–2.89464200
H	2.00841000	4.74298300	–2.27698500
H	3.39172200	4.12681400	–1.32872700
N	0.75380700	1.03738700	0.44858100
O	0.20858800	–0.02095800	–2.03451400
O	1.71937900	2.90583300	–1.37111600
Si	–0.35086200	–0.39196500	0.36600200
Si	2.30576600	–2.30858900	–0.05933100
Li	1.44963500	0.99563100	–1.45202700
H	0.01633800	–2.81648700	0.57159600
H	0.13309700	–2.26872900	–1.09860700
O	–0.59473100	–0.52601100	2.06397000
C	–1.11260800	–1.65899700	2.72102500
H	–1.94219700	–2.11846900	2.17131800
H	–0.33621800	–2.41792300	2.86959900
H	–1.48491700	–1.35210100	3.70091600
C	–2.10085900	–0.07646900	–0.31614700
C	–2.72477900	–1.39919400	–0.80923300
C	–3.06240300	0.60053100	0.67527900
H	–1.98665500	0.57237700	–1.19227400
C	–4.10546700	–1.17347300	–1.43220700
H	–2.83006400	–2.09610700	0.03322800
H	–2.07015700	–1.88321600	–1.53524100
C	–4.44444100	0.82719600	0.05213300
H	–3.16800400	–0.01965500	1.57288400
H	–2.65950400	1.55880000	1.01191200
C	–5.04952700	–0.48593700	–0.44507400
H	–4.52906000	–2.12576200	–1.76552100
H	–3.99155400	–0.54249800	–2.32244800
H	–5.11144100	1.30229200	0.77829600
H	–4.34601400	1.51832400	–0.79431800
H	–6.02416100	–0.30667700	–0.90826100
H	–5.21876800	–1.14995600	0.41201100
C	2.93214200	–2.62649200	1.69843000
C	2.67501000	–3.86203800	–1.07320600
C	3.29109800	–0.90075000	–0.86266500
H	2.71437300	–1.80962900	2.38911800
H	2.46105400	–3.52984800	2.09722500
H	4.01356900	–2.78971100	1.69820500

H	3.22457700	0.03230300	–0.29716900
H	4.34879000	–1.17142900	–0.92618300
H	2.92328600	–0.74896600	–1.88243900
H	2.13167300	–4.72417000	–0.67676500
H	2.36934400	–3.72431200	–2.11409900
H	3.74228000	–4.10033200	–1.06121500

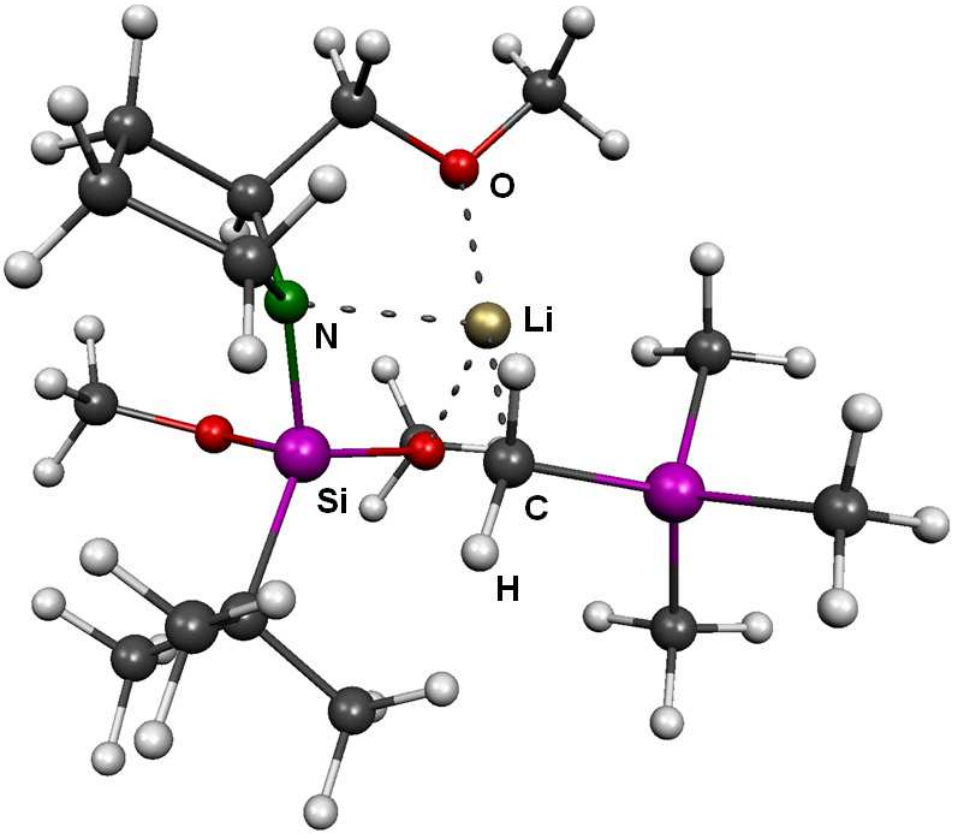

Abbildung 9.20 Molekel-Darstellung von **[TS4]**‡ [M052X/6-31+G(d)].

Tabelle 9.38 Standardorientierung von **[TS4]**‡ [M052X/6-31+G(d)].

Atomsymbol	x	y	z
C	–0.24469300	–0.06064300	2.86682600
C	2.90702300	0.83342200	–2.23730600
C	3.31115200	1.73056800	–1.04583200
C	1.39698200	0.63002900	–2.05011000
C	2.10407600	1.64408800	–0.07204100
C	–1.52334300	–0.33763700	–1.20510700
C	1.36784500	2.98295300	–0.06365000
C	–0.48478200	4.09066300	0.90680500
H	0.49294000	0.72260000	3.04727100

H	0.10541700	–0.98324500	3.32872100
H	3.40917200	–0.13472600	–2.16720300
H	–1.20327100	0.22552200	3.30298000
H	4.23075300	1.38683300	–0.57207400
H	3.15928600	1.27433900	–3.20308400
H	2.39191500	1.41101500	0.95241700
H	1.01308000	–0.27351800	–2.51365800
H	3.47940400	2.76387400	–1.36475800
H	0.84537200	1.47474800	–2.48500600
H	1.97563900	3.73989700	0.44539900
H	1.16756800	3.33001500	–1.08490200
H	–1.42170200	3.89115100	1.42034300
H	0.16819000	4.68617700	1.54988500
H	–0.68222400	4.63767400	–0.02027000
N	1.23297100	0.59207600	–0.59688500
O	–0.46502400	–0.24522700	1.46939500
O	0.12358600	2.83627900	0.62388100
Si	0.70620900	–0.80366100	0.36750800
Si	–3.19608700	–0.02525000	–0.47329800
Li	–0.78717100	1.13472300	0.10230800
H	–1.35150000	0.42047400	–1.99344500
H	–1.55191500	–1.28826900	–1.74070900
O	1.96281100	–0.83227700	1.53406100
C	3.34075300	–0.94787500	1.27766900
H	3.72891400	–1.87180400	1.71255200
H	3.56810700	–0.95011600	0.20426800
H	3.87162000	–0.10658600	1.73535700
C	0.62753900	–2.63534900	–0.22539000
C	0.81196400	–2.81896800	–1.73874500
C	1.72423400	–3.47266100	0.45804200
H	1.79626800	–2.46717200	–2.06596100
H	0.05013400	–2.30431700	–2.32155200
H	2.72234200	–3.19973300	0.11075300
H	1.70050700	–3.37650000	1.54492500
C	–3.14924500	1.66452100	0.45186200
C	–4.63970400	0.15603000	–1.70043800
C	–3.72648500	–1.30142000	0.82141200
H	–2.94778700	–1.41910200	1.57835700
H	–4.65015400	–0.98070100	1.31282100
H	–3.91364700	–2.28063700	0.37187600
H	–4.44583300	0.96476200	–2.41110600
H	–4.76619700	–0.76489400	–2.27668200

H	–5.58396500	0.36896900	–1.18891800
H	–2.80265100	2.48226000	–0.19319400
H	–4.16225900	1.92772300	0.76800900
H	–2.53790400	1.64235500	1.36277300
C	–0.72191000	–3.22334500	0.21674000
H	–1.56375800	–2.68430800	–0.20927000
H	–0.77808800	–4.27234800	–0.09923200
H	–0.82652100	–3.19732800	1.30581500
H	0.75410400	–3.88779400	–1.97821100
H	1.56822100	–4.52770400	0.20391900

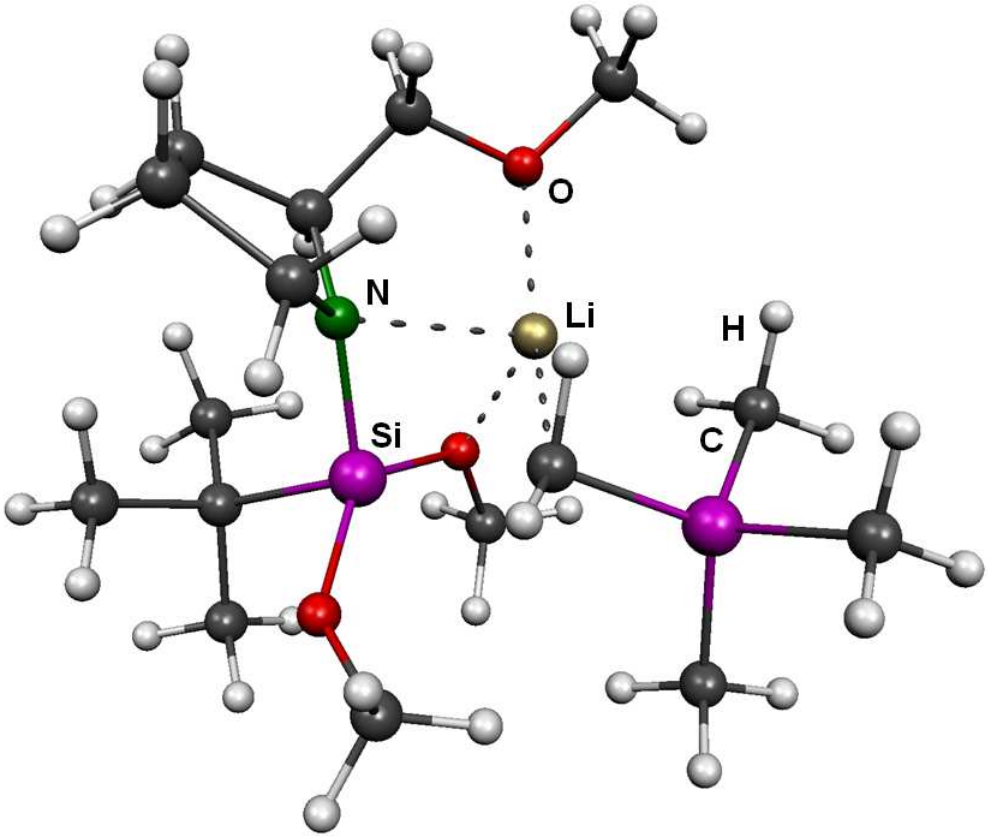

Abbildung 9.21 Molekel-Darstellung von **[TS5]**‡ [M052X/6-31+G(d)].

Tabelle 9.39 Standardorientierung von **[TS5]**‡ [M052X/6-31+G(d)].

Atomsymbol	x	y	z
C	0.62844900	–1.30246300	–2.48709500
C	–2.76282200	1.54235500	2.14319900
C	–3.24447000	1.84727300	0.70447400
C	–1.31145100	1.01762200	1.99018100
C	–1.97675100	1.68020900	–0.15552400

C	1.51797700	0.01780000	1.05953700
C	–1.28153200	3.03963300	–0.26558600
C	0.64279700	4.11721800	–1.13751600
H	1.51053100	–0.87676800	–2.96895300
H	–0.16191900	–1.41689800	–3.23174200
H	–3.39978400	0.79100500	2.61061800
H	0.88965200	–2.28854900	–2.09855100
H	–3.99848800	1.12691800	0.38698800
H	–2.79135300	2.43064500	2.77673500
H	–2.17771300	1.32978600	–1.16638200
H	–1.12773900	0.12279500	2.58739100
H	–3.68236800	2.84532800	0.61219900
H	–0.59541400	1.77702100	2.32961800
H	–1.89010400	3.72407100	–0.86676500
H	–1.12654800	3.48491100	0.72486500
H	1.58401900	3.90263200	–1.63832900
H	0.02409500	4.74877800	–1.77991400
H	0.83475900	4.63327400	–0.19221900
N	–1.14661000	0.72567900	0.56457500
O	0.21021600	–0.43077400	–1.45092000
O	–0.00896100	2.87673200	–0.89998800
Si	–0.53672200	–0.88120500	0.05275600
Si	3.20963000	–0.11124700	0.30222700
Li	0.74350800	1.14408900	–0.53985000
O	–0.27778200	–2.17825300	1.08337500
C	0.72725300	–2.70547400	1.91486300
H	0.69809200	–2.24548600	2.90615600
H	0.53075200	–3.77453200	2.02180000
H	1.72002200	–2.56790800	1.48793500
H	1.38375600	1.09502000	1.29775700
H	1.51536800	–0.42918300	2.05533600
C	–2.12464200	–1.80253700	–0.64866000
C	–1.78817700	–3.20958300	–1.18031100
C	–3.11700900	–1.99701800	0.51216500
H	–1.20215500	–3.78087800	–0.45876300
H	–1.24267200	–3.17881700	–2.12629800
H	–2.70830600	–2.66814500	1.26930500
H	–3.36544600	–1.04817600	0.99755100
C	3.65890900	–1.83784700	–0.34138100
C	3.27654100	1.11665700	–1.17011100
C	4.64962600	0.41426200	1.42644600
H	2.84272900	–2.30223500	–0.89802800

H	4.53181400	–1.78242300	–0.99865100
H	3.91792800	–2.50255000	0.48777700
H	5.61135500	0.34886800	0.90796500
H	4.51871500	1.44302200	1.77365600
H	4.69936400	–0.22806900	2.31035300
H	2.53292700	0.92961000	–1.95275800
H	3.15777800	2.14531100	–0.80842400
H	4.25597200	1.06865900	–1.65412600
C	–2.87356200	–1.06507100	–1.77196800
H	–4.05413900	–2.43200200	0.13823300
H	–2.71934100	–3.75999800	–1.37209600
H	–2.21021000	–0.70808100	–2.56486400
H	–3.60576000	–1.74203200	–2.23173700
H	–3.43973200	–0.21248500	–1.39191500

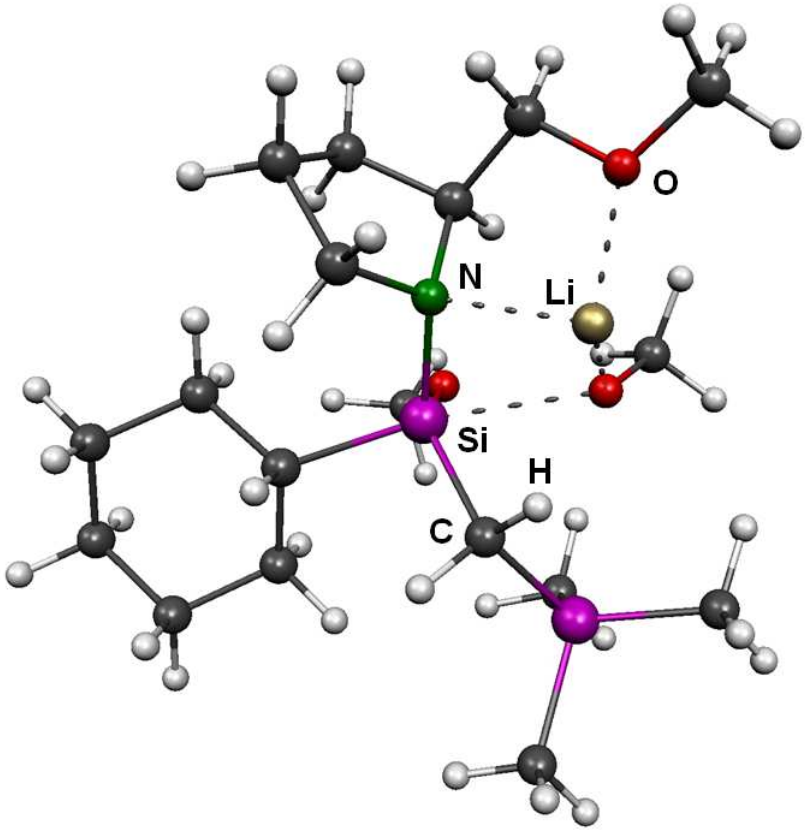

Abbildung 9.22 Molekel-Darstellung von **[TS6]**‡ [M052X/6-31+G(d)].

Tabelle 9.40 Standardorientierung von **[TS6]**‡ [M052X/6-31+G(d)].

Atomsymbol	x	y	z
C	2.00216000	1.94385600	1.72280600

C	1.54042600	–3.37628500	–0.77824400
C	1.82544100	–2.93124000	0.66776900
C	1.17477600	–2.05955900	–1.52305500
C	2.21350700	–1.45630300	0.49815100
C	–0.53374300	1.37275400	–1.18716000
C	3.68012100	–1.38979100	0.05784700
C	5.36437800	0.09020700	–0.71813900
H	2.01093600	3.03715900	1.86885000
H	3.04447400	1.59890100	1.85874800
H	0.74336000	–4.11757500	–0.83102600
H	1.41086000	1.51049400	2.54230400
H	0.92175800	–2.97938300	1.27807800
H	2.42441000	–3.83459000	–1.22643600
H	2.08254300	–0.86774600	1.40538700
H	0.17109900	–2.08714500	–1.94584200
H	2.60016900	–3.53248600	1.15133700
H	1.86845400	–1.89946300	–2.35533600
H	4.32485400	–1.58126400	0.92279800
H	3.90269900	–2.13689600	–0.71345800
H	5.49032100	1.08728800	–1.13361400
H	5.92654200	0.01090900	0.21596400
H	5.72940600	–0.65602300	–1.43023600
N	1.29463800	–0.96088800	–0.54174200
O	1.48388900	1.60055800	0.48089400
O	3.98063200	–0.09852200	–0.47214600
Si	–0.18955800	–0.05603800	0.01117100
Si	–0.95230600	3.07609000	–0.46605400
Li	2.33433400	0.78210300	–0.78990300
H	0.37364600	1.54739100	–1.77862600
H	–1.31071100	1.07094000	–1.89792100
O	–0.15838400	–0.04061900	1.68030900
C	–1.06267700	–0.22241700	2.74222800
H	–0.47855700	–0.28047400	3.66332100
H	–1.74891000	0.62310000	2.82334800
H	–1.64433600	–1.14056500	2.64222300
C	–1.74141400	–1.14133900	–0.40923000
C	–1.82839400	–2.57596800	0.13356800
C	–3.03128500	–0.37669500	–0.03796300
H	–1.75225200	–1.21758800	–1.50943800
C	–3.08297000	–3.30066800	–0.36955000
H	–1.84972400	–2.56663600	1.22882600
H	–0.94475800	–3.14939700	–0.14838700

C	–4.28585000	–1.09559700	–0.54515100
H	–3.10677400	–0.28023900	1.05116700
H	–3.00835900	0.64175800	–0.43715400
C	–4.35039200	–2.52559400	–0.00589600
H	–3.12695200	–4.31433700	0.04110300
H	–3.02405800	–3.39845500	–1.46109100
H	–5.18405100	–0.54049400	–0.25790900
H	–4.26188700	–1.12442900	–1.64160400
H	–5.23617000	–3.03994700	–0.38969700
H	–4.44840400	–2.49153700	1.08667000
C	0.43590400	4.31949800	–0.76133900
C	–2.47256200	3.71137300	–1.41644400
C	–1.44085200	3.04047400	1.35465700
H	–0.62572300	2.66865400	1.97587400
H	–1.70828800	4.04770100	1.68757900
H	–2.31585200	2.40011700	1.50227400
H	–2.26468300	3.77639100	–2.48872600
H	–3.33288500	3.04809000	–1.28399000
H	–2.76428600	4.70738500	–1.07057300
H	0.66323800	4.39430100	–1.82957600
H	0.14615800	5.31488100	–0.41253700
H	1.33478000	3.99882300	–0.23400700

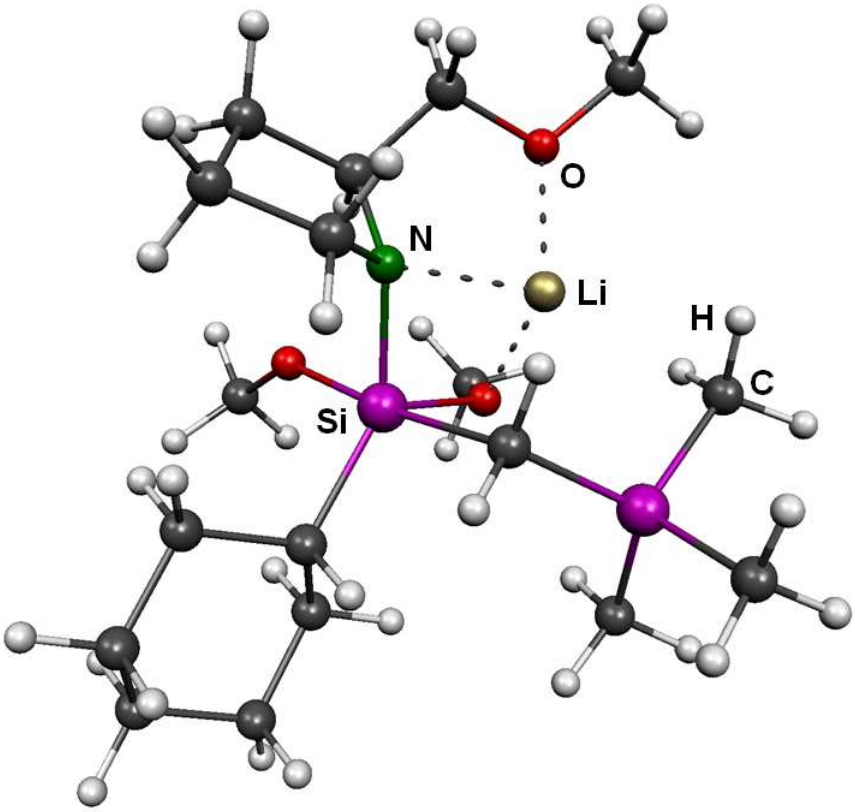

Abbildung 9.23 Molekel-Darstellung von **[BPR1]‡** [M052X/6-31+G(d)].

Tabelle 9.41 Standardorientierung von **[BPR1]‡** [M052X/6-31+G(d)].

Atomsymbol	x	y	z
C	0.63586200	0.37423500	2.70788500
C	0.76714200	–3.09455100	–1.89720500
C	1.69155500	–3.48759200	–0.73045500
C	1.02956700	–1.59116600	–2.05398800
C	1.94621000	–2.15026800	0.01500100
C	0.18411400	1.30986200	–1.21676800
C	3.42448400	–1.77616800	–0.03493000
C	4.94356200	–0.08102900	0.66056600
H	1.40107400	1.02176600	3.14321400
H	0.91341500	–0.66936300	2.86517800
H	–0.27486200	–3.24490700	–1.60762200
H	–0.31312400	0.57181800	3.21292000
H	1.22865900	–4.22405400	–0.07419200
H	0.96282700	–3.66316400	–2.80855900
H	1.63426300	–2.20376100	1.05561000
H	0.22790900	–1.06346900	–2.57273800
H	2.63072500	–3.91377400	–1.10023000
H	1.95243600	–1.42997800	–2.63126600

H	4.02605600	–2.47832400	0.55336200
H	3.79799300	–1.76720600	–1.06639500
H	4.96309300	0.93418300	1.05242800
H	5.44771000	–0.75203700	1.36090900
H	5.45503800	–0.11350900	–0.30632800
N	1.17482200	–1.11179800	–0.67471700
O	0.53443500	0.68588000	1.32929600
O	3.58196900	–0.45663500	0.51522900
Si	–0.27357800	–0.26080100	0.09923100
Si	0.44197700	3.03952500	–0.53699200
Li	2.02130000	0.61323000	0.05356900
H	1.07841200	1.11043000	–1.83680200
H	–0.61512100	1.37661400	–1.96320600
O	–0.49370600	–1.69812000	1.12320000
C	–1.27250600	–2.16457000	2.18414600
H	–2.25745100	–2.51302500	1.84980600
H	–0.75993900	–3.01756300	2.64613400
H	–1.43523400	–1.41371900	2.96603400
C	–2.16319600	–0.07574200	–0.27782200
C	–2.76667600	–1.33802800	–0.91749500
C	–2.98204900	0.35855100	0.95302100
H	–2.27781300	0.73267200	–1.00810200
C	–4.25141700	–1.14882400	–1.24971000
H	–2.64786900	–2.18939500	–0.24034700
H	–2.22007900	–1.59358900	–1.83335500
C	–4.45760100	0.56086200	0.59022700
H	–2.92671800	–0.39614000	1.73999200
H	–2.57116100	1.28352900	1.37023500
C	–5.04375700	–0.71715200	–0.01349300
H	–4.66850900	–2.07155600	–1.66516400
H	–4.34995900	–0.37588300	–2.02199200
H	–5.02871500	0.86023900	1.47462100
H	–4.54301800	1.37586300	–0.13934800
H	–6.09762100	–0.57203700	–0.26891900
H	–5.00269600	–1.51746000	0.73665400
C	0.45348600	4.32000500	–1.93719700
C	–0.83871500	3.59705300	0.73103900
C	2.18822700	3.14531800	0.24997600
H	1.22161900	4.08256000	–2.67880700
H	–0.51060800	4.33542200	–2.45331200
H	0.64755100	5.32779200	–1.55776700
H	2.96387200	2.76248000	–0.42869600

H	2.44653200	4.19128800	0.43683700
H	2.25590700	2.62617700	1.21115600
H	–1.84943700	3.50762400	0.32204000
H	–0.78115700	2.98635500	1.63330600
H	–0.68057200	4.64409600	1.00507000

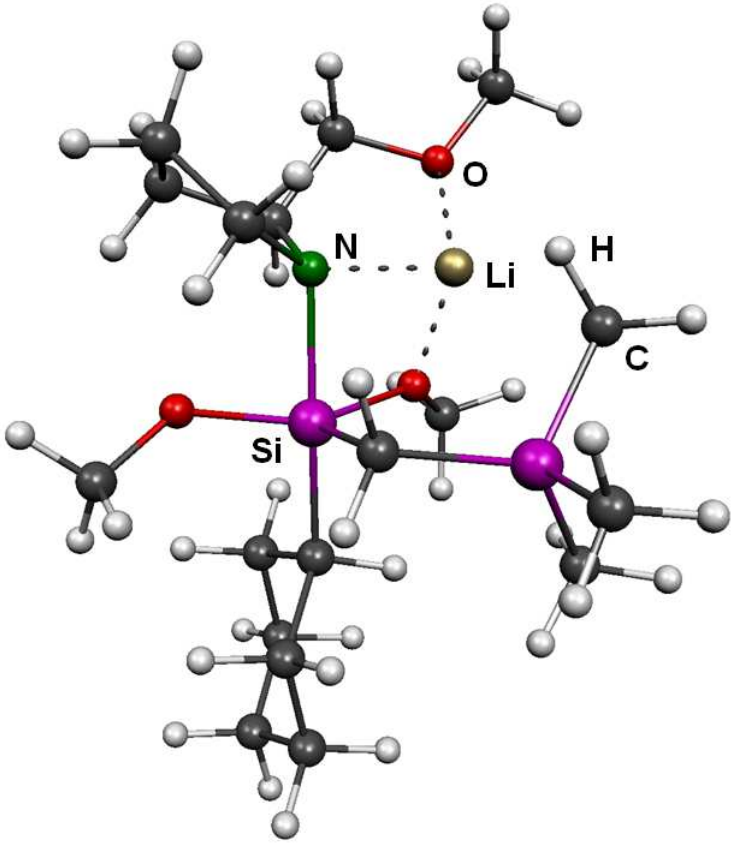

Abbildung 9.24 Molekel-Darstellung von **[BPR2]‡** [M052X/6-31+G(d)].

Tabelle 9.42 Standardorientierung von **[BPR2]‡** [M052X/6-31+G(d)].

Atomsymbol	x	y	z
C	–0.11165000	0.06056300	2.59775100
C	3.05225400	–1.86589700	–2.08427100
C	2.65820700	–2.67019500	–0.84159000
C	2.16548800	–0.60719900	–1.99854200
C	2.32848700	–1.56696400	0.17281600
C	–0.37581900	1.21539400	–1.47928400
C	3.62165000	–1.13221400	0.86782400
C	4.54236700	0.50031300	2.32621000
H	0.32723600	0.85976600	3.20447300
H	0.23449200	–0.89826200	2.99725900

H	2.88525600	–2.41940500	–3.00963100
H	–1.19690900	0.10974300	2.70692100
H	1.75320800	–3.24374700	–1.03338000
H	4.11227100	–1.59920400	–2.05318100
H	1.63959600	–1.92167800	0.94551300
H	1.30342200	–0.72558000	–2.65868200
H	3.44797200	–3.34610900	–0.49923600
H	2.71514100	0.28042900	–2.33235300
H	3.98555600	–1.91965400	1.53786300
H	4.39916900	–0.90490200	0.12841200
H	4.27405500	1.40064400	2.87544700
H	4.88589000	–0.26505800	3.02730900
H	5.34297400	0.72645200	1.61507100
N	1.71617900	–0.46216200	–0.59596600
O	0.31210500	0.22553800	1.26485700
O	3.38330700	0.05312500	1.64330200
Si	–0.23999200	–0.34388200	–0.38319300
Si	–0.34583100	2.86221500	–0.57570200
Li	1.93402300	0.89886300	0.74200800
H	0.43597300	1.25806400	–2.21216100
H	–1.30781200	1.18558200	–2.05410400
O	–0.25589500	–1.85574200	–1.23598800
C	–1.18242800	–2.29005200	–2.20012400
H	–1.56404100	–1.45913000	–2.80466400
H	–0.67192800	–2.98999000	–2.86953600
H	–2.03524200	–2.81005700	–1.75262300
C	–2.07666100	–0.49136100	0.30106200
C	–3.26913000	–0.25341200	–0.64544600
C	–2.29750000	–1.81539100	1.05804300
H	–2.16419200	0.32020600	1.03584500
C	–4.59411500	–0.24291000	0.12904700
H	–3.32771500	–1.03015300	–1.41321200
H	–3.16159300	0.69978300	–1.17202300
C	–3.61876700	–1.82338800	1.83419700
H	–2.30537700	–2.64257800	0.34001300
H	–1.46595800	–2.02687300	1.73905100
C	–4.79692100	–1.55085600	0.89683700
H	–5.43348700	–0.07123400	–0.55286600
H	–4.58247600	0.59208400	0.84172900
H	–3.75876500	–2.77959600	2.34903400
H	–3.58792900	–1.04387200	2.60703500
H	–5.73576700	–1.52326400	1.45819400

H	–4.87797400	–2.37652500	0.17840200
C	–0.58873800	4.25790200	–1.83211700
C	–1.65896200	3.04456600	0.76791100
C	1.35463200	3.18447400	0.24891600
H	0.18856400	4.23556500	–2.60111300
H	–1.55485800	4.15801000	–2.33435600
H	–0.56092300	5.23857200	–1.34845700
H	2.18790000	2.76583000	–0.32977100
H	1.53470100	4.26105900	0.30363000
H	1.38082500	2.82483300	1.28471400
H	–2.65082500	2.77616300	0.39450000
H	–1.43681600	2.40152300	1.62187200
H	–1.69791600	4.08085300	1.11650500

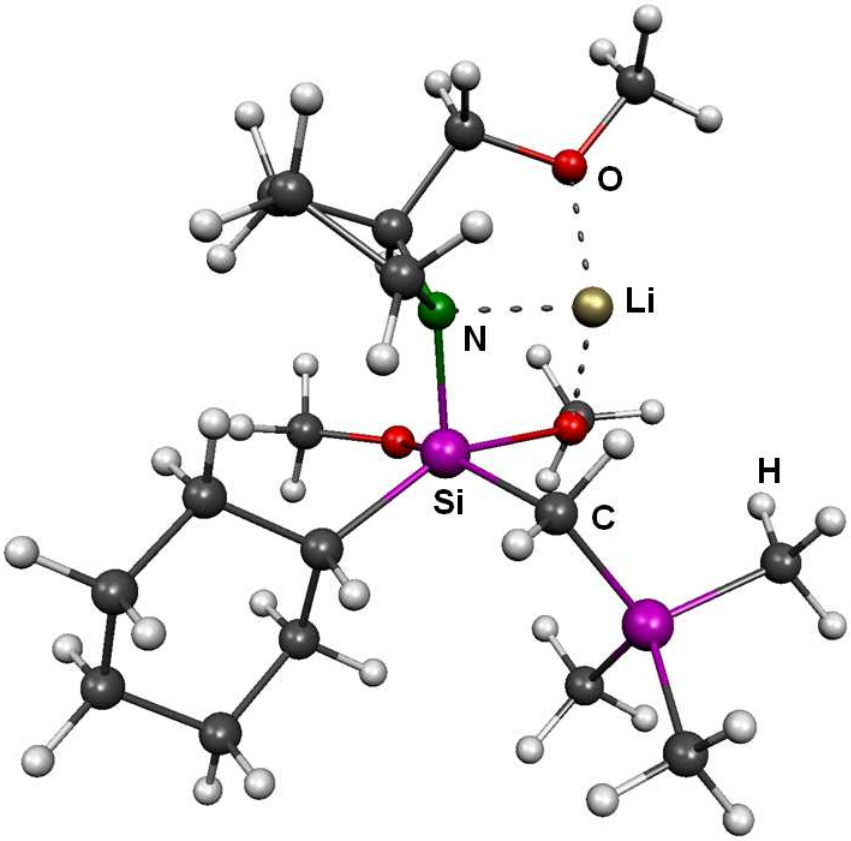

Abbildung 9.25 Molekel-Darstellung von **[BPR3]‡** [M052X/6-31+G(d)].

Tabelle 9.43 Standardorientierung von **[BPR3]‡** [M052X/6-31+G(d)].

Atomsymbol	x	y	z
C	1.26136300	1.87767300	2.18230400
C	1.86066500	–2.70827000	–1.80009300

C	2.18776100	–2.88833000	–0.30530400
C	1.35015400	–1.24449000	–1.92245800
C	2.39804800	–1.44679000	0.17909800
C	–0.52317300	1.34250400	–1.19626700
C	3.82647000	–0.99521400	–0.13205000
C	5.23915900	0.91753000	–0.04829200
H	1.70269800	2.88131000	2.19247500
H	1.99883900	1.15913800	2.55605800
H	1.11701600	–3.43044200	–2.13769700
H	0.41102600	1.86322200	2.86585600
H	1.33259900	–3.30999900	0.22533600
H	2.75049800	–2.85565900	–2.41597300
H	2.22323000	–1.31767900	1.24802400
H	0.32972500	–1.18590300	–2.30208700
H	3.05080700	–3.53791100	–0.13445500
H	1.97999000	–0.69165800	–2.63139800
H	4.53614500	–1.46752300	0.55534800
H	4.11196300	–1.24622400	–1.16083600
H	5.19952500	1.99812700	0.07129800
H	5.84185600	0.48507600	0.75405800
H	5.68460000	0.66807000	–1.01581000
N	1.42498400	–0.65811900	–0.57259500
O	0.85961000	1.58675400	0.85760200
O	3.90678700	0.42905800	0.02452000
Si	–0.06599600	0.05572500	0.23019300
Si	–1.38109500	2.92383700	–0.61825500
Li	2.18209500	1.19002600	–0.32533700
H	0.40584500	1.71087700	–1.66384300
H	–1.09053300	0.87670000	–2.00650400
O	0.10678300	–0.41896800	1.88886300
C	–0.06102400	–1.62081900	2.58772600
H	–0.81041000	–1.49806700	3.37509200
H	–0.36484500	–2.45417200	1.95287300
H	0.88698200	–1.89277100	3.06928000
C	–1.68372300	–1.04733800	–0.12478200
C	–1.54438400	–2.54066400	–0.48925800
C	–2.76919700	–0.90523400	0.96070200
H	–2.11619800	–0.58646300	–1.02242500
C	–2.88155600	–3.11736400	–0.97395800
H	–1.21996600	–3.12895000	0.37558200
H	–0.78811200	–2.68796500	–1.26302300
C	–4.11295000	–1.47493800	0.49131200

H	–2.46462300	–1.43822400	1.86619900
H	–2.89374700	0.14068500	1.25034700
C	–3.97069300	–2.94370500	0.08671000
H	–2.76990200	–4.17600500	–1.23130200
H	–3.18398300	–2.59354900	–1.88923200
H	–4.86763100	–1.37172300	1.27765000
H	–4.46607600	–0.89624400	–0.37149200
H	–4.92462600	–3.33605600	–0.27812500
H	–3.70089300	–3.53227200	0.97282000
C	–0.14248100	4.35475800	–0.52841000
C	–2.71439300	3.41084000	–1.87796400
C	–2.25171600	2.79389800	1.06046500
H	–1.66761700	2.23052100	1.79207500
H	–2.41097300	3.79972400	1.46141500
H	–3.23182700	2.32104200	0.96193600
H	–2.27780000	3.59031200	–2.86466500
H	–3.45593400	2.61287500	–1.98154800
H	–3.23984400	4.31954700	–1.56984600
H	0.38474000	4.47682000	–1.47995400
H	–0.65316600	5.29659200	–0.30781700
H	0.59330200	4.16868500	0.25658700