Supporting Information for –

Stereoselectivity induced by Support Confinement Effects. Aza-pyridinoxazolines: A New Family of C_1-Symmetric Ligands for Copper-Catalyzed Enantioselective Cyclopropanation Reactions

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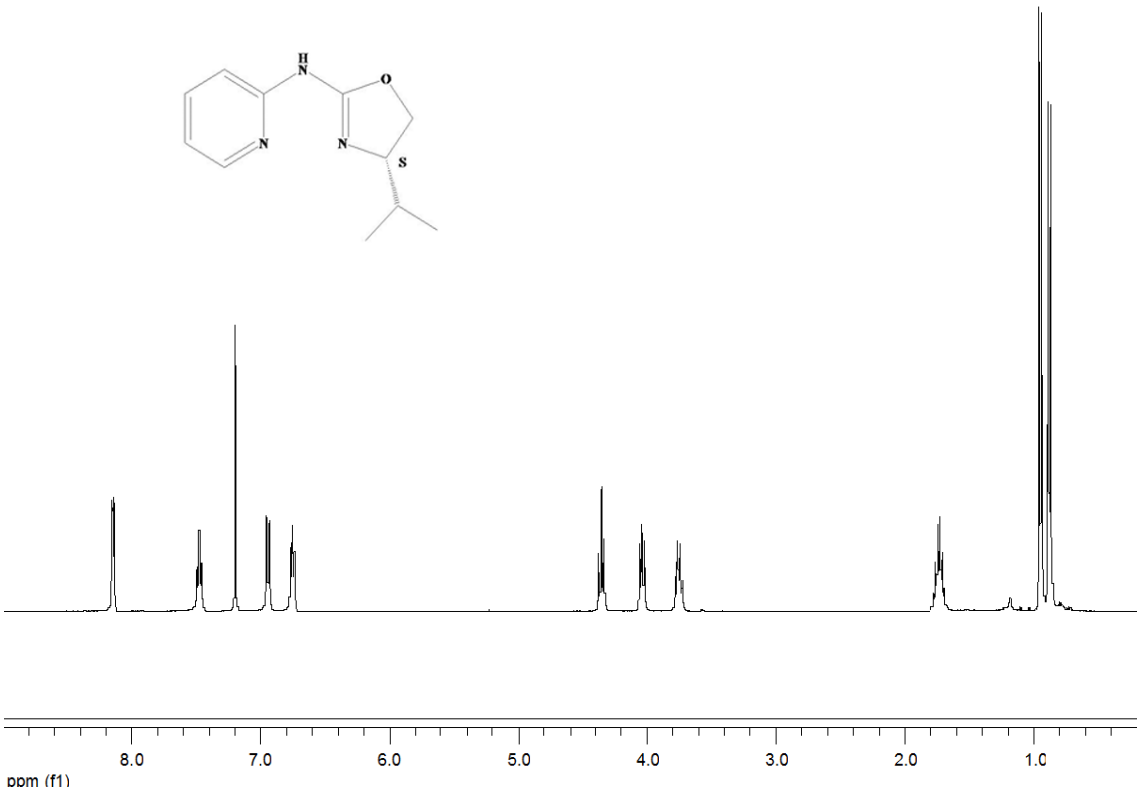
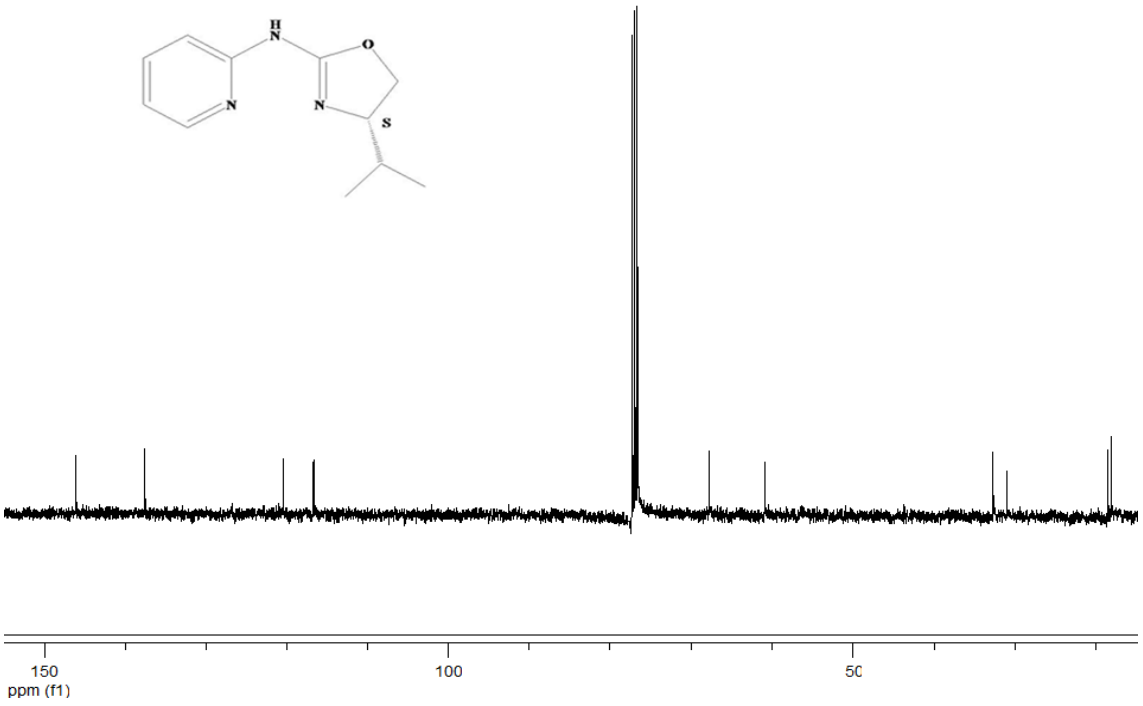
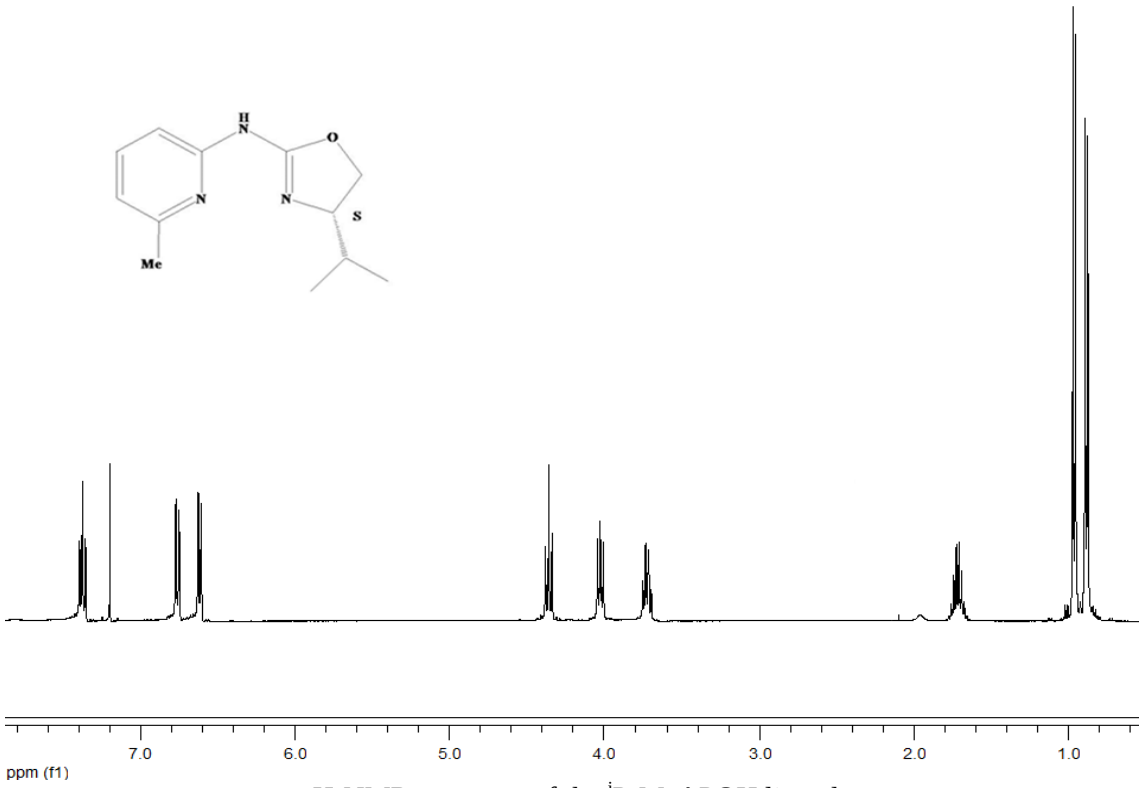


^{1}H-NMR spectrum of the ^{i}PrAPOH ligand



^{13}C-NMR spectrum of the ^{i}PrAPOH ligand



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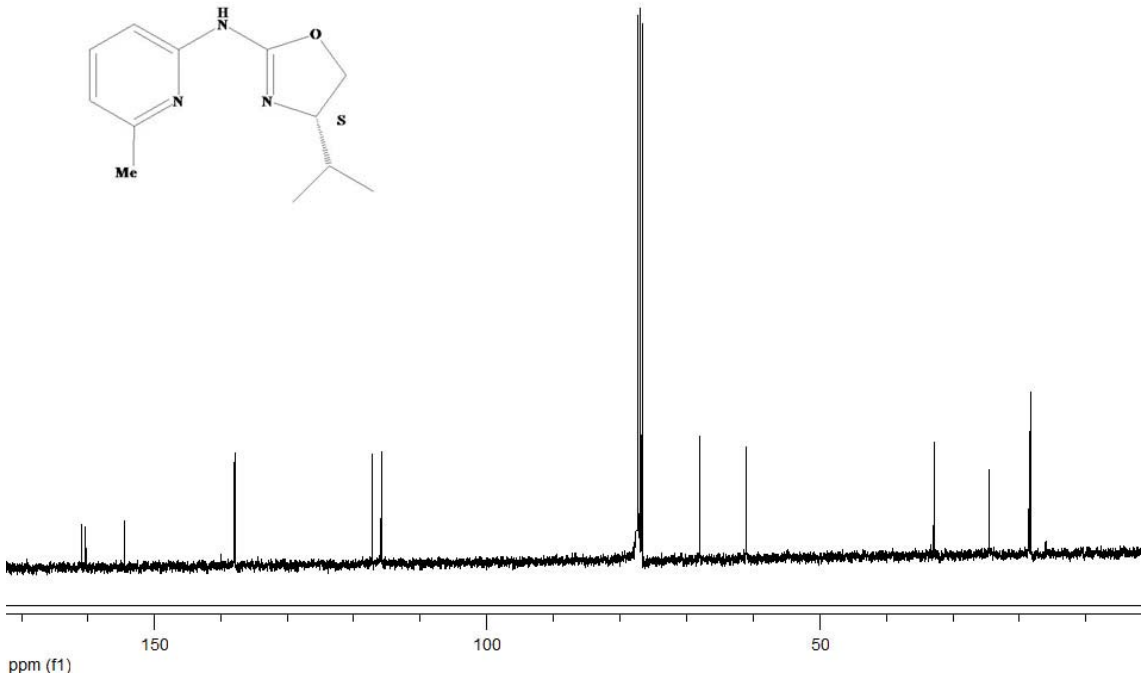

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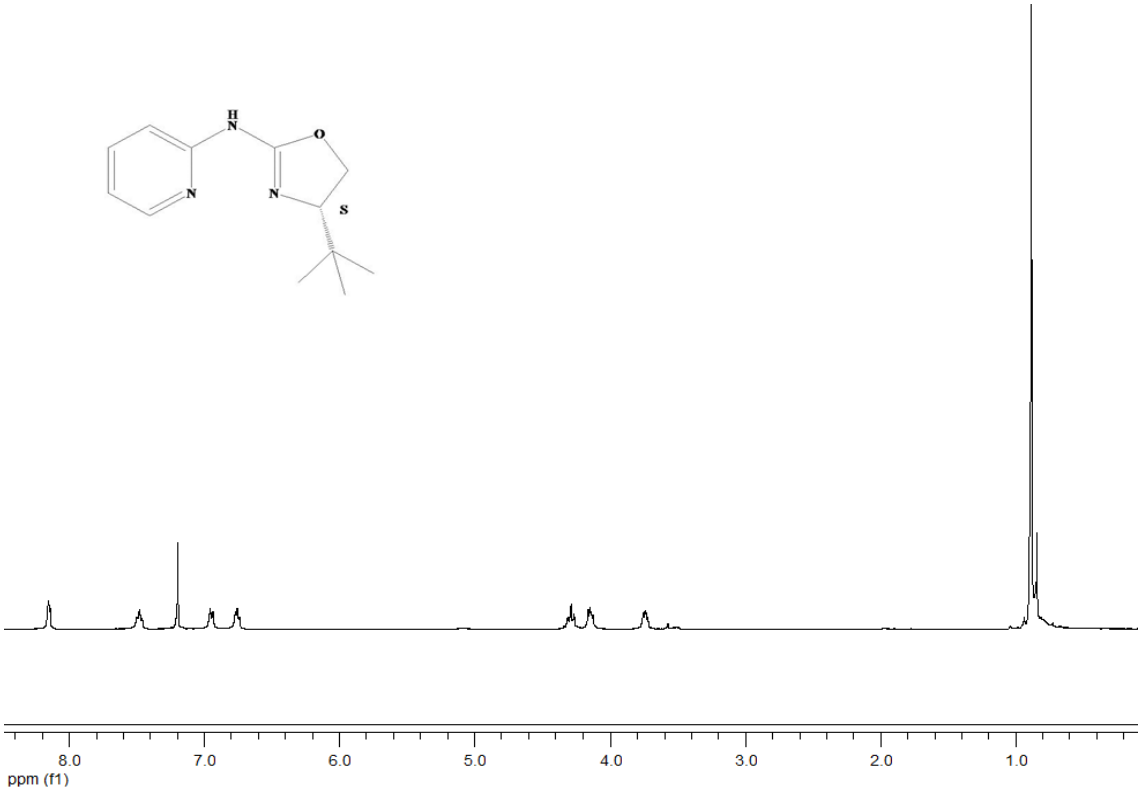

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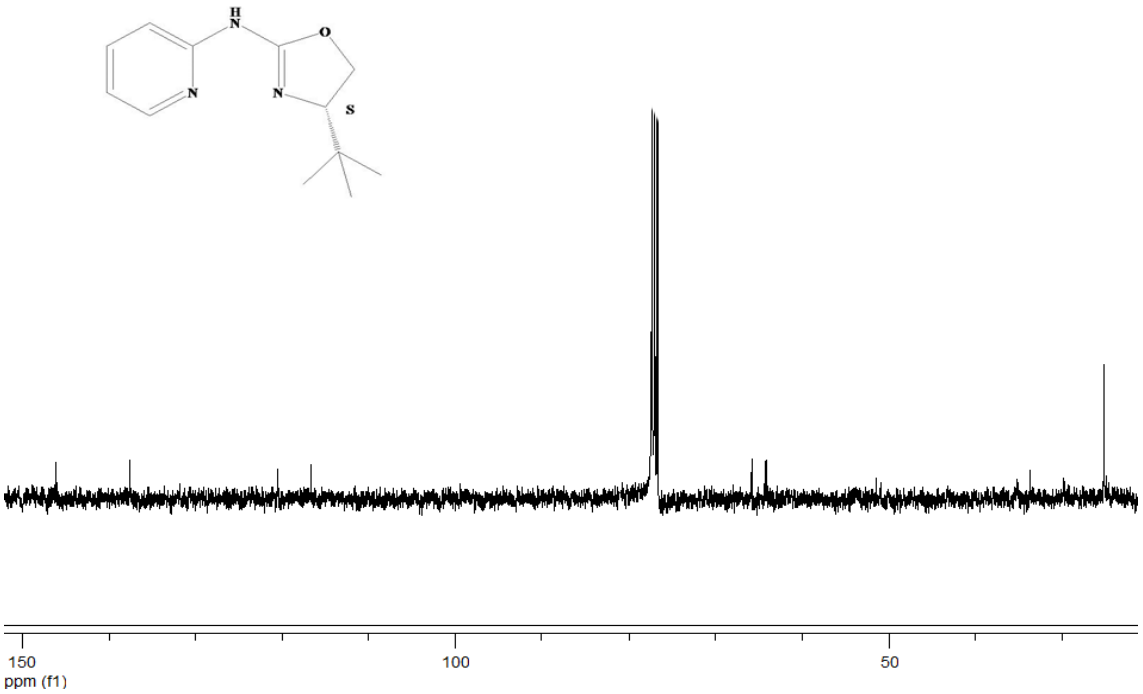

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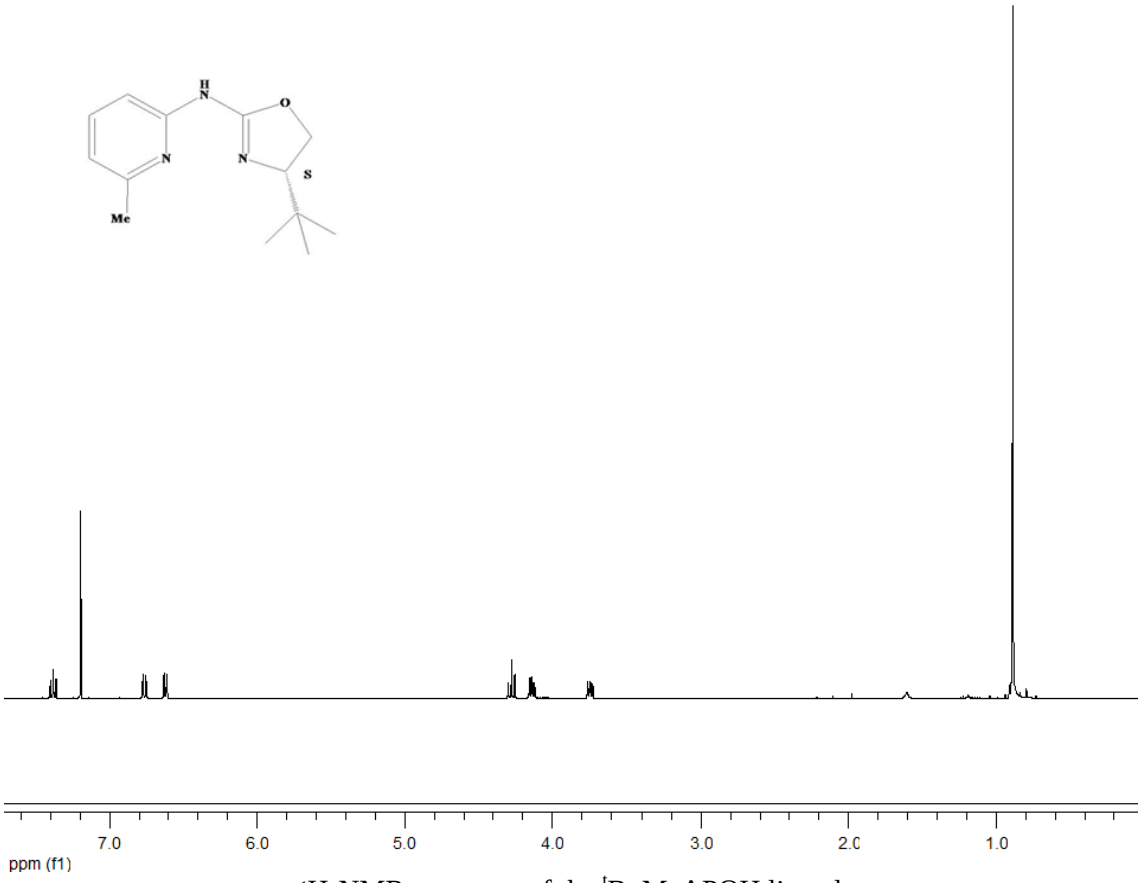

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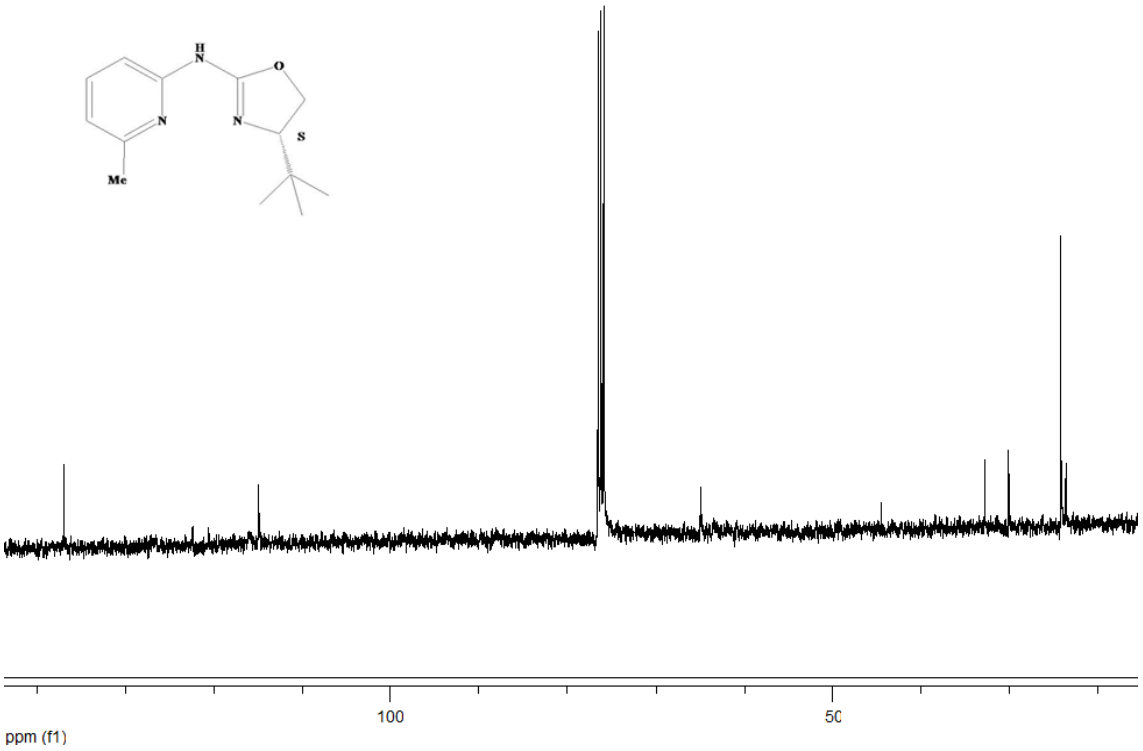

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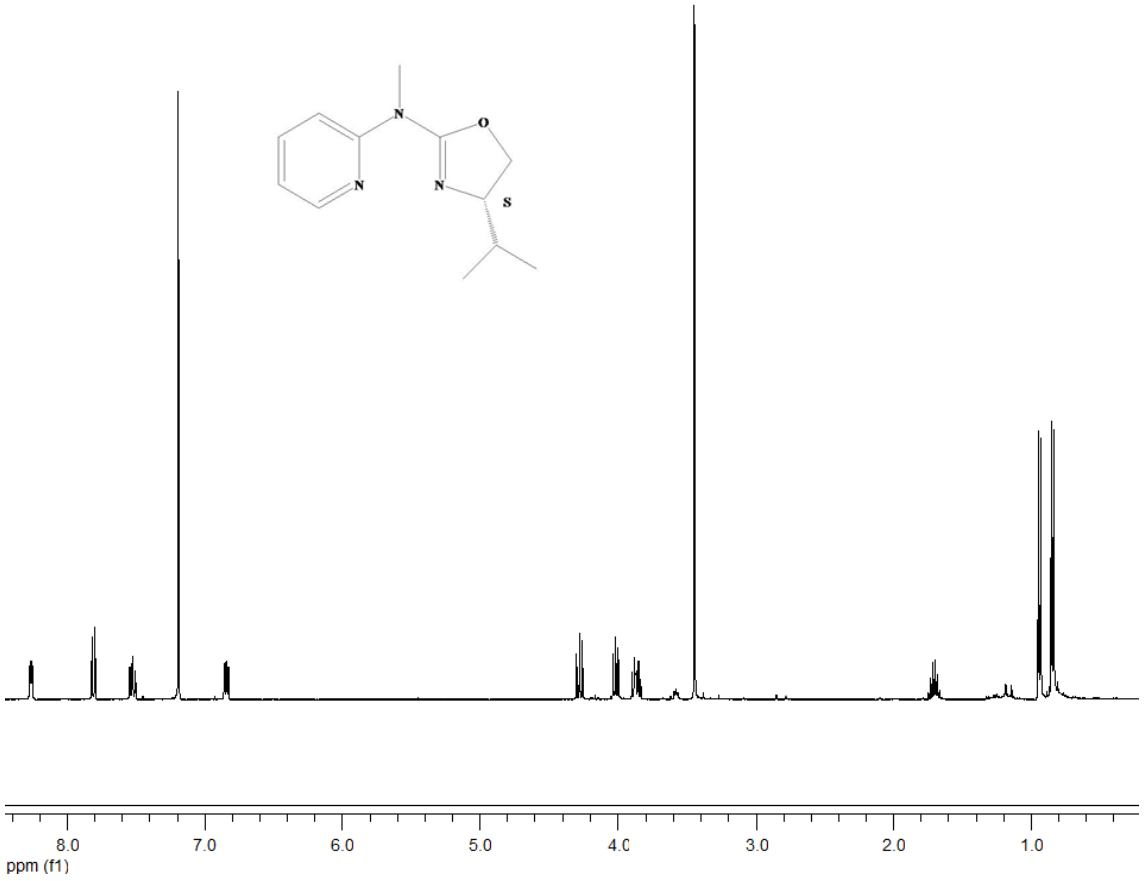

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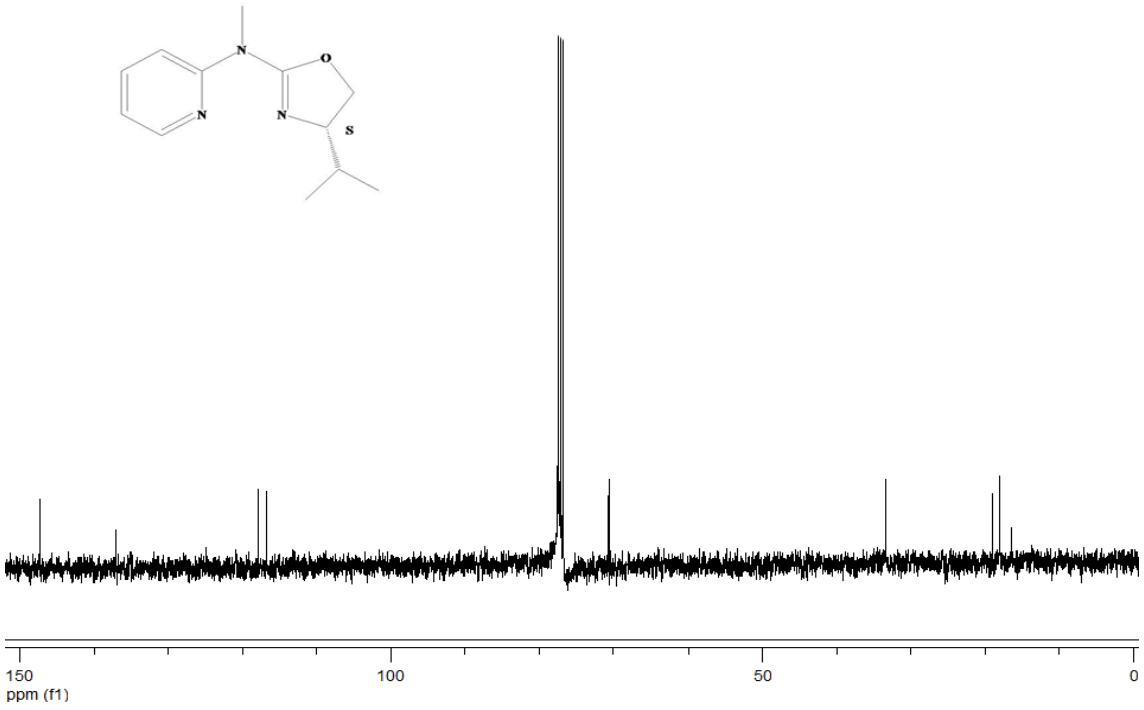

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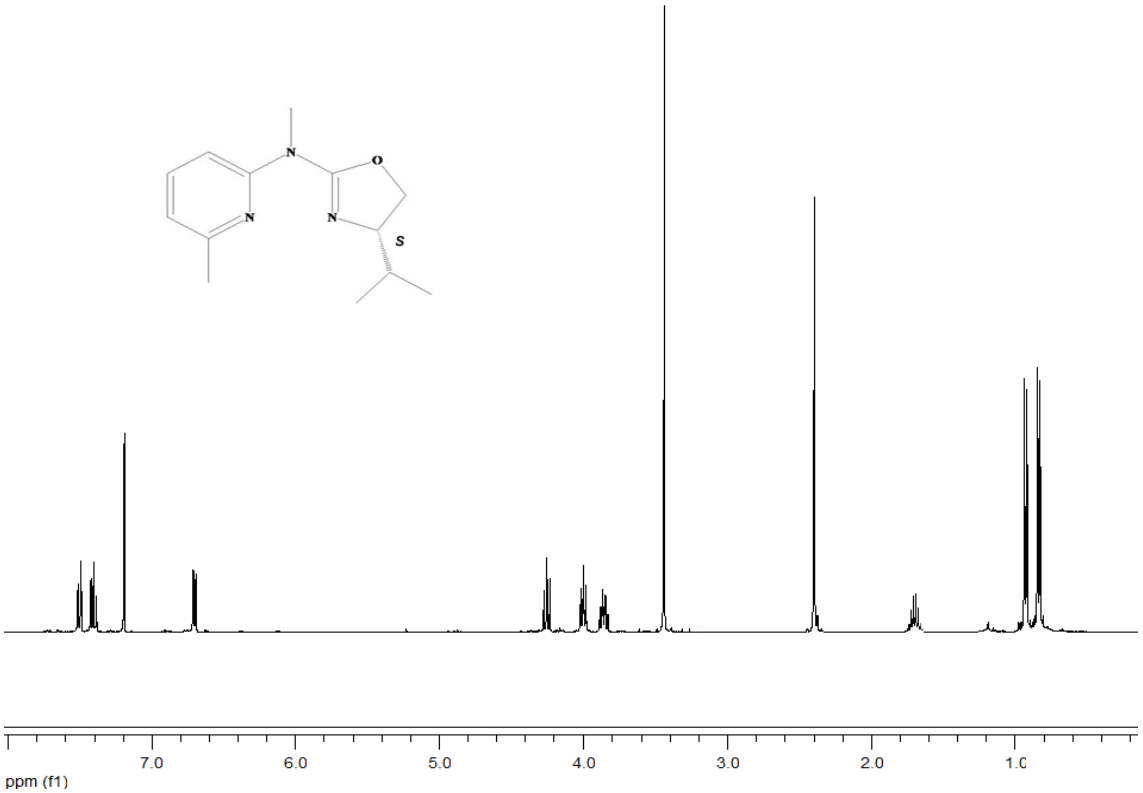

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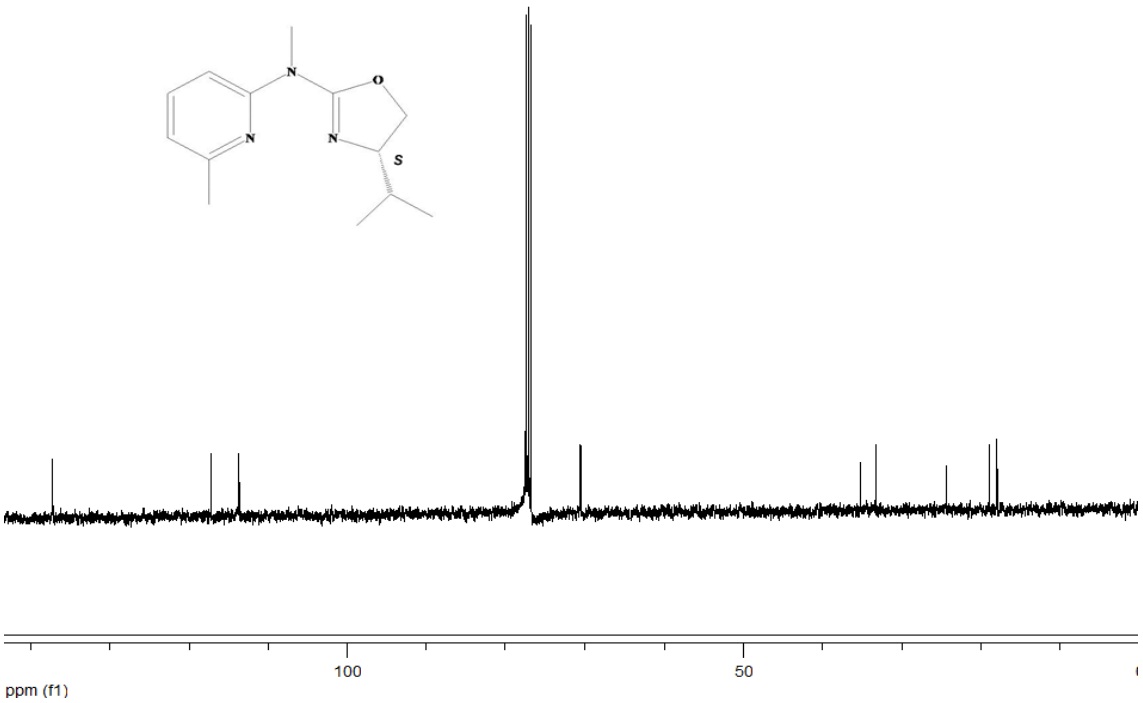

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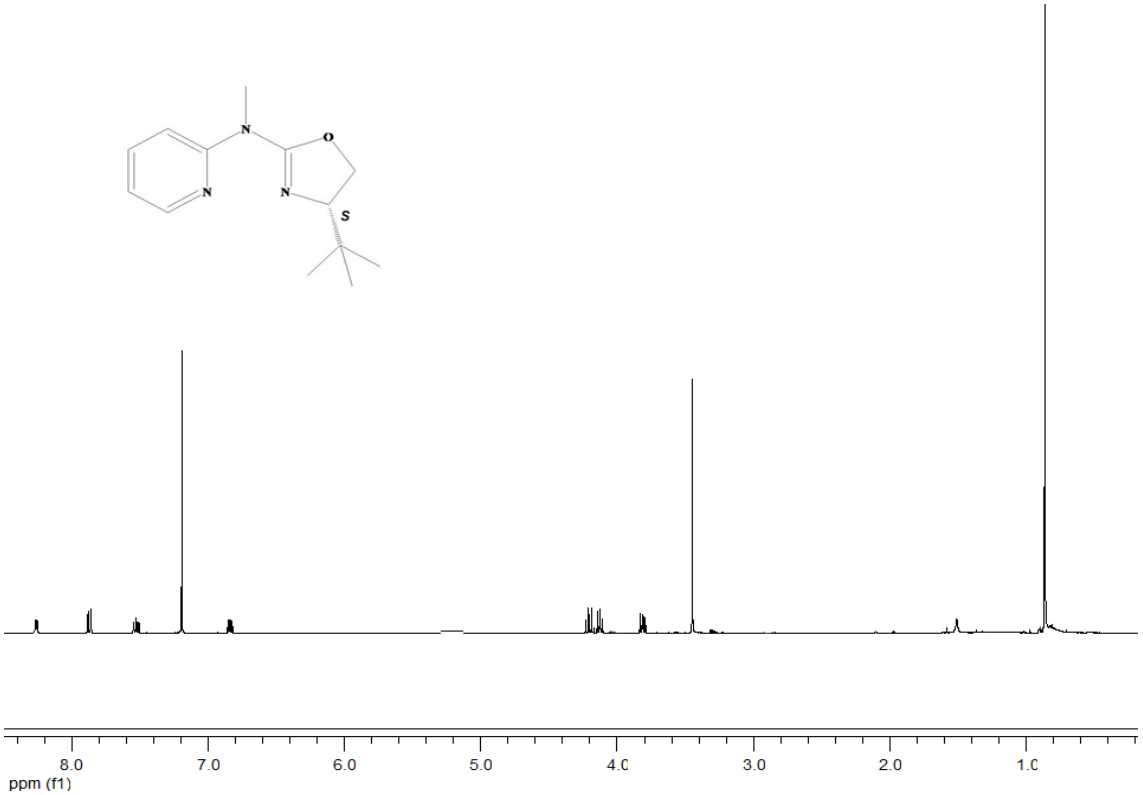

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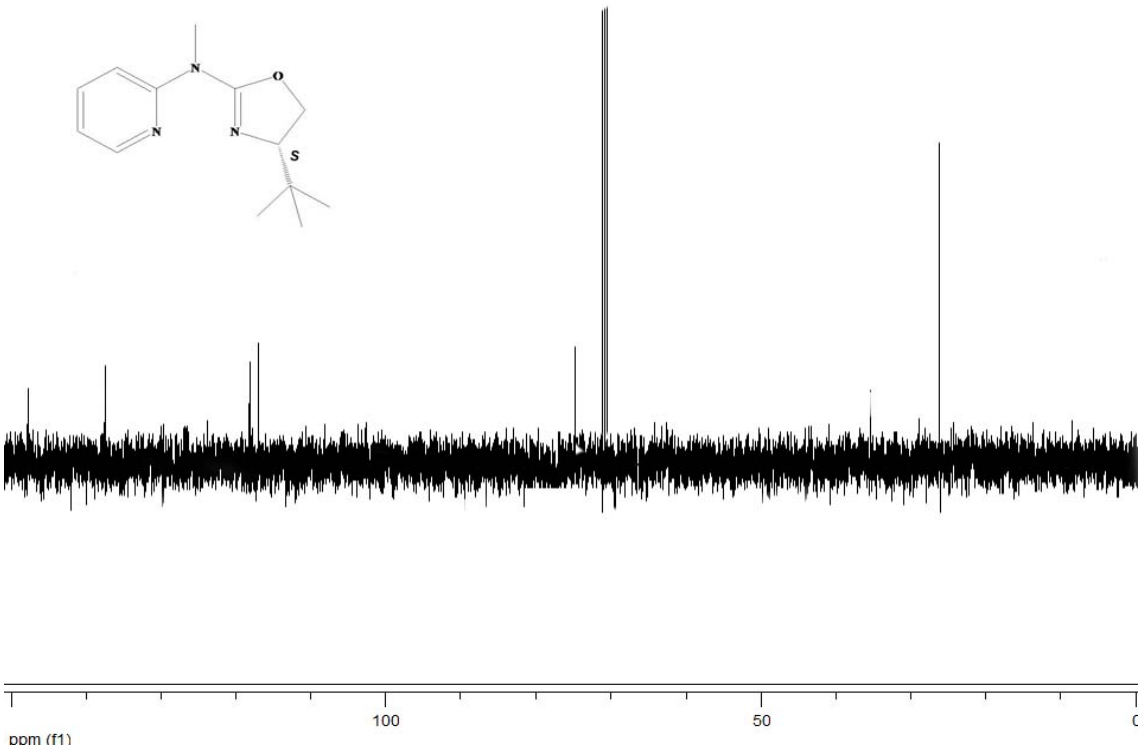
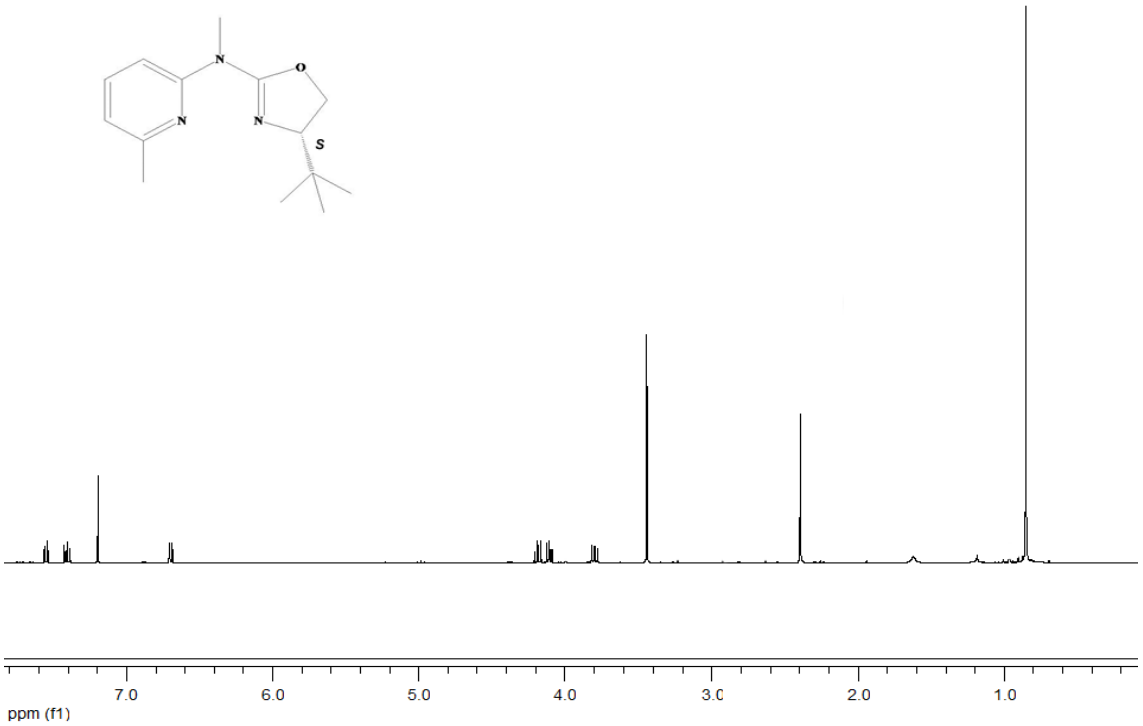
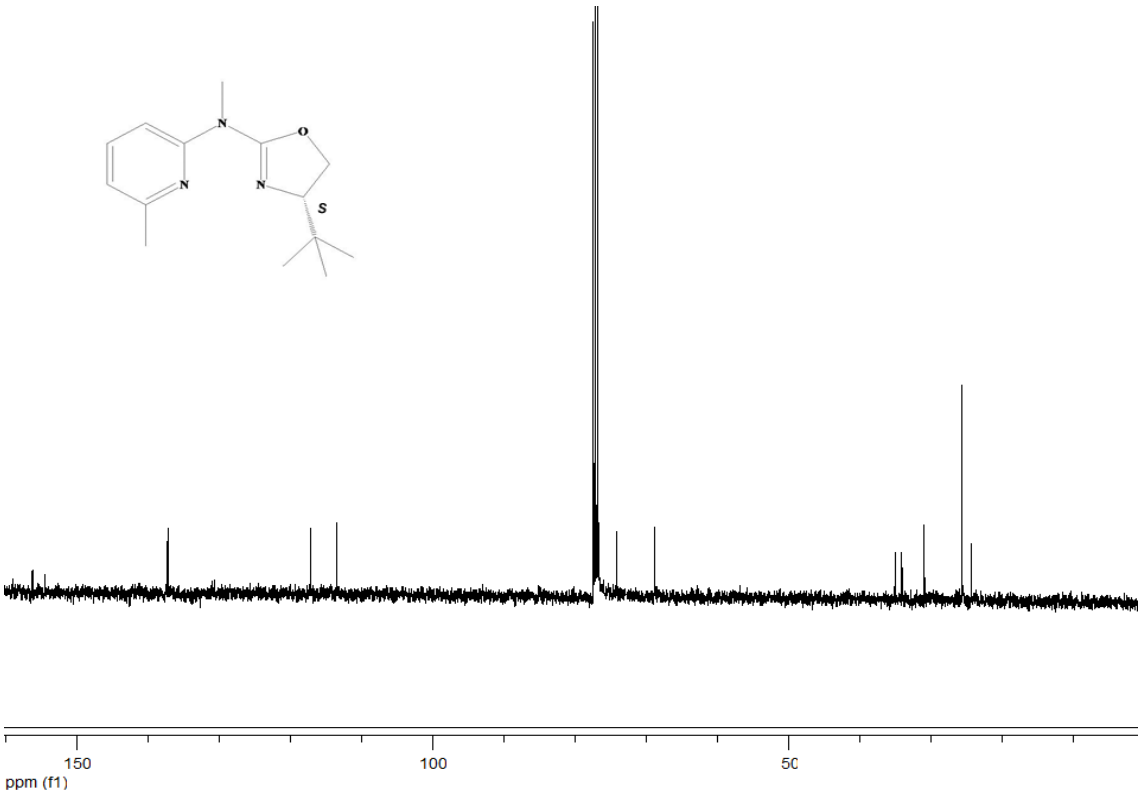


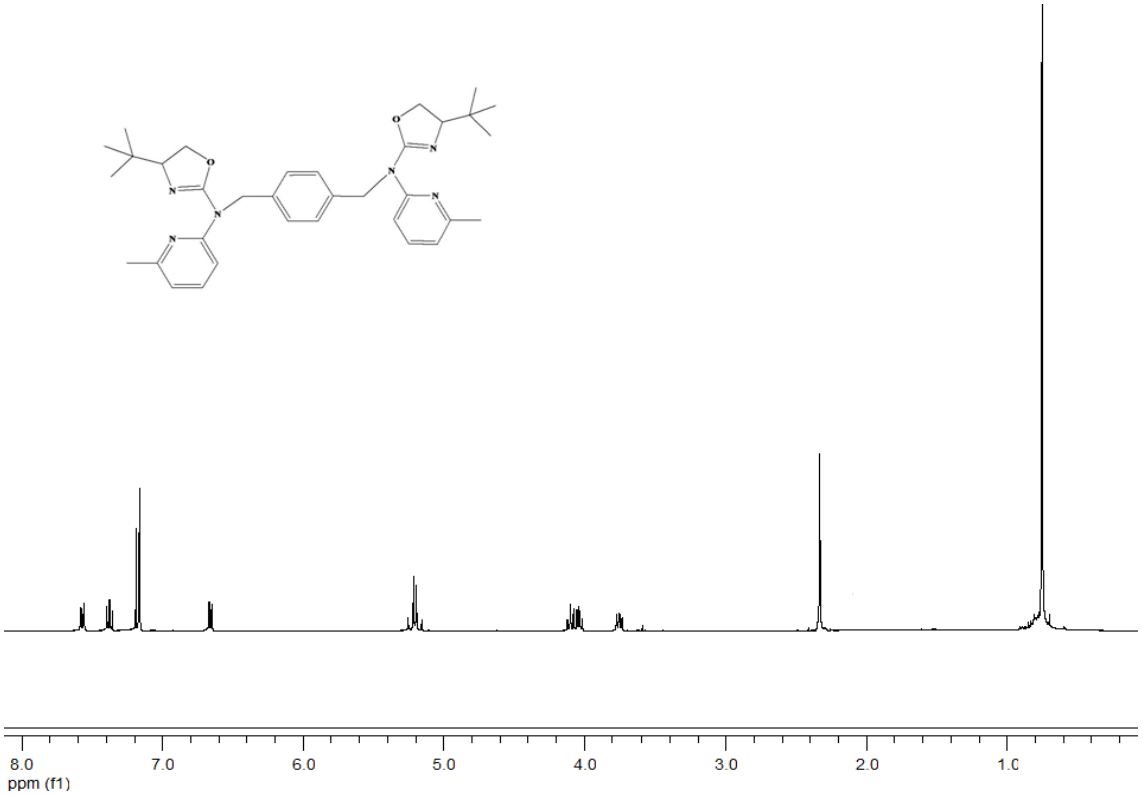
^{13}C-NMR spectrum of the ^{t}BuAPOMe ligand



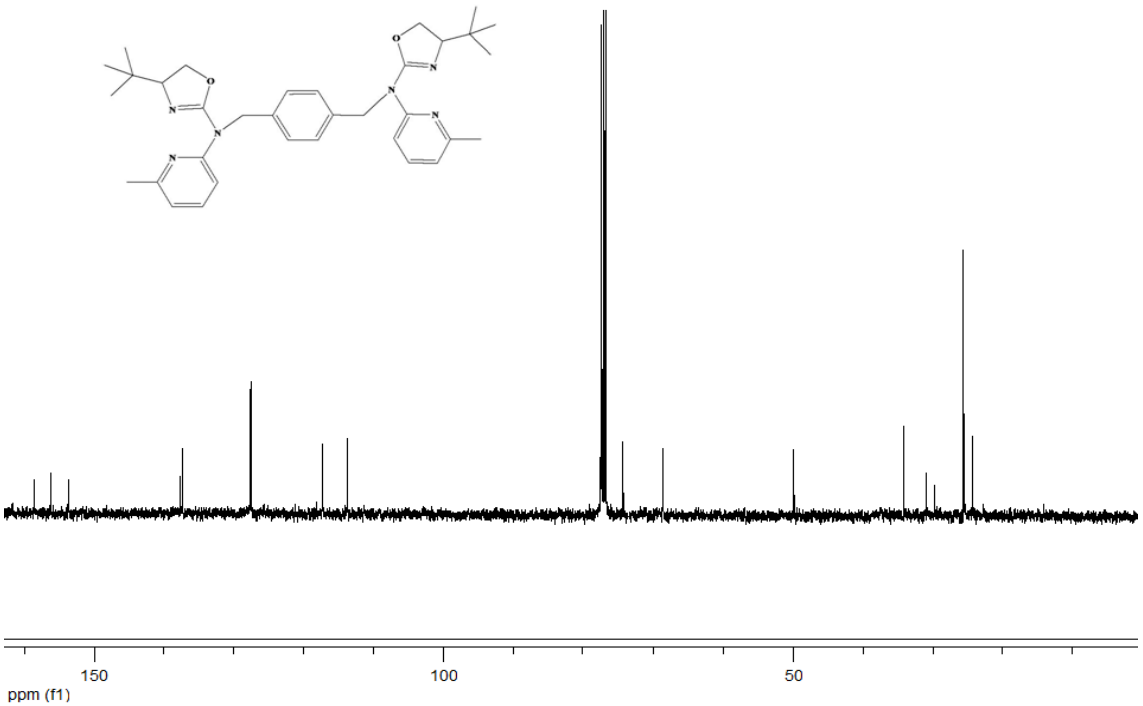
^{1}H-NMR spectrum of the ^{t}BuMeAPOMe ligand



^{13}C-NMR spectrum of the ^{t}BuMeAPOMe ligand



^{1}H-NMR spectrum of the ^{t}BuDaxMeAPO ligand



^{13}C-NMR spectrum of the ^{t}BuDaxMeAPO ligand

Table S1. M05-2X/6-31G(d)//B3LYP/6-31G(d) calculated absolute energies, enthalpies, free energies, and entropies of the structures* considered in this work.

Structure	$E_{M05\text{-}2X}$ (Hartree)[a]	E_{B3LYP} (Hartree)[a]	$H_{M05\text{-}2X/B3LYP}$ (Hartree)[b]	$S_{M05\text{-}2X/B3LYP}$ (cal mol^{-1} K^{-1})[b]	$G_{M05\text{-}2X/B3LYP}$ (Hartree)[b]	Lowest freq. (cm^{-1})
ts15a'-anti-I-Re-Λ	–2613.952088	–2614.233486	–2613.857879	166.2	–2613.936841	–132.3
ts15a'-anti-I-Re-V	–2613.950657	–2614.234167	–2613.858789	168.1	–2613.938666	–99.8
ts15a'-anti-II-Re-Λ	–2613.949500	–2614.231948	–2613.856587	167.6	–2613.936234	–107.0
ts15a'-anti-II-Re-V	–2613.945955	–2614.230638	–2613.855488	171.0	–2613.936721	–78.4
ts15a'-syn-I-Re-Λ	–	–	–	–	–	–
ts15a'-syn-I-Re-V	–2613.947463	–2614.232095	–2613.856944	169.9	–2613.937648	–67.2
ts15a'-syn-II-Re-Λ	–	–	–	–	–	–
ts15a'-syn-II-Re-V	–2613.953327	–2614.236108	–2613.860692	167.8	–2613.940416	–104.5
ts15a'-anti-I-Si-Λ	–	–	–	–	–	–
ts15a'-anti-I-Si-V	–2613.945582	–2614.230709	–2613.855659	171.9	–2613.937343	–55.6
ts15a'-anti-II-Si-Λ	–2613.951784	–2614.233988	–2613.858452	164.4	–2613.936541	–105.4
ts15a'-anti-II-Si-V	–2613.951513	–2614.235071	–2613.859677	167.2	–2613.939140	–73.6
ts15a'-syn-I-Si-Λ	–2613.949100	–2614.231092	–2613.855812	167.6	–2613.935435	–116.5
ts15a'-syn-I-Si-V	–2613.951421	–2614.234449	–2613.859108	166.8	–2613.938351	–97.7
ts15a'-syn-II-Si-Λ	–2613.946753	–2614.229445	–2613.854250	170.4	–2613.935234	–98.8
ts15a'-syn-II-Si-V	–2613.948347	–2614.231577	–2613.856153	170.6	–2613.937208	–103.3
ts15c'-anti-I-Re-Λ	–2653.265377	–2653.552315	–2653.147639	174.4	–2653.230479	–126.5
ts15c'-anti-I-Re-V	–2653.262441	–2653.553374	–2653.148861	175.3	–2653.232170	–71.0
ts15c'-anti-II-Re-Λ	–2653.263528	–2653.551363	–2653.146832	174.9	–2653.229911	–109.9
ts15c'-anti-II-Re-V	–2653.256422	–2653.548929	–2653.144793	180.5	–2653.230542	–54.2
ts15c'-syn-I-Re-Λ	–2653.262726	–2653.548917	–2653.144588	175.5	–2653.227966	–62.7
ts15c'-syn-I-Re-V	–2653.264191	–2653.551174	–2653.146580	174.7	–2653.229570	–108.6
ts15c'-syn-II-Re-Λ	–2653.263400	–2653.551422	–2653.146798	172.1	–2653.228564	–83.5
ts15c'-syn-II-Re-V	–2653.266396	–2653.552505	–2653.147907	173.7	–2653.230453	–135.9
ts15c'-anti-I-Si-Λ	–	–	–	–	–	–
ts15c'-anti-I-Si-V	–2653.262916	–2653.552109	–2653.147594	176.4	–2653.231394	–77.7
ts15c'-anti-II-Si-Λ	–2653.263079	–2653.549891	–2653.145281	171.6	–2653.226800	–115.4
ts15c'-anti-II-Si-V	–2653.265974	–2653.553941	–2653.149241	173.7	–2653.231772	–100.7
ts15c'-syn-I-Si-Λ	–2653.262726	–2653.550927	–2653.146382	173.2	–2653.228667	–101.8
ts15c'-syn-I-Si-V	–2653.266180	–2653.554103	–2653.149554	175.2	–2653.232785	–104.8
ts15c'-syn-II-Si-Λ	–2653.259407	–2653.549032	–2653.144667	176.3	–2653.228413	–65.6
ts15c'-syn-II-Si-V	–2653.261007	–2653.551049	–2653.146623	177.0	–2653.230728	–90.5
ts15d-anti-I-Re-Λ	–2771.191230	–2771.488162	–2770.994848	190.1	–2771.085181	–143.6
ts15d-anti-I-Re-V	–2771.191618	–2771.493551	–2771.000264	192.9	–2771.091919	–74.1
ts15d-anti-II-Re-V	–	–	–	–	–	–
ts15d-anti-II-Re-Λ	–2771.190196	–2771.488105	–2770.994897	191.6	–2771.085909	–134.0
ts15d-syn-I-Re-Λ	–2771.184906	–2771.486422	–2770.993193	190.6	–2771.083732	–59.2
ts15d-syn-I-Re-V	–2771.192520	–2771.491694	–2770.998339	191.1	–2771.089140	–98.9
ts15d-syn-II-Re-Λ	–2771.189627	–2771.489620	–2770.996146	188.5	–2771.085689	–73.6
ts15d-syn-II-Re-V	–2771.194993	–2771.493163	–2770.999626	189.6	–2771.089693	–131.0
ts15d-anti-I-Si-Λ	–2771.184680	–2771.484971	–2770.991561	189.1	–2771.081404	–93.5
ts15d-anti-I-Si-V	–2771.189832	–2771.492372	–2770.999146	192.6	–2771.090658	–61.8
ts15d-anti-II-Si-Λ	–2771.186930	–2771.486851	–2770.993410	189.5	–2771.083431	–111.3
ts15d-anti-II-Si-V	–2771.194023	–2771.494804	–2771.001294	189.9	–2771.091541	–82.6
ts15d-syn-I-Si-Λ	–2771.187360	–2771.486693	–2770.993427	191.5	–2771.084404	–109.7
ts15d-syn-I-Si-V	–2771.193112	–2771.494232	–2771.000868	190.9	–2771.091593	–91.5
ts15d-syn-II-Si-Λ	–2771.186328	–2771.486678	–2770.993432	191.4	–2771.084374	–99.7
ts15d-syn-II-Si-V	–2771.190791	–2771.491562	–2770.998230	193.0	–2771.089916	–106.7

[a] 1 Hartree = 627.5 kcal mol^{-1}. [b] Thermal corrections at 298.15 K.

Cartesian coordinates of the structures considered in this work calculated at the B3LYP/6–31G(d) level.

Structure **ts15a'-*anti*-I-*Re*-Λ**

Cu	-0.36246300	-0.01222900	0.29771600
N	1.01684700	-1.40849000	-0.00573700
C	2.34694500	-1.19875200	-0.10130700
C	2.15820100	1.24727700	-0.01745600
N	0.87150800	1.40251300	-0.09142800
C	0.54289700	-2.64689900	-0.27653700
C	3.22755300	-2.23766700	-0.45118800
C	0.61506500	2.83848300	-0.39940100
O	2.91711000	2.34562100	-0.13358600
C	1.34437100	-3.72135900	-0.61531400
C	2.72063200	-3.50404800	-0.70328100
C	2.00147700	3.47959200	-0.17842400
H	0.32494900	2.90286600	-1.45525400
C	-2.11200100	0.12386200	0.76480500
C	-3.12323900	0.49355600	-0.25538900
O	-3.74470400	-0.51200100	-0.88753400
C	-4.65234600	-0.11393400	-1.94417800
H	-2.34588700	0.59344400	1.72086900
O	-3.26941000	1.67147000	-0.53542400
H	-5.43043200	0.54186100	-1.54815700
H	-4.10587800	0.40630000	-2.73359900
H	-5.08142400	-1.04287300	-2.31736400
C	-3.70861200	-1.45225800	2.06396800
C	-2.65609100	-2.04003100	1.45288800
H	-1.75076700	-2.27873300	2.00186700
H	-2.75535900	-2.44299600	0.45078400
H	-4.64353400	-1.28431500	1.53960800
H	-3.65663600	-1.12422800	3.09869000
H	-0.53212600	-2.75713700	-0.20222900
H	2.33257200	4.13337500	-0.98542600
H	2.07906000	4.00185400	0.78023400
H	0.90457700	-4.69276900	-0.81010900
H	3.39467300	-4.30870700	-0.98020300
N	2.86706000	0.08457100	0.16548000
C	-0.47666700	3.45747700	0.46423400
H	-0.55980700	4.52734100	0.24108600
H	-1.44762600	2.99878600	0.26291500
H	-0.23701700	3.34840200	1.52832200
C	4.30950000	0.20448400	0.46876200
H	4.59350100	-0.60768200	1.13925800
H	4.91813400	0.17018500	-0.44028500
H	4.48449500	1.15295700	0.96963700
H	4.28797100	-2.05285300	-0.55335100

Structure **ts15a'-*anti*-I-*Re*-V**

Cu	-0.38305600	0.30854600	-0.37590500
N	1.23721600	1.38863900	-0.01805100
C	2.44916800	0.90080000	0.32988200
C	1.75428000	-1.45246400	0.21174800
N	0.60259400	-1.31952500	-0.36877700
C	1.13683900	2.70608300	-0.31233600
C	3.58078900	1.73354000	0.38277300
C	0.15266900	-2.67058200	-0.79552200
O	2.20626200	-2.70095300	0.38731000
C	2.19873700	3.59005000	-0.26409700
C	3.45080100	3.08265100	0.08705600
C	1.12700100	-3.59487800	-0.03190300
H	-0.87519500	-2.80626400	-0.45172100
C	-2.17029900	0.32818100	-0.64185000
C	-2.98896500	-0.42747800	0.33715900
O	-3.68464500	0.26426500	1.24443700
C	-4.39358900	-0.53060300	2.22688000
H	-2.56167100	0.19059900	-1.65171700
O	-2.92096200	-1.64678300	0.30708600
H	-5.10725700	-1.19337500	1.73347000
H	-3.68746400	-1.12471800	2.81079700
H	-4.90800000	0.19117500	2.85972200
C	-4.01874000	2.18780400	-1.11032100
C	-2.90352900	2.60925600	-0.47906000
H	-2.10336700	3.09018400	-1.03332000
H	-2.83620800	2.62361200	0.60297200
H	-4.85514400	1.77038700	-0.55993800
H	-4.11902200	2.24869200	-2.19091200
H	0.14361300	3.04399700	-0.58323800
H	0.69700500	-4.03206600	0.87292800
H	1.57906200	-4.37540100	-0.64525600
H	2.05086700	4.63731300	-0.50129200
H	4.32318700	3.72781500	0.12162700
C	0.21728900	-2.81895700	-2.31522800
H	-0.14293100	-3.80898200	-2.61507900
H	-0.41591300	-2.06901800	-2.79968200
H	1.24219700	-2.69600900	-2.68370100
N	2.58499000	-0.46143800	0.67284700
C	3.77062700	-0.86935000	1.45700300
H	4.65770200	-0.96645300	0.82327900
H	3.94863300	-0.12794700	2.23713300
H	3.56808600	-1.83030500	1.92215400
H	4.55311900	1.32864200	0.62712600

Structure **ts15a'-*anti*-II-*Re*-Λ**

Cu	-0.35790400	-0.12031800	0.25666400
N	1.19171700	-1.30823800	-0.09633500
C	2.48694100	-0.93068300	-0.11698700
C	1.98506600	1.45649400	0.08040300
N	0.69535000	1.44477200	-0.07660000
C	0.88282400	-2.56586800	-0.48778100
C	3.50351700	-1.82199200	-0.49711700
C	0.27245100	2.84341800	-0.36016500
O	2.59200600	2.65101600	0.06490500
C	1.82605500	-3.50303800	-0.86935500
C	3.16721800	-3.11649400	-0.86837200
C	1.53174100	3.65156000	0.01513100
H	0.07720600	2.91831000	-1.43751400
C	-2.10234700	-0.27279300	0.70267500
C	-3.15880300	-0.25048500	-0.35121100
O	-3.73912000	0.96794200	-0.38611200
C	-4.68064300	1.18161000	-1.46422600
H	-2.46725100	0.09507700	1.66218900
O	-3.42178200	-1.15171300	-1.12178500
H	-4.19671400	1.01983000	-2.43025200
H	-5.52505800	0.49654900	-1.36424100
H	-5.00754400	2.21538800	-1.36010900
C	-3.42089400	-2.21097800	1.94678300
C	-2.28079300	-2.59129900	1.33306800
H	-1.35398100	-2.70678300	1.88695200
H	-2.30138300	-2.92451800	0.30115000
H	-4.36102700	-2.16590900	1.40560900
H	-3.44301100	-1.94222700	2.99967800
H	-0.17284900	-2.80753200	-0.48006600
H	1.82594400	4.40088100	-0.71960900
H	1.46316200	4.10807900	1.00770700
H	1.51811800	-4.49974000	-1.16383500
H	3.94614200	-3.80964900	-1.17052700
N	2.82558500	0.38782300	0.25849400
C	-0.97186400	3.26464400	0.41062500
H	-1.20746900	4.31278600	0.19469700
H	-1.83694600	2.66030000	0.12485400
H	-0.81377600	3.16406000	1.49021100
C	4.22116200	0.66934100	0.65688600
H	4.57517700	-0.14854400	1.28569000
H	4.87550100	0.78348000	-0.21306900
H	4.24202400	1.59160400	1.23217600
H	4.53579000	-1.50128600	-0.53206600

Structure **ts15a'-*anti*-II-*Re*-V**

Cu	0.39165900	0.33782200	0.31286200
N	-1.30079700	1.31597600	-0.00073600
C	-2.49935300	0.76490300	-0.29449300
C	-1.68348300	-1.54657800	-0.13936800
N	-0.49989500	-1.33928500	0.35103800
C	-1.24699600	2.64800000	0.23518600
C	-3.66656400	1.54659900	-0.34508700
C	0.04389800	-2.64777200	0.79529900
O	-2.08632400	-2.82057600	-0.22990000
C	-2.34669500	3.48415100	0.18323000
C	-3.58551900	2.91110600	-0.10750200
C	-0.95095900	-3.65004400	0.16523700
C	2.16699700	0.54684600	0.50021900
C	3.06138100	0.11397400	-0.61364600
O	3.33390200	-1.20301800	-0.46335800
C	4.12795200	-1.79556100	-1.51900300
O	3.44143200	0.78370900	-1.55004500
N	-2.58806700	-0.61581000	-0.57868600
C	-3.79371900	-1.10838200	-1.28078400
C	0.13020400	-2.72603700	2.31869400
H	-0.26127300	3.03540600	0.46083900
H	-4.62765900	1.09344200	-0.54398100
H	1.04185400	-2.76274200	0.36366200
H	-2.23623500	4.54582700	0.37155200
H	-4.48540200	3.51732700	-0.14140500
H	-0.57198000	-4.13561400	-0.73755700
H	-1.32963700	-4.40077100	0.86032200
H	2.65861400	0.46745800	1.47144200
H	3.62004900	-1.69428200	-2.48091000
H	5.10363400	-1.30834000	-1.57318000
H	4.23637500	-2.84404700	-1.24373600
H	-4.64370000	-1.20402900	-0.59820400

H	-4.03813600	-0.41621300	-2.08763500
H	-3.57652400	-2.08408900	-1.70657600
H	0.76795100	-1.92513600	2.70587200
H	0.56370400	-3.68360200	2.62683700
H	-0.86076900	-2.63021100	2.77660100
C	3.84211700	2.69005000	0.92048000
C	2.64438800	3.01735200	0.40017000
H	4.65685800	2.35832100	0.28476700
H	4.03955700	2.75538500	1.98755300
H	1.85378900	3.40799900	1.03543700
H	2.47813900	3.01234300	-0.67140100

Structure **ts15a'-*syn*-I-*Re*-V**

Cu	0.40430900	-0.12840100	-0.38358400
N	-0.78810100	1.42471300	-0.20725900
C	-2.13776200	1.39893200	-0.16141200
C	-2.26482200	-1.04865200	-0.03470900
N	-1.00600000	-1.34934000	0.06550200
C	-0.15632500	2.61475300	-0.04993600
C	-2.88168500	2.57545000	0.03218700
C	-0.91885200	-2.75402900	0.53740000
O	-3.14424500	-2.03936500	0.16447200
C	-0.82303600	3.81249400	0.13037300
C	-2.21777000	3.78561200	0.17277900
C	-2.36527000	-3.26170600	0.33602700
H	-0.22923600	-3.29590600	-0.11589000
C	2.14860600	-0.06608900	-0.80142000
C	3.17379300	0.34803900	0.19534300
O	3.37058100	1.68197500	0.07561600
C	4.26818800	2.27006700	1.04905000
H	2.49509400	0.06643700	-1.82773100
O	3.70252100	-0.34659400	1.03638100
H	3.88826600	2.11199200	2.06105600
H	5.26006600	1.82281300	0.96047800
H	4.30041300	3.33131400	0.80556100
C	3.83200500	-2.15202900	-1.60823300
C	2.74839200	-2.55836400	-0.92279000
H	1.86915200	-2.93774700	-1.43644600
H	2.75964300	-2.60711200	0.16047900
H	4.72743800	-1.81728600	-1.09359300
H	3.85595400	-2.15164700	-2.69513500
H	0.92639500	2.57404000	-0.08142400
H	-2.49693100	-3.86386600	-0.56659500
H	-2.77837100	-3.78732500	1.19800300
H	-0.26517900	4.73553800	0.23861400
H	-2.78773200	4.69658400	0.32699500
C	-0.42259600	-2.82457100	1.98123700
H	-0.32675200	-3.86751000	2.30211900
H	0.55866800	-2.34791100	2.07209500
H	-1.11606900	-2.31572200	2.66027100
H	-3.96022000	2.54395000	0.09871400
C	-4.26275300	0.20932500	-0.64335800
H	-4.86783400	0.43606000	0.23985200
H	-4.42991500	0.96254400	-1.41461300
H	-4.55939500	-0.76227700	-1.02931800
N	-2.82017800	0.17222000	-0.31917600

Structure **ts15a'-*syn*-II-*Re*-V**

Cu	0.38478800	-0.09698900	-0.38087200
N	-0.86207100	1.41740400	-0.18046300
C	-2.20711200	1.33202100	-0.09739800
C	-2.24353900	-1.12303600	-0.03821400
N	-0.97468400	-1.38088400	0.07165800
C	-0.27800100	2.62896700	-0.00749200
C	-2.99680900	2.46346400	0.16121700
C	-0.84740900	-2.79506200	0.50253300
O	-3.08873200	-2.15355700	0.11529600
C	-0.99429400	3.78896000	0.23256100
C	-2.38283800	3.69840000	0.32230300
C	-2.26729900	-3.35018800	0.24912700
H	-0.12155500	-3.29300900	-0.14724500
C	2.10932200	0.11055100	-0.89100900
C	3.06879800	0.83748900	-0.03099300
O	3.94748400	0.13343500	0.68525600
C	4.79599000	0.90695300	1.57098800
H	2.30769100	0.32108700	-1.94426800
O	2.94730100	2.05296100	0.03111000
H	5.39407000	1.61629600	0.99553500
H	4.18696000	1.44758600	2.29825000
H	5.43262100	0.17491300	2.06569000
C	3.84669400	-1.66062300	-1.79567600
C	2.88431000	-2.13910800	-0.97859900
H	1.99304800	-2.60853100	-1.38245500
H	3.03817300	-2.20796700	0.09250700
H	4.76947100	-1.24906900	-1.40080200
H	3.73042900	-1.66606500	-2.87632800
H	0.80498900	2.64163900	-0.07625900
H	-2.35574300	-3.91677500	-0.68166400
H	-2.67539100	-3.93051900	1.07782100
H	-0.47308400	4.73201600	0.35123000
H	-2.98734900	4.57672100	0.52678700
C	-4.28338000	0.07450600	-0.62203500
H	-4.90279400	0.22657900	0.26735400
H	-4.47825700	0.86217500	-1.35096300
H	-4.53716800	-0.88585900	-1.06332700
C	-0.38805200	-2.89553400	1.95709900
H	-0.26571100	-3.94437600	2.24875000
H	0.57339000	-2.38934700	2.09109100
H	-1.11619200	-2.43117500	2.63156400
H	-4.07023100	2.37910600	0.26054400
N	-2.84223600	0.08176500	-0.29094900

Structure **ts15a'-*anti*-I-*Si*-V**

Cu	-0.43581300	-0.13470500	-0.28530400
N	0.76994100	1.42109800	-0.31052000
C	2.08907700	1.42205400	-0.01692500
C	2.18052200	-0.98769100	0.45518200
N	1.00590500	-1.35277200	0.03776000
C	0.22270800	2.55266900	-0.82243400
C	2.88932000	2.55114000	-0.26319400
C	1.00855300	-2.83520100	-0.05292200
O	3.02788400	-1.96304000	0.80943600
C	0.94257100	3.70709600	-1.06771700
C	2.31043500	3.69581000	-0.79154200
C	2.27617800	-3.21212300	0.74503200
C	-2.21130300	-0.08072000	-0.52786300
C	-3.13554400	0.43260300	0.52027500
O	-3.37135300	1.73847900	0.26348000
C	-4.15582800	2.44073600	1.25806800
H	-2.67256100	-0.05327600	-1.51748900
O	-3.55974700	-0.16556900	1.48517200
H	-3.66750800	2.38819300	2.23379600
H	-5.15232400	1.99981000	1.32695300
H	-4.21259500	3.46983700	0.90562400
C	-4.03164100	-2.23174700	-0.95245100
C	-2.92375700	-2.62674000	-0.30328400
H	-2.11678400	-3.13159100	-0.82749300
H	-2.83833700	-2.52336000	0.77312800
H	-4.85832400	-1.76964300	-0.42123700
H	-4.15120100	-2.37414000	-2.02370200
H	-0.84257900	2.50748000	-1.01170300
H	2.91470600	-3.94668200	0.25279500
H	2.06942700	-3.52383400	1.77212900
H	0.44647100	4.58304100	-1.46958000
H	2.92589400	4.56811800	-0.98844400
H	3.95200300	2.52917300	-0.06558300
C	3.97766200	0.44856900	1.26307800
H	3.95062100	1.36927500	1.84717800
H	4.80699500	0.48076000	0.54996100
H	4.12750800	-0.39177400	1.93526400
N	2.67793200	0.28291800	0.57485800
H	0.11353200	-3.21375300	0.44804900
C	1.02793100	-3.30039200	-1.50897700
H	0.16797900	-2.89579200	-2.05233100
H	0.98386900	-4.39360300	-1.56249600
H	1.93976300	-2.96581600	-2.01635500

Structure **ts15a'-*anti*-II-*Si*-Λ**

Cu	0.35309100	-0.11779900	0.20393300
N	-0.90183000	1.40784500	0.10788600
C	-2.24703900	1.30800300	0.14779100
C	-2.27163000	-1.12483100	-0.12202200
N	-1.01516700	-1.36347500	-0.35740000
C	-0.34975000	2.63329500	-0.06590500
C	-3.07085200	2.43714100	0.02753100
C	-0.95159700	-2.70074100	-1.00885700
O	-3.13671700	-2.12647400	-0.34698600
C	-1.09878300	3.79230400	-0.18084600
C	-2.48825200	3.68754600	-0.13310900
C	-2.32852500	-3.29608300	-0.66561500
C	2.04534300	0.18000500	0.78854000
C	3.00728400	0.90798800	-0.07006400
O	3.96591100	0.20978800	-0.68132500
C	4.81708900	0.96651800	-1.57883200
O	2.82120800	2.10600000	-0.23494800
C	-4.24069100	-0.02564900	0.79940100
N	-2.84248100	0.03611900	0.32432200
C	0.21997600	-3.55195500	-0.54429200
H	0.73465500	2.65901500	-0.09688000
H	-4.14794700	2.33950400	0.03084700
H	-0.87083400	-2.53674500	-2.09168000
H	-0.60107300	4.74713900	-0.30638800
H	-3.11824300	4.56614200	-0.23253100
H	-2.30372700	-3.93602400	0.22303400
H	-2.81782100	-3.81763500	-1.48788900
H	2.16710900	0.48286500	1.83050300

H	5.33514700	1.75625500	-1.03114500
H	4.22076000	1.40767500	-2.37997400
H	5.52569900	0.24163000	-1.97671500
H	-4.95321500	0.16755500	-0.00861500
H	-4.37075500	0.70956600	1.59461100
H	-4.43072400	-1.01821000	1.20085900
H	1.16925000	-3.07472100	-0.80145200
H	0.19392300	-4.53032800	-1.03613300
H	0.18530500	-3.71013300	0.53912400
C	3.91737700	-1.32493100	1.98135800
C	3.03520400	-1.95961800	1.18154100
H	4.82601700	-0.88456300	1.58415600
H	3.74699100	-1.22393100	3.05022600
H	2.16090200	-2.45272500	1.59215700
H	3.25114200	-2.12804400	0.13252900

Structure **ts15a'-*anti*-II-*Si*-V**

Cu	-0.40745900	-0.14999500	-0.26205200
N	0.78707000	1.41995100	-0.21997300
C	2.11742200	1.40819100	0.01647600
C	2.22014400	-1.01366800	0.45080200
N	1.02766200	-1.37452800	0.08093600
C	0.22003500	2.57162900	-0.66092500
C	2.91320800	2.53841200	-0.23391600
C	1.02532400	-2.85564900	-0.01999500
O	3.07996600	-1.99568400	0.76233800
C	0.93714700	3.73075500	-0.89961700
C	2.31638300	3.70301100	-0.69704900
C	2.32572600	-3.24162700	0.71840100
C	-2.16770100	-0.02091700	-0.64553000
C	-3.06919300	0.82630600	0.16195900
O	-3.86821600	0.25896700	1.06408900
C	-4.65199100	1.17568300	1.87019400
H	-2.47395400	0.00988600	-1.69444300
O	-2.96309900	2.03315000	-0.01027800
H	-5.29765900	1.78138000	1.23139700
H	-3.99139800	1.82667100	2.44629300
H	-5.24257900	0.54091800	2.52898400
C	-3.99771900	-1.95554800	-1.10776900
C	-3.00187700	-2.31325000	-0.27379500
H	-2.14546900	-2.87484600	-0.63338800
H	-3.07935100	-2.16191100	0.79724700
H	-4.88294000	-1.44412400	-0.74377800
H	-3.95498700	-2.16881400	-2.17280700
H	-0.85636300	2.54148800	-0.78730700
H	2.94082800	-3.97283600	0.19212800
H	2.16232600	-3.56467500	1.74997900
H	0.42561300	4.62326400	-1.24130800
H	2.92787700	4.57764100	-0.89645900
H	3.98387000	2.50610300	-0.08774200
C	4.05559100	0.40478700	1.19448200
H	4.05415800	1.31376200	1.79731400
H	4.85320400	0.45310900	0.44686600
H	4.23567000	-0.44861000	1.84212800
N	2.72739200	0.25241700	0.55999900
H	0.15304200	-3.23879800	0.51761600
C	0.97860400	-3.31222400	-1.47830500
H	0.09710200	-2.90039500	-1.98066600
H	0.92865400	-4.40488900	-1.53785100
H	1.86797700	-2.97614900	-2.02309000

Structure **ts15a'-*syn*-I-*Si*-Λ**

Cu	-0.39151700	-0.15090100	-0.61182900
N	1.12778100	-1.38133400	-0.23533200
C	2.29321500	-0.99989000	0.32940200
C	1.83468900	1.39237800	0.12577400
N	0.78448200	1.36399200	-0.63759900
C	1.00434500	-2.66323500	-0.64547200
C	3.34902600	-1.90692900	0.51447400
C	0.65786500	2.72327700	-1.23777000
O	2.41394200	2.58521900	0.32442800
C	1.99402000	-3.61789400	-0.49218600
C	3.19293400	-3.22377900	0.10415900
C	1.51721600	3.56734000	-0.28317700
C	-2.20282900	-0.14500300	-0.68438800
C	-2.88353200	0.40644400	0.51473500
O	-3.16755800	-0.46460100	1.49487000
C	-3.74114300	0.11400900	2.69140000
O	-3.05205300	1.61046500	0.59872100
N	2.44704100	0.33832500	0.75431700
C	3.48205600	0.64439700	1.76353900
C	-0.77741900	3.20379200	-1.38485900
H	0.05451200	-2.91476200	-1.10195700
H	4.28681500	-1.58217900	0.94495700
H	1.13189700	2.68384900	-2.22788800
H	1.83157500	-4.63440300	-0.83184200
H	4.00687500	-3.92978600	0.23656500
H	0.93135400	4.02361700	0.52182300
H	2.13927000	4.31799400	-0.76958400
H	-2.75100400	0.10428800	-1.59218500
H	-4.66834900	0.63933800	2.45278200
H	-3.03671700	0.81264500	3.14813200
H	-3.93347700	-0.72936600	3.35332600
H	4.47804000	0.71473900	1.31496300
H	3.46981700	-0.13760500	2.52391300
H	3.24338400	1.59688800	2.23093400
H	-1.31621500	3.16929400	-0.43426000
H	-1.31868000	2.58145800	-2.10345400
H	-0.78748200	4.23169100	-1.76411300
C	-4.04701800	-1.99542900	-1.02605300
C	-2.79405200	-2.44064500	-0.79278700
H	-4.72856700	-1.77530200	-0.21120700
H	-4.41775100	-1.83946100	-2.03564900
H	-2.15049500	-2.73122700	-1.61776900
H	-2.45682400	-2.67413600	0.21094000

Structure **ts15a'-*syn*-I-*Si*-V**

Cu	-0.36297700	-0.21170500	-0.36512000
N	1.15674100	-1.39346100	0.09771500
C	2.45535000	-1.02138200	0.12385800
C	1.98621800	1.35192500	-0.28254100
N	0.69620100	1.35875900	-0.14875200
C	0.83346900	-2.63221400	0.53645700
C	3.45479100	-1.89735000	0.58123200
C	0.27105600	2.77419000	0.01357900
O	2.59482600	2.54110500	-0.38008000
C	1.76044100	-3.55348600	0.98841500
C	3.10234600	-3.16897700	1.01008800
C	1.53129400	3.54342000	-0.44054300
C	-2.09394700	-0.18214700	-0.87721800
C	-3.08755700	0.47737400	0.00044800
O	-3.89808000	-0.29503900	0.73020100
C	-4.78678200	0.41041300	1.63169600
H	-2.30838000	0.03570700	-1.92564700
O	-3.05145300	1.69636800	0.06547800
H	-5.43517400	1.08655700	1.07082600
H	-4.20822900	0.98149500	2.36081600
H	-5.36986300	-0.36678600	2.12367100
C	-3.76303400	-2.02796000	-1.81461900
C	-2.76743400	-2.48199700	-1.02560600
H	-1.85921400	-2.89430500	-1.45448100
H	-2.90514000	-2.58559500	0.04545300
H	-4.69956000	-1.67553500	-1.39543500
H	-3.66322500	-1.99765700	-2.89648400
H	-0.22295900	-2.87299100	0.50483300
H	1.82260300	4.35838100	0.22306200
H	1.47905700	3.90095800	-1.47235700
H	1.44112800	-4.53556200	1.31784800
H	3.86945100	-3.84741400	1.37035000
N	2.82200600	0.26362800	-0.33159300
C	4.23158000	0.49760900	-0.71086100
H	4.58929600	-0.36263800	-1.27832700
H	4.86545400	0.65628600	0.16729300
H	4.28135600	1.38226600	-1.34055000
H	4.48777900	-1.58083900	0.62739400
H	-0.57159800	2.96091000	-0.65584100
C	-0.15334900	3.06476600	1.45239100
H	0.66635400	2.87331400	2.15447500
H	-1.01013900	2.44284500	1.72446700
H	-0.45630000	4.11301900	1.55007900

Structure **ts15a'-*syn*-II-*Si*-Λ**

Cu	-0.34118200	-0.29969600	-0.53884500
N	1.37658100	-1.23041700	-0.16826400
C	2.48314100	-0.63954100	0.32995600
C	1.62823300	1.63217400	0.04011700
N	0.54896200	1.39169300	-0.64209700
C	1.44536100	-2.53792100	-0.50445000
C	3.67406800	-1.35818000	0.52156400
C	0.14056300	2.67541500	-1.27573300
O	2.01555900	2.91195700	0.13695100
C	2.57711900	-3.31577000	-0.33805300
C	3.71577300	-2.70522300	0.18950700
C	0.94445200	3.70465800	-0.46017500
C	-2.11202600	-0.65712000	-0.58018600
C	-2.85702700	-0.31649000	0.66973700
O	-3.65141300	0.75383300	0.46193700
C	-4.32365800	1.26866700	1.63390400
H	-2.74686600	-0.62546300	-1.46541900
O	-2.71772400	-0.86345000	1.74620600
H	-3.59676900	1.54369600	2.40205800
H	-5.00373300	0.51535500	2.03753800
H	-4.87630600	2.14201400	1.28956000
C	-3.57062000	-2.90790100	-0.60052300
C	-2.24074600	-3.06717800	-0.43885300
H	-1.61071400	-3.32250900	-1.28614700

H	-1.79472600	-3.08984100	0.54933200
H	-4.22236700	-2.72933800	0.24907300
H	-4.03777000	-2.95595700	-1.58060300
H	0.53478400	-2.95986000	-0.91090200
H	0.36385700	4.14460500	0.35741600
H	1.41255100	4.49042100	-1.05242100
H	2.56644500	-4.36348400	-0.61581100
H	4.63446000	-3.26650400	0.32875800
N	2.44035300	0.73007500	0.67415200
C	3.45930600	1.25579000	1.60713500
H	4.41240500	1.44276200	1.10255400
H	3.59853500	0.53466400	2.41363100
H	3.09818700	2.19123700	2.02765600
H	4.56137000	-0.86660100	0.89668200
H	0.49572600	2.65660400	-2.31448700
C	-1.36282000	2.90860100	-1.26263100
H	-1.75977700	2.88477400	-0.24307700
H	-1.87935700	2.14331400	-1.84842400
H	-1.59502600	3.88323000	-1.70565600

Structure **ts15a'-*syn*-II-*Si*-V**

Cu	0.37411100	-0.15485800	0.34134200
N	-1.16329500	-1.31713700	-0.12960400
C	-2.46229500	-0.94976300	-0.14481300
C	-1.98656800	1.41493300	0.29671300
N	-0.69469600	1.41953300	0.17646600
C	-0.83503600	-2.54081200	-0.60525700
C	-3.46095500	-1.82036000	-0.61361500
C	-0.23847900	2.83195900	0.18074600
O	-2.59468900	2.60197300	0.41416600
C	-1.75999000	-3.45513900	-1.07517200
C	-3.10428500	-3.07973600	-1.07455000
C	-1.56456600	3.62637700	0.28134400
C	2.11967300	-0.30566500	0.77581100
C	3.18939600	-0.14964600	-0.25377600
O	3.65329900	1.11792400	-0.22811100
C	4.62574100	1.44669200	-1.24912300
H	2.46438600	-0.02653700	1.77244200
O	3.55150100	-0.99171300	-1.05000100
H	4.21015900	1.26864800	-2.24346700
H	5.52379300	0.83923900	-1.11884000
H	4.84979300	2.50260400	-1.10302300
C	3.47334400	-2.32761100	1.86741100
C	2.35961900	-2.67748400	1.19104600
H	1.42551400	-2.87469900	1.70869200
H	2.41164700	-2.90129700	0.13098100
H	4.42229400	-2.19853000	1.35620000
H	3.46410200	-2.16851400	2.94260000
H	0.22258600	-2.77367300	-0.59214900
H	-1.79508600	4.19660000	-0.62225800
H	-1.63263900	4.27576300	1.15528100
H	-1.43611200	-4.42456300	-1.43602900
H	-3.87041100	-3.75404700	-1.44449300
N	-2.82821800	0.33109900	0.32316900
C	-4.24436900	0.57218800	0.67312200
H	-4.61720900	-0.28843400	1.22995300
H	-4.85868800	0.73657100	-0.21775900
H	-4.30412500	1.45320900	1.30670100
H	-4.49601800	-1.50960000	-0.64628600
H	0.36633400	2.98189900	1.08202800
C	0.60113900	3.16874300	-1.04721800
H	0.03351000	3.00081500	-1.96912900
H	1.50217300	2.54886200	-1.06743200
H	0.91314100	4.21858100	-1.01760100

Structure **ts15c'-*anti*-I-*Re*-Λ**

C	2.13425400	3.52240300	-0.41440200
C	0.77083700	2.88589200	-0.77861600
N	0.92684700	1.48609900	-0.29954800
C	2.16668600	1.32479800	0.04141500
O	2.97281300	2.39219100	-0.03097000
N	2.77292500	0.17384400	0.49147600
C	4.08113800	0.31514500	1.16108100
Cu	-0.33068800	0.08569100	0.14668600
C	-1.99966800	0.33054200	0.83250200
C	-3.15027000	0.61461100	-0.05973900
O	-3.31771400	1.75281200	-0.46385700
C	-0.41281000	3.60779600	-0.14524200
N	1.05948200	-1.31346000	-0.23195900
C	2.36151000	-1.11312700	0.07446000
C	3.30906100	-2.13917800	-0.02445000
C	2.89710700	-3.38645300	-0.47734700
C	1.57358200	-3.57375600	-0.86080300
C	0.68003500	-2.51160100	-0.74795400
O	-3.87427800	-0.43972400	-0.46402700
C	-4.92660900	-0.14122300	-1.41445400
C	-2.47491200	-1.74912700	1.86826900
C	-3.41076300	-1.05618800	2.55255700
H	0.63874100	2.85234000	-1.86673700
H	-2.08374000	0.90009300	1.75846200
H	-5.62681700	0.58109600	-0.98999500
H	-4.49947700	0.26468000	-2.33385600
H	-5.41980700	-1.09385300	-1.60296700
H	-1.49997700	-1.95486900	2.29907800
H	-2.72435500	-2.25470700	0.94344000
H	-4.41049700	-0.91445100	2.15496500
H	-3.19904100	-0.61362000	3.52237300
C	-0.73796500	-2.64443600	-1.23226600
H	2.63139800	4.02867900	-1.24230300
H	2.07336400	4.19270600	0.44797700
H	1.23262600	-4.52403000	-1.25743400
H	3.61718400	-4.19455100	-0.56208500
H	-0.46048800	4.63662900	-0.51976600
H	-1.35985000	3.11714800	-0.38288900
H	-0.30196900	3.64763400	0.94469900
H	4.17939000	-0.47876000	1.90288000
H	4.91249800	0.26787900	0.45031900
H	4.11240800	1.27660300	1.66859300
H	4.34960300	-1.96491000	0.21128000
H	-0.75307200	-2.82192000	-2.31396800
H	-1.24910200	-3.48871600	-0.75743700
H	-1.29769500	-1.73032200	-1.02753600

Structure **ts15c'-*anti*-I-*Re*-V**

C	0.61686900	3.72044000	0.41208600
C	0.05378800	2.62085800	1.33949300
N	0.45132400	1.38558100	0.63250200
C	1.32217200	1.71703000	-0.26852400
O	1.56757800	3.01917800	-0.43949500
N	2.02415600	0.86844400	-1.09023900
C	2.69606300	1.44981000	-2.26230500
Cu	-0.34881400	-0.35853700	0.47328700
C	-2.14715000	-0.57217800	0.55434700
C	-3.01735500	0.32243100	-0.24442400
O	-3.06030300	1.49257600	0.10714800
C	0.60191800	2.65731800	2.76479800
N	1.45660300	-1.14008000	0.05601500
C	2.34221400	-0.45293800	-0.70210500
C	3.56028500	-1.01184300	-1.10447800
C	3.87211800	-2.30216500	-0.69376300
C	2.99328900	-2.98478700	0.13897000
C	1.80118500	-2.36877100	0.51740400
O	-3.63306200	-0.16856100	-1.32156100
C	-4.41581800	0.77362400	-2.08425300
C	-2.68150000	-2.83728700	-0.27387800
C	-3.78749800	-2.75475900	0.49545200
H	-1.03754400	2.66018600	1.35984700
H	-2.60723300	-0.73100200	1.53547200
H	-5.19555100	1.21706600	-1.46081300
H	-3.77673500	1.56368400	-2.48590600
H	-4.85592000	0.18946600	-2.89209700
H	-1.79868300	-3.36454400	0.06995900
H	-2.68582200	-2.51231200	-1.30822100
H	-4.69884800	-2.28982800	0.13196300
H	-3.80991000	-3.15171300	1.50779300
C	0.86735900	-3.04021300	1.48426100
H	-0.13962800	4.16625400	-0.24034800
H	1.17074600	4.50571700	0.92895200
H	3.22724300	-3.97778700	0.50788400
H	4.81301200	-2.75308000	-0.99568700
H	0.27646200	3.57249200	3.27064100
H	0.22973100	1.80557300	3.34230300
H	1.69677400	2.62766200	2.77421200
H	3.70058300	1.81478600	-2.02474300
H	2.75141200	0.69151700	-3.04445000
H	2.10200100	2.28504300	-2.62849900
H	4.26698000	-0.44496200	-1.69514000
H	1.34838500	-3.14685400	2.46342400
H	-0.03920300	-2.44790700	1.61601500
H	0.59143600	-4.04445500	1.14693800

Structure **ts15c'-*anti*-II-*Re*-Λ**

Cu	-0.33266300	-0.04062800	0.11143000
N	1.28289500	-1.15586000	-0.28879900
C	2.52147600	-0.74684900	0.06782700
C	1.90177900	1.61567100	0.11840000
N	0.66986400	1.55973200	-0.28415800
C	1.12910300	-2.37471800	-0.86892400
C	3.63526500	-1.58618300	-0.03903700
C	0.28092200	2.92249900	-0.72825600
O	2.48825600	2.82029200	0.13670900
C	2.19878500	-3.25965000	-0.99184400
C	3.45797600	-2.86507200	-0.55486300
C	1.45518900	3.78847000	-0.21574900
H	0.25436800	2.92147000	-1.82507600
C	-2.00686500	-0.15356800	0.79450300

C	-3.19999000	-0.24753200	-0.09687400
O	-3.86007900	0.92797900	-0.12309900
C	-4.95381100	1.01145800	-1.06740000
H	-2.24527000	0.30752200	1.75318600
O	-3.49936100	-1.21304600	-0.77294700
H	-4.59984000	0.80602600	-2.08031600
H	-5.73065600	0.29087100	-0.80326600
H	-5.32807600	2.03095700	-0.98442200
C	-3.11550500	-1.96397300	2.41684200
C	-2.04605300	-2.39809000	1.71772700
H	-1.05485900	-2.42357300	2.16060600
H	-2.17210000	-2.85992900	0.74620900
H	-4.11653200	-2.00804000	1.99812800
H	-3.01955700	-1.56020200	3.42139400
H	1.88076000	4.46009800	-0.96144000
H	1.20659000	4.34853400	0.69101000
H	2.03915800	-4.23486900	-1.43891700
H	4.30931900	-3.53263900	-0.64590500
N	2.69008000	0.57562200	0.54651300
C	-1.07553200	3.35990800	-0.18899800
H	-1.31409200	4.36759300	-0.54662200
H	-1.87058500	2.68631500	-0.51988300
H	-1.07269700	3.37595400	0.90658000
C	3.93185900	0.91311200	1.27020800
H	4.14336100	0.11806700	1.98670800
H	4.78033000	1.03764100	0.58965300
H	3.77989300	1.84442100	1.81106800
H	4.62274500	-1.24508200	0.23905300
C	-0.22485400	-2.72287200	-1.42185900
H	-0.97332400	-1.98137800	-1.13886000
H	-0.18270400	-2.75616100	-2.51748500
H	-0.55786700	-3.70931000	-1.08328500

Structure **ts15c'-*anti*-II-*Re*-V**

C	0.52827900	3.79588800	0.38112500
C	-0.13176300	2.68430700	1.23630400
N	0.37362900	1.44710400	0.59429500
C	1.30491200	1.78259400	-0.24444200
O	1.53114500	3.09052400	-0.41351600
N	2.08459200	0.94424900	-0.99912000
C	2.85978000	1.53966100	-2.10685600
Cu	-0.36058600	-0.31783000	0.46263700
C	-2.11969100	-0.67486800	0.43472700
C	-2.97882200	-0.14105800	-0.66154000
O	-3.11672400	-0.60466800	-1.77347300
C	0.23315300	2.73955300	2.71899100
N	1.46055700	-1.06526400	0.13128700
C	2.36832100	-0.38768400	-0.60989000
C	3.58389400	-0.96456400	-0.99267100
C	3.86958900	-2.25972400	-0.57759800
C	2.96823100	-2.93091000	0.24068900
C	1.77951800	-2.30010300	0.60028700
O	-3.53743100	1.01699400	-0.24569200
C	-4.32101800	1.72278200	-1.23688300
C	-2.42107800	-3.27154400	-0.37518100
C	-3.59981900	-3.13493600	0.25304000
C	0.82804300	-2.94732900	1.56770300
H	4.30599100	-0.40975800	-1.57516400
H	-1.21958000	2.70338700	1.12185100
H	3.18126700	-3.92695000	0.61312500
H	4.80684700	-2.72482800	-0.86704300
H	-0.15901900	4.28093800	-0.31620900
H	1.05670900	4.55006200	0.96632500
H	-2.70945600	-0.88340500	1.33077100
H	-3.71067000	1.95297400	-2.11342600
H	-5.17453900	1.11398300	-1.54233400
H	-4.65549500	2.63462500	-0.74354700
H	3.86073000	1.84403800	-1.78493300
H	2.93321700	0.80835200	-2.91293500
H	2.32958000	2.41591700	-2.47256600
H	-0.19457100	1.88532800	3.25332900
H	-0.16149900	3.65472600	3.17368000
H	1.32000900	2.72439100	2.85712300
H	-4.44695200	-2.66228400	-0.23587600
H	-3.76367500	-3.51455500	1.25874800
H	-1.59041800	-3.79074400	0.09376600
H	-2.28187100	-2.92413500	-1.39291800
H	1.23933300	-2.90045800	2.58395200
H	-0.13265900	-2.42926300	1.56782200
H	0.66719700	-4.00309800	1.32937900

Structure **ts15c'-*syn*-I-*Re*-Λ**

C	0.65896600	3.77557700	-0.61682400
C	0.22567400	2.68014300	-1.60657800
N	0.50281300	1.44353200	-0.82537300
C	1.32885200	1.77481700	0.11794200
O	1.58796300	3.08063000	0.27608500
N	1.97938900	0.93163300	0.98596100
C	2.62441900	1.52963400	2.17079200
Cu	-0.31586200	-0.29583800	-0.64551100
C	-2.11474600	-0.53461500	-0.56942300
C	-2.81679000	0.16632600	0.53767700
O	-3.02447100	1.36378500	0.43052400
C	-1.21197800	2.79590800	-2.09040600
N	1.47512200	-1.07956500	-0.18719100
C	2.31525000	-0.39637200	0.62326800
C	3.50090100	-0.96273400	1.10165700
C	3.82899600	-2.25525500	0.70754700
C	2.99853000	-2.93419000	-0.17751100
C	1.83548700	-2.31143400	-0.62552300
O	-3.09041100	-0.54419000	1.63968300
C	-3.70065300	0.19801200	2.72281600
C	-2.51518000	-2.88248300	-0.12011700
C	-3.77878800	-2.61644500	-0.51030300
C	0.94260700	-2.96624500	-1.64316600
H	4.17003300	-0.40132900	1.73941300
H	0.90149000	2.67312300	-2.47260800
H	3.24691800	-3.92928300	-0.53046400
H	4.74558800	-2.71284400	1.06689500
H	-0.17143100	4.14604000	-0.00663100
H	1.20116600	4.60794500	-1.06424200
H	-2.72727000	-0.52790300	-1.47219000
H	-4.64341500	0.64120400	2.39541000
H	-3.02854500	0.98782100	3.06532500
H	-3.87026500	-0.53462600	3.51070200
H	3.65041500	1.84943200	1.96134700
H	2.62167600	0.79449400	2.97699800
H	2.04689400	2.39809400	2.48067900
H	-1.91964300	2.72773600	-1.26010600
H	-1.43868800	1.99806300	-2.80522200
H	-1.35449600	3.75097000	-2.60797700
H	-4.51963700	-2.24070100	0.18775300
H	-4.10270600	-2.77031300	-1.53649100
H	-1.80157300	-3.32282200	-0.80735800
H	-2.21596500	-2.80062300	0.91853800
H	1.45084600	-3.03110700	-2.61264000
H	0.66962200	-3.98456600	-1.34736700
H	0.03378700	-2.37436800	-1.77514400

Structure **ts15c'-*syn*-I-*Re*-V**

C	-2.40742800	-3.26260700	0.44269400
C	-1.04914300	-2.68463800	0.90671900
N	-1.03843900	-1.34880900	0.26146600
C	-2.24958100	-1.10052000	-0.12888700
O	-3.14548800	-2.09161800	-0.02091600
N	-2.72962600	0.07274400	-0.65109900
C	-4.03084500	0.02765600	-1.34806900
Cu	0.37721100	-0.11213300	-0.21627800
C	2.07303700	-0.21731900	-0.84768300
C	3.27171000	0.00522700	0.01203300
O	3.57822800	-0.65140500	0.98809800
C	-0.90216200	-2.57446500	2.42444000
N	-0.86902900	1.42973900	-0.01219800
C	-2.18506900	1.33431600	-0.30573300
C	-3.03328200	2.44873100	-0.26959700
C	-2.50608900	3.67829700	0.09883400
C	-1.16189200	3.76978700	0.44808100
C	-0.36845500	2.62807200	0.39466000
O	3.93370700	1.10817400	-0.39594100
C	5.04020500	1.51893800	0.44025400
C	2.17955400	-2.60068900	-0.99277200
C	3.27573900	-2.39602700	-1.75428900
H	-0.22386900	-3.27638300	0.50194600
H	2.29564000	-0.05891000	-1.90405100
H	4.70340300	1.68766700	1.46579000
H	5.81459200	0.74880300	0.43889000
H	5.41171300	2.44092400	-0.00515400
H	1.21172100	-2.78844100	-1.44703000
H	2.26363100	-2.71991700	0.08176400
H	4.25760300	-2.27820100	-1.30625900
H	3.21844600	-2.34267100	-2.83820300
C	1.08259900	2.67103100	0.78012800
H	-2.32470300	-3.95420500	-0.40007200
H	-2.99501300	-3.71784200	1.24104000
H	-0.72815700	4.71098000	0.76588000
H	-3.14894200	4.55221400	0.13936700
H	-0.89656800	-3.57110900	2.87921300
H	0.03734200	-2.07721400	2.68551400
H	-1.72902300	-2.00096400	2.85832300
H	-4.08764800	2.35387800	-0.48880900
H	-4.86758800	0.20317800	-0.66441900
H	-4.02973400	0.78115900	-2.13692500
H	-4.15066200	-0.95506800	-1.79893000
H	1.32507900	1.86224900	1.47762500
H	1.73110600	2.55845800	-0.09546700
H	1.32721800	3.62161500	1.26002900

Structure **ts15c'-*syn*-II-*Re*-Λ**

C	2.01417600	3.58504700	0.23056400
C	1.11062600	2.98846700	-0.86448500
N	0.95123000	1.58362000	-0.40283600
C	1.91117300	1.36172900	0.44317700
O	2.65329000	2.41436400	0.82068200
N	2.26745100	0.16401600	1.00424200
C	3.14084600	0.19851100	2.19392100
Cu	-0.38080900	0.18354000	-0.60140200
C	-2.14306200	-0.24077200	-0.56656200
C	-2.65492600	-1.05310800	0.56256400
O	-2.47105900	-2.25983900	0.51376900
C	-0.20479000	3.72736300	-1.05397200
N	1.03461200	-1.21653400	-0.49984600
C	2.09819200	-1.06636500	0.31839100
C	3.04223200	-2.08225500	0.50241800
C	2.88307800	-3.27254200	-0.19540300
C	1.81287500	-3.41363000	-1.07246000
C	0.90556700	-2.36640900	-1.21355200
O	-3.18675400	-0.41312500	1.60836900
C	-3.58405400	-1.25591100	2.71796700
C	-3.40672600	1.87166000	-0.36725100
C	-4.47438200	1.15063200	-0.76098600
C	-0.27069200	-2.47908400	-2.14027400
H	3.89918700	-1.93800000	1.14602600
H	1.64837800	2.96192000	-1.82177400
H	1.67544700	-4.32220000	-1.64756700
H	3.60695400	-4.07233800	-0.07293900
H	2.80475900	4.23906400	-0.13636300
H	1.44609700	4.08821300	1.02052200
H	-2.66665800	-0.51571600	-1.48333700
H	-4.32249400	-1.99056600	2.39038900
H	-2.71412100	-1.77317000	3.12813100
H	-4.01335200	-0.57627900	3.45276200
H	2.92610400	-0.67791200	2.80684000
H	4.20167300	0.21445700	1.92405000
H	2.91470400	1.09535200	2.76714500
H	-0.78527700	3.74505200	-0.12566600
H	-0.80254200	3.25158500	-1.83710500
H	-0.01568000	4.76091000	-1.36334300
H	-5.07828500	0.59669700	-0.04925100
H	-4.77421200	1.09839800	-1.80460300
H	-2.84391600	2.46937600	-1.07527700
H	-3.15284000	1.97740300	0.68168300
H	-0.12659900	-3.29091600	-2.85715200
H	-1.18047900	-2.68485000	-1.56432300
H	-0.42104300	-1.54803700	-2.69601600

Structure **ts15c'-*syn*-II-*Re*-V**

C	-1.94890600	-3.49658900	0.45630100
C	-0.68270100	-2.74526600	0.93091700
N	-0.84361800	-1.41722900	0.29073300
C	-2.07700600	-1.32873200	-0.10177000
O	-2.83440900	-2.43148700	-0.00068300
N	-2.70819000	-0.22926000	-0.62191900
C	-3.98970600	-0.44692400	-1.32254200
Cu	0.38856100	0.00337900	-0.20998200
C	2.03855300	0.12612600	-0.97152100
C	3.24390900	0.70133400	-0.33146700
O	3.50097000	1.87883000	-0.51523400
C	-0.56346700	-2.62346600	2.45055500
N	-1.05163400	1.36649000	0.02683900
C	-2.34172500	1.09501500	-0.26906900
C	-3.33454100	2.08183400	-0.22888900
C	-2.97940700	3.37060900	0.14567500
C	-1.66141100	3.64181200	0.49923000
C	-0.71912400	2.61864300	0.44342600
O	3.91317700	-0.09448700	0.51691000
C	5.03136800	0.52593700	1.19639800
C	2.43211400	-2.16916500	-1.11675400
C	3.39908200	-1.82793500	-1.99771300
H	0.21700800	-3.22211900	0.53170400
H	2.07277900	0.30574800	-2.04740700
H	5.75651200	0.89966800	0.47028200
H	4.68314100	1.35292500	1.81866100
H	5.46763300	-0.26219600	1.80866600
H	1.45206500	-2.48282100	-1.46042700
H	2.65464900	-2.29908200	-0.06357200
H	4.40357000	-1.58537600	-1.66729700
H	3.20600100	-1.77851800	-3.06591600
C	0.71095200	2.85249700	0.83167700
H	-1.77037100	-4.16409100	-0.39123000
H	-2.47236900	-4.03390500	1.24825000
H	-1.35937400	4.63150600	0.82218600
H	-3.73510900	4.14895000	0.18793100
H	-4.84317500	-0.40040300	-0.63866700
H	-4.09383300	0.31101000	-2.10006200
H	-3.97074200	-1.43001200	-1.78811800
H	-0.42466800	-3.61166300	2.90273000
H	0.29615900	-2.00187900	2.72082400
H	-1.46383800	-2.16995800	2.87989900
H	-4.36614800	1.84533800	-0.44962400
H	0.82394800	3.81161400	1.34261000
H	1.06331000	2.06304800	1.50445800
H	1.37287500	2.85697500	-0.04063500

Structure **ts15c'-*anti*-I-*Si*-V**

C	2.18235500	-3.34003300	0.58400100
C	1.12037800	-2.88833500	-0.44664400
N	1.00570800	-1.43543300	-0.17165800
C	2.01090300	-1.10339100	0.57876400
O	2.79992600	-2.09181900	1.01991800
N	2.37010700	0.15480200	0.98358500
C	3.36847000	0.26540400	2.06753000
Cu	-0.42723100	-0.16952000	-0.43922000
C	-2.23014600	-0.15025300	-0.47868900
C	-2.97959400	0.22099100	0.75552700
O	-3.07348100	-0.43866800	1.77020300
C	1.51083200	-3.15372100	-1.90072900
N	0.84532000	1.35649000	-0.41252300
C	2.01268900	1.32318300	0.26922500
C	2.88596900	2.41865700	0.29380700
C	2.54187500	3.56504600	-0.40733000
C	1.35339500	3.59304000	-1.13117200
C	0.52808000	2.47290200	-1.12555900
O	-3.47157900	1.47119400	0.61159800
C	-4.08697200	2.04185900	1.79021200
C	-2.72794900	-2.59588300	-0.45729300
C	-3.98617300	-2.23259600	-0.77157200
H	-2.82564700	0.00151300	-1.37967400
H	-3.37561000	2.06313900	2.61918200
H	-4.95994900	1.45250100	2.07840700
H	-4.37978100	3.05081800	1.50258400
H	-2.03346200	-2.92599300	-1.22441100
H	-2.41072500	-2.67217500	0.57705000
H	-4.69993400	-1.95621800	-0.00148100
H	-4.33584300	-2.20913000	-1.80052300
C	-0.75934100	2.45965900	-1.90178100
H	2.97481800	-3.96150300	0.16457000
H	1.75751700	-3.82293800	1.46778300
H	1.06622100	4.46798400	-1.70286900
H	3.20925500	4.42133800	-0.40570900
H	3.82832400	2.36647400	0.82126800
H	3.16083100	1.16968200	2.64077100
H	4.39102100	0.29519100	1.67824600
H	3.26998300	-0.59770200	2.72204700
H	0.15765600	-3.35921600	-0.23057000
H	0.76892600	-2.72766200	-2.58391900
H	1.56894400	-4.23119000	-2.08992300
H	2.48482600	-2.70868400	-2.13289000
H	-0.82495100	3.33082200	-2.55770000
H	-0.83487400	1.55768200	-2.51716100
H	-1.62335600	2.47550300	-1.22705500

Structure **ts15c'-*anti*-II-*Si*-Λ**

C	-2.10892400	-3.41960800	-0.80745500
C	-0.89816300	-2.64030000	-1.35532200
N	-0.92097100	-1.40939700	-0.51999200
C	-2.11450500	-1.32822800	-0.01772800
O	-2.92515800	-2.38611100	-0.17989100
N	-2.65631800	-0.26886200	0.66520200
C	-3.85618700	-0.52821100	1.48388800
Cu	0.34142300	-0.02519800	0.03516800
C	1.93866400	0.20104500	0.88186100
C	3.15318200	0.82086900	0.30139900
O	3.30935200	2.02562700	0.41248100
C	0.41413200	-3.40737200	-1.29922900
N	-1.09697700	1.35261500	-0.12097400
C	-2.34342700	1.07118500	0.31388700
C	-3.33473600	2.05365300	0.40967500
C	-3.02543100	3.34939700	0.01514300
C	-1.76034200	3.62825700	-0.49242700
C	-0.81552600	2.60722600	-0.56089800
O	3.95328000	0.02053100	-0.41648900
C	5.08345900	0.67363300	-1.04392800
C	2.54154600	-2.04955800	1.29070800
C	3.38790900	-1.56045900	2.22244000
C	0.56113300	2.84527500	-1.10696400
H	-4.33261900	1.81070000	0.74789300
H	-1.08762600	-2.33425600	-2.39306000
H	-1.50079800	4.62274800	-0.83710200
H	-3.78036100	4.12730100	0.07572700
H	-1.83175900	-4.14246100	-0.03240100
H	-2.72182300	-3.90364800	-1.56734500
H	1.88250400	0.44644700	1.94394000

H	5.70414100	1.16428700	-0.29116700
H	4.73634200	1.41494200	-1.76670100
H	5.63460300	-0.12338800	-1.54112900
H	-4.77879200	-0.44657900	0.90017300
H	-3.87395500	0.18456600	2.30971300
H	-3.79006900	-1.53600500	1.88954600
H	1.24231400	-2.78166400	-1.64561000
H	0.36424500	-4.28475100	-1.95277900
H	0.63121400	-3.75018600	-0.28272100
H	4.39729600	-1.25578900	1.96512600
H	3.09074000	-1.44679100	3.26166800
H	1.55892600	-2.41706500	1.56632800
H	2.87149000	-2.23468300	0.27548800
H	0.60687200	3.79252200	-1.64970900
H	1.31030300	2.87959900	-0.30852200
H	0.84889400	2.04320000	-1.79598300

Structure **ts15c'-*anti*-II-*Si*-V**

C	-1.85101100	3.53680700	0.49030600
C	-0.87594300	2.95400900	-0.56031200
N	-0.86264700	1.51136000	-0.21910800
C	-1.86053600	1.29505800	0.58185400
O	-2.54759400	2.36501800	1.00832100
N	-2.30211000	0.08980100	1.05844100
C	-3.24162300	0.10934800	2.19855100
Cu	0.42962500	0.10004300	-0.50373500
C	2.22125800	-0.15613600	-0.61369900
C	2.93326800	-0.86467400	0.47515200
O	2.95406100	-2.08464900	0.43761300
C	-1.31040400	3.18443500	-2.00792800
N	-0.98968600	-1.29431000	-0.38572800
C	-2.09990300	-1.13229800	0.36816800
C	-3.06603300	-2.13836100	0.49172400
C	-2.87645200	-3.33383300	-0.18731100
C	-1.75073300	-3.49274200	-0.98877200
C	-0.82805200	-2.45429000	-1.08064000
O	3.41299300	-0.13119200	1.48626800
C	4.01247400	-0.88368500	2.56961400
C	3.01436100	2.10806800	-0.52253700
C	4.17585700	1.59369600	-0.97719900
H	2.69379200	-0.37412200	-1.57235000
H	4.84539700	-1.48412000	2.19800000
H	3.26951100	-1.53859500	3.02960600
H	4.36135900	-0.13435900	3.27885600
H	2.30143800	2.56163900	-1.20358800
H	2.82202900	2.21209400	0.53949900
H	4.92220800	1.19681500	-0.29694100
H	4.40717400	1.55753400	-2.03851900
C	0.39482400	-2.58338600	-1.94334900
H	-2.60770200	4.20384400	0.07472600
H	-1.34929900	4.02126300	1.33218400
H	-1.58463100	-4.40718200	-1.54655600
H	-3.61633600	-4.12443500	-0.10874300
H	-3.96119500	-1.98139200	1.07727000
H	-3.07741200	-0.78599100	2.79940300
H	-4.28434300	0.15138100	1.86814000
H	-3.03405000	0.98671700	2.80701200
H	0.12990100	3.35663800	-0.40927900
H	-0.63642200	2.66975600	-2.70038600
H	-1.29266600	4.25351700	-2.24653400
H	-2.32587400	2.80910600	-2.17686400
H	1.29296200	-2.70442600	-1.32612700
H	0.31344000	-3.45034100	-2.60322600
H	0.52891900	-1.69004700	-2.56186100

Structure **ts15c'-*syn*-I-*Si*-Λ**

C	0.65896600	3.77557700	-0.61682400
C	0.22567400	2.68014300	-1.60657800
N	0.50281300	1.44353200	-0.82537300
C	1.32885200	1.77481700	0.11794200
O	1.58796300	3.08063000	0.27608500
N	1.97938900	0.93163300	0.98596100
C	2.62441900	1.52963400	2.17079200
Cu	-0.31586200	-0.29583800	-0.64551100
C	-2.11474600	-0.53461500	-0.56942300
C	-2.81679000	0.16632600	0.53767700
O	-3.02447100	1.36378500	0.43052400
C	-1.21197800	2.79590800	-2.09040600
N	1.47512200	-1.07956500	-0.18719100
C	2.31525000	-0.39637200	0.62326800
C	3.50090100	-0.96273400	1.10165700
C	3.82899600	-2.25525500	0.70754700
C	2.99853000	-2.93419000	-0.17751100
C	1.83548700	-2.31143400	-0.62552300
O	-3.09041100	-0.54419000	1.63968300
C	-3.70065300	0.19801200	2.72281600
C	-2.51518000	-2.88248300	-0.12011700
C	-3.77878800	-2.61644500	-0.51030300
C	0.94260700	-2.96624500	-1.64316600
H	4.17003300	-0.40132900	1.73941300
H	0.90149000	2.67312300	-2.47260800
H	3.24691800	-3.92928300	-0.53046400
H	4.74558800	-2.71284400	1.06689500
H	-0.17143100	4.14604000	-0.00663100
H	1.20116600	4.60794500	-1.06424200
H	-2.72727000	-0.52790300	-1.47219000
H	-4.64341500	0.64120400	2.39541000
H	-3.02854500	0.98782100	3.06532500
H	-3.87026500	-0.53462600	3.51070200
H	3.65041500	1.84943200	1.96134700
H	2.62167600	0.79449400	2.97699800
H	2.04689400	2.39809400	2.48067900
H	-1.91964300	2.72773600	-1.26010600
H	-1.43868800	1.99806300	-2.80522200
H	-1.35449600	3.75097000	-2.60797700
H	-4.51963700	-2.24070100	0.18775300
H	-4.10270600	-2.77031300	-1.53649100
H	-1.80157300	-3.32282200	-0.80735800
H	-2.21596500	-2.80062300	0.91853800
H	1.45084600	-3.03110700	-2.61264000
H	0.66962200	-3.98456600	-1.34736700
H	0.03378700	-2.37436800	-1.77514400

Structure **ts15c'-*syn*-I-*Si*-V**

C	-1.31023200	3.69534900	0.25174500
C	-0.16361600	2.83355700	-0.32777900
N	-0.62561100	1.45447800	-0.02699600
C	-1.87059500	1.52383200	0.32485300
O	-2.40435200	2.74541300	0.45250700
N	-2.72037500	0.47953500	0.59479700
C	-4.00515400	0.79833600	1.25007400
Cu	0.33495900	-0.17880300	0.26123300
C	2.03106400	-0.05959800	0.89437000
C	3.08117200	0.51278300	0.01889600
O	3.00688700	1.70239800	-0.24950100
C	0.07195300	3.02842400	-1.82462700
N	-1.28480000	-1.26903400	-0.18081600
C	-2.53918600	-0.81626200	0.05468000
C	-3.66841100	-1.59644700	-0.22245900
C	-3.49268100	-2.86165100	-0.76747700
C	-2.20770000	-3.31110000	-1.05143600
C	-1.12329000	-2.48798700	-0.76062900
O	3.98981400	-0.32011400	-0.49803700
C	4.94009800	0.28188900	-1.41173700
C	2.79122900	-2.25691300	1.49342800
C	3.67812300	-1.61770300	2.28401400
H	2.13739900	0.32958600	1.90940700
H	5.49803100	1.07426300	-0.90877100
H	4.41950800	0.69591000	-2.27778500
H	5.60248500	-0.52969200	-1.70943700
H	1.86020700	-2.64532200	1.89423600
H	3.04344600	-2.52814000	0.47443600
H	4.63664100	-1.28265900	1.90161300
H	3.46570900	-1.41363300	3.33031500
C	0.28045000	-2.92867200	-1.07533100
H	-1.67717900	4.46567500	-0.42796100
H	-1.07936800	4.13631400	1.22497200
H	-2.03921200	-4.28271700	-1.50294600
H	-4.35761500	-3.47724900	-0.99458500
H	-4.29961400	-0.04849800	1.87133700
H	-4.79196600	1.01857700	0.52142200
H	-3.86597000	1.67070300	1.88459500
H	-4.66476300	-1.21304000	-0.05158200
H	0.77347500	3.00536200	0.20615200
H	-0.84099800	2.83707100	-2.40017200
H	0.85878500	2.35324500	-2.17261900
H	0.39962600	4.05472800	-2.02341800
H	0.33154800	-3.39075300	-2.06585500
H	0.96263500	-2.07676700	-1.04326000
H	0.63074700	-3.67113400	-0.34798800

Structure **ts15c'-*syn*-II-*Si*-Λ**

C	-0.13029400	3.81953500	-0.57059400
C	-0.42483900	2.64228300	-1.52179500
N	0.18320200	1.49955600	-0.79315600
C	0.97589800	1.99617700	0.10726700
O	0.96367900	3.32748100	0.26350300
N	1.83156700	1.31147900	0.93118300
C	2.38745500	2.02702000	2.09677000
Cu	-0.24017900	-0.37211200	-0.61226800
C	-1.88544800	-1.10427900	-0.46019200
C	-2.69041500	-0.64301200	0.71252400
O	-2.34716700	-0.71525400	1.87747100
C	-1.90065700	2.43894900	-1.83483100
N	1.68466000	-0.76112800	-0.23404600
C	2.39880800	0.06790600	0.55970400

C	3.68092500	-0.26521000	1.00842600
C	4.23637200	-1.47260200	0.60062300
C	3.53035200	-2.29289800	-0.27289200
C	2.26193000	-1.89997100	-0.69398600
O	-3.82412000	-0.03964700	0.29894900
C	-4.62238000	0.57248000	1.33679900
C	-1.45805600	-3.38824200	0.50380200
C	-2.74328500	-3.60393000	0.16125700
H	-2.52147300	-1.46463200	-1.27021300
H	-4.03390400	1.30980900	1.88838700
H	-4.98150200	-0.19004200	2.03158700
H	-5.45551000	1.04648900	0.81928900
H	-0.64690300	-3.73032800	-0.13003700
H	-1.19364600	-2.96274300	1.46564100
H	-3.56041100	-3.32890100	0.82215200
H	-3.01501300	-4.07549100	-0.77960700
C	1.49853900	-2.69748400	-1.71509400
H	-0.97131900	4.05172100	0.09130500
H	0.21911200	4.72627000	-1.06358900
H	3.95557000	-3.22131900	-0.63846800
H	5.22945700	-1.75127300	0.93932900
H	3.32682800	2.53377100	1.85360300
H	2.54814400	1.30798800	2.90124900
H	1.66554700	2.77066900	2.42711100
H	4.24649100	0.41029000	1.63548900
H	0.12933500	2.76886000	-2.46111000
H	-2.47959000	2.25015100	-0.92517500
H	-2.03790000	1.58953700	-2.51084300
H	-2.30787400	3.32715400	-2.32996200
H	1.52671100	-3.76969200	-1.49759300
H	0.45947300	-2.36313000	-1.75705600
H	1.93899800	-2.55425200	-2.70970400

Structure **ts15c'-*syn*-II-*Si*-V**

C	-1.40420700	3.72453200	0.31741900
C	-0.26854800	2.91999800	-0.36123200
N	-0.64731200	1.51925300	-0.05566500
C	-1.86634500	1.52910900	0.38865400
O	-2.43700900	2.72538400	0.58071200
N	-2.64753400	0.44556100	0.70118400
C	-3.88447900	0.69034400	1.46955000
Cu	0.37954700	-0.08826000	0.18628400
C	2.05829900	-0.16390400	0.84678900
C	3.25155000	-0.04468600	-0.03906600
O	3.67831000	-0.91035700	-0.77750500
C	-0.15442500	3.15471700	-1.86726900
N	-1.22091700	-1.19215200	-0.28549600
C	-2.46645200	-0.82017800	0.08963200
C	-3.57634800	-1.64475900	-0.11802200
C	-3.38861100	-2.86922800	-0.74974500
C	-2.12026000	-3.22318600	-1.19422000
C	-1.05379900	-2.35454300	-0.96781100
O	3.74156100	1.20955900	0.02607800
C	4.81191700	1.51283100	-0.89893600
C	2.34859000	-2.53143300	1.52340300
C	3.35634400	-2.07133400	2.29075300
H	2.26502800	0.18748300	1.85857800
H	4.49266900	1.32593700	-1.92693200
H	5.68537400	0.89670400	-0.67493100
H	5.03478600	2.56802300	-0.74577600
H	1.36272400	-2.71978800	1.93876900
H	2.52850100	-2.83664200	0.49964100
H	4.35662000	-1.94411200	1.88730900
H	3.21164500	-1.81682700	3.33761600
C	0.31651700	-2.66450800	-1.50476100
H	-1.85205000	4.48767300	-0.32060300
H	-1.11898500	4.16180900	1.27767000
H	-1.95027600	-4.15408200	-1.72439400
H	-4.23763900	-3.52384400	-0.92086100
H	-4.08696400	-0.18379700	2.08991800
H	-4.73901300	0.88951100	0.81490700
H	-3.73112300	1.55318600	2.11385700
H	-4.56884700	-1.33014600	0.17364900
H	0.69286500	3.12782600	0.11712600
H	-1.10985700	2.96438300	-2.36891100
H	0.60112300	2.49434300	-2.30432200
H	0.14214000	4.18988500	-2.06877000
H	0.28708200	-2.73219500	-2.59838400
H	1.03179400	-1.88734500	-1.23078100
H	0.68453500	-3.62642300	-1.13186300

Structure **ts15d-*anti*-I-*Re*-Λ**

C	1.32060000	3.63730000	0.09740000
C	0.31110000	2.74350000	-0.65130000
N	0.67830000	1.38400000	-0.15930000
C	1.86850000	1.48250000	0.34110000
O	2.38820000	2.71140000	0.47040000
N	2.68750000	0.45480000	0.75770000
C	3.82350000	0.80340000	1.63140000
Cu	-0.17780000	-0.35670000	0.10760000
C	-1.69350000	-0.84990000	1.00610000
C	-3.06460000	-0.87810000	0.43780000
O	-3.79120000	0.08910000	0.57130000
C	-1.18370000	3.12180000	-0.50720000
N	1.54640000	-1.25460000	-0.43130000
C	2.70710000	-0.78660000	0.07530000
C	3.91040000	-1.48680000	-0.06540000
C	3.90190000	-2.68470000	-0.77070000
C	2.71920000	-3.13390000	-1.35070000
C	1.55690000	-2.38430000	-1.18260000
O	-3.36580000	-1.95590000	-0.30770000
C	-4.67080000	-1.92890000	-0.93420000
C	-1.17110000	-3.08880000	1.45580000
C	-2.12000000	-2.95830000	2.41010000
H	0.54540000	2.76160000	-1.72530000
H	-1.74240000	-0.54540000	2.05260000
H	-5.45230000	-1.81880000	-0.17930000
H	-4.73140000	-1.09910000	-1.64150000
H	-4.76220000	-2.88440000	-1.44920000
H	-0.11700000	-2.99170000	1.69440000
H	-1.42400000	-3.46240000	0.47100000
H	-3.16780000	-3.13960000	2.19270000
H	-1.87260000	-2.66990000	3.42810000
C	0.27330000	-2.76410000	-1.86700000
H	1.77090000	4.41660000	-0.51590000
H	0.92670000	4.07020000	1.02070000
H	2.69270000	-4.04600000	-1.93680000
H	4.82350000	-3.24580000	-0.89200000
H	4.06830000	-0.06470000	2.24540000
H	4.70350000	1.11580000	1.05960000
H	3.52420000	1.62270000	2.28230000
H	4.83580000	-1.09740000	0.33660000
H	0.26030000	-2.35840000	-2.88710000
H	0.16130000	-3.84920000	-1.94550000
H	-0.58820000	-2.34950000	-1.33820000
C	-1.67790000	3.00350000	0.94560000
H	-1.14640000	3.68080000	1.62420000
H	-2.74110000	3.25770000	0.99880000
H	-1.57010000	1.98250000	1.32140000
C	-1.35830000	4.57270000	-1.00200000
H	-0.98210000	4.69920000	-2.02460000
H	-2.41950000	4.84260000	-1.00510000
H	-0.84250000	5.29440000	-0.35670000
C	-1.99300000	2.17600000	-1.41490000
H	-1.72910000	2.31630000	-2.47020000
H	-1.79270000	1.13430000	-1.14610000
H	-3.06750000	2.34680000	-1.30210000

Structure **ts15d-*anti*-I-*Re*-V**

C	-1.20020000	-2.82540000	-0.98810000
N	-1.08990000	-1.74650000	-0.17050000
C	-2.06170000	-1.51460000	0.74460000
C	-3.13340000	-2.39710000	0.92100000
C	-3.20630000	-3.53160000	0.12220000
C	-2.23750000	-3.74500000	-0.85150000
Cu	0.48040000	-0.51520000	-0.33920000
C	2.26610000	-0.27020000	-0.51040000
C	2.98980000	0.42120000	0.58440000
O	3.81160000	-0.29060000	1.35980000
C	4.43130000	0.43770000	2.44830000
N	-1.99010000	-0.35110000	1.54610000
C	-2.74530000	-0.31830000	2.81430000
C	-0.16660000	-2.99430000	-2.06840000
C	-1.46580000	0.83330000	1.08590000
N	-0.61810000	0.99400000	0.11990000
C	-0.41120000	2.45140000	-0.07240000
C	-1.10670000	3.04380000	1.17910000
O	-1.88090000	1.93030000	1.72800000
C	-0.93200000	2.96840000	-1.44560000
O	2.74080000	1.60560000	0.75520000
C	3.36400000	-2.49140000	-0.60200000
C	4.35180000	-1.84150000	-1.24770000
H	0.66530000	2.63520000	-0.02370000
H	2.66450000	0.05480000	-1.47550000
H	5.01220000	1.27670000	2.06020000
H	3.66790000	0.80910000	3.13520000
H	5.07760000	-0.28590000	2.94310000
H	2.60990000	-3.04850000	-1.14690000
H	3.35770000	-2.58120000	0.47830000
H	5.14130000	-1.33100000	-0.70580000
H	4.39910000	-1.80850000	-2.33340000
H	-0.40170000	3.35970000	1.95170000
H	-1.81400000	3.84650000	0.97570000
H	-2.28400000	-4.60500000	-1.51090000
H	-4.03230000	-4.22570000	0.24320000
C	-0.63710000	4.48040000	-1.53090000

C	-0.16050000	2.25510000	-2.57330000
C	-2.44040000	2.71270000	-1.61840000
H	-3.80620000	-0.10120000	2.65300000
H	-2.63470000	-1.28320000	3.31110000
H	-2.32550000	0.45780000	3.45040000
H	-3.91240000	-2.18890000	1.64160000
H	-0.64230000	-3.03370000	-3.05460000
H	0.53480000	-2.15760000	-2.05520000
H	0.39440000	-3.92690000	-1.93920000
H	-0.45960000	2.65280000	-3.54910000
H	0.92150000	2.40220000	-2.47090000
H	-0.36250000	1.17780000	-2.58200000
H	-2.77820000	3.09070000	-2.58930000
H	-2.67160000	1.64170000	-1.58520000
H	-3.04130000	3.21640000	-0.85180000
H	-0.93520000	4.86740000	-2.51110000
H	-1.18550000	5.05800000	-0.77770000
H	0.43210000	4.68720000	-1.40270000

Structure **ts15d-*anti*-II-*Re*-Λ**

C	0.46000000	3.81890000	0.13960000
C	-0.32210000	2.72480000	-0.61660000
N	0.35500000	1.48180000	-0.14950000
C	1.49320000	1.84580000	0.35250000
O	1.71280000	3.16020000	0.49870000
N	2.52800000	1.03230000	0.75720000
C	3.56140000	1.62710000	1.62580000
Cu	-0.08020000	-0.40870000	0.10120000
C	-1.45500000	-1.28710000	0.90960000
C	-2.57120000	-1.90630000	0.13710000
O	-2.44590000	-2.81960000	-0.65830000
C	-1.86210000	2.74780000	-0.44860000
C	-2.45370000	1.65940000	-1.36420000
N	1.79700000	-0.88400000	-0.43720000
C	2.82470000	-0.17260000	0.07160000
C	4.15320000	-0.58580000	-0.07240000
C	4.40970000	-1.75040000	-0.78770000
C	3.35600000	-2.44400000	-1.37490000
C	2.05470000	-1.97470000	-1.20320000
C	0.89220000	-2.61800000	-1.90520000
O	-3.72700000	-1.26120000	0.37490000
C	-4.85120000	-1.66730000	-0.43990000
C	-2.29210000	2.49130000	1.00720000
C	-2.37220000	4.12900000	-0.90940000
C	-0.27200000	-3.24900000	1.56760000
C	-1.34550000	-3.45450000	2.36230000
H	-0.11430000	2.81290000	-1.69240000
H	-1.74950000	-1.03520000	1.92850000
H	-4.61630000	-1.54570000	-1.49980000
H	-5.09850000	-2.71250000	-0.24220000
H	-5.67130000	-1.01390000	-0.14510000
H	0.63510000	-2.79430000	1.95340000
H	-0.23230000	-3.67550000	0.57280000
H	-2.22090000	-3.98410000	1.99920000
H	-1.37310000	-3.10440000	3.39080000
H	0.71510000	4.68800000	-0.46530000
H	-0.01870000	4.13920000	1.06880000
H	3.53240000	-3.33240000	-1.97110000
H	5.43250000	-2.09280000	-0.91160000
H	3.99290000	0.83770000	2.24310000
H	4.34950000	2.12140000	1.04830000
H	3.09120000	2.36440000	2.27350000
H	4.96930000	-0.00390000	0.33360000
H	-0.04240000	-2.50460000	-1.35060000
H	0.74710000	-2.14370000	-2.88520000
H	1.06980000	-3.68200000	-2.08380000
H	-2.05700000	4.35320000	-1.93560000
H	-3.46680000	4.15130000	-0.88790000
H	-2.01930000	4.93860000	-0.25910000
H	-2.21670000	1.85110000	-2.41750000
H	-2.05040000	0.67850000	-1.09530000
H	-3.54290000	1.61650000	-1.26370000
H	-3.38470000	2.49630000	1.07920000
H	-1.94080000	1.51700000	1.36050000
H	-1.92030000	3.25850000	1.69580000

Structure **ts15d-*syn*-I-*Re*-Λ**

C	-3.33230000	-1.88920000	-0.68620000
C	-2.80730000	-0.92760000	0.39910000
N	-1.35620000	-0.84560000	0.06100000
C	-1.09630000	-1.87290000	-0.68490000
O	-2.13270000	-2.59810000	-1.12430000
N	0.14260000	-2.32600000	-1.07000000
C	0.20220000	-3.24240000	-2.22530000
Cu	0.13950000	0.36340000	0.39650000
C	0.85770000	2.01660000	0.29560000
C	1.74760000	2.36350000	-0.85090000
O	1.39850000	2.63550000	-1.98000000
C	-3.53710000	0.43100000	0.52070000
N	1.36230000	-1.19640000	0.63420000
C	1.25020000	-2.26030000	-0.19000000
C	2.18800000	-3.29970000	-0.18720000
C	3.24520000	-3.23960000	0.71040000
C	3.33610000	-2.16600000	1.59210000
C	2.37890000	-1.15680000	1.53560000
O	3.03760000	2.24190000	-0.46300000
C	4.02470000	2.40830000	-1.50840000
C	-0.93620000	3.86650000	-0.29060000
C	-0.02730000	4.77100000	0.11020000
H	1.09160000	2.62600000	1.17010000
H	3.84280000	1.70100000	-2.32080000
H	3.98460000	3.42660000	-1.90070000
H	4.98510000	2.21610000	-1.03180000
H	-1.73490000	3.54140000	0.36790000
H	-0.94730000	3.49590000	-1.30990000
H	0.74430000	5.13370000	-0.56330000
H	-0.03480000	5.18660000	1.11510000
C	2.45320000	0.03480000	2.44850000
H	-4.03290000	-2.63910000	-0.32120000
H	-3.74920000	-1.38200000	-1.55990000
H	4.13880000	-2.10370000	2.31790000
H	3.97840000	-4.03980000	0.73700000
H	2.07610000	-4.15130000	-0.84420000
H	1.17540000	-3.13210000	-2.70570000
H	0.04430000	-4.28560000	-1.93300000
H	-0.57390000	-2.95800000	-2.93350000
H	-2.87580000	-1.42130000	1.37900000
H	3.15690000	-0.14450000	3.26500000
H	2.79890000	0.91580000	1.89480000
H	1.47620000	0.26620000	2.88530000
C	-3.42240000	1.25860000	-0.77240000
H	-3.89170000	2.23830000	-0.63320000
H	-2.37730000	1.42050000	-1.05390000
H	-3.93040000	0.78130000	-1.61780000
C	-2.90530000	1.19630000	1.70000000
H	-3.03560000	0.65180000	2.64310000
H	-1.83160000	1.33780000	1.53470000
H	-3.36670000	2.18250000	1.81880000
C	-5.02130000	0.15220000	0.83510000
H	-5.13440000	-0.45990000	1.73800000
H	-5.55350000	1.09390000	1.00600000
H	-5.52850000	-0.36080000	0.00900000

Structure **ts15d-*syn*-I-*Re*-V**

C	-2.84820000	-2.49140000	-0.58380000
C	-1.39380000	-2.30320000	-0.07480000
N	-1.13930000	-0.87000000	-0.35890000
C	-2.25610000	-0.33180000	-0.72880000
O	-3.31060000	-1.14080000	-0.88530000
N	-2.49040000	0.99620000	-0.99160000
C	-3.70280000	1.32610000	-1.76700000
Cu	0.47940000	0.19760000	-0.39080000
C	2.18200000	0.05050000	-0.99950000
C	3.39240000	-0.13420000	-0.14770000
O	3.65010000	-1.10730000	0.53170000
C	-1.13050000	-2.67800000	1.41420000
N	-0.54820000	1.83840000	0.12170000
C	-1.81510000	2.03630000	-0.30850000
C	-2.48900000	3.24580000	-0.08970000
C	-1.84240000	4.25600000	0.60680000
C	-0.55720000	4.03680000	1.09340000
C	0.06300000	2.81600000	0.84640000
O	4.13880000	0.99170000	-0.17130000
C	5.27510000	1.00760000	0.72410000
C	2.03980000	-2.20750000	-1.88140000
C	3.14890000	-1.89420000	-2.58290000
H	-0.70840000	-2.89860000	-0.68820000
H	2.44050000	0.48340000	-1.96780000
H	4.95310000	0.84040000	1.75460000
H	5.98580000	0.22910000	0.43840000
H	5.71840000	1.99600000	0.60940000
H	1.05740000	-2.16400000	-2.34180000
H	2.10940000	-2.62900000	-0.88550000
H	4.13800000	-1.99870000	-2.14730000
H	3.09680000	-1.53090000	-3.60600000
C	1.44270000	2.53460000	1.37030000
H	-2.91530000	-3.07450000	-1.50480000
H	-3.53560000	-2.90020000	0.15670000
H	-0.03670000	4.79750000	1.66380000
H	-2.35110000	5.19720000	0.79130000
H	-3.50750000	3.38500000	-0.42380000
H	-4.57210000	1.48760000	-1.12150000
H	-3.50560000	2.22170000	-2.35800000
H	-3.91950000	0.50050000	-2.44130000
H	1.46700000	1.59600000	1.93550000
H	2.17060000	2.45140000	0.55660000

H	1.77130000	3.33660000	2.03580000
C	-1.94530000	-1.78420000	2.36680000
H	-3.02260000	-1.83530000	2.16540000
H	-1.79650000	-2.10650000	3.40250000
H	-1.63700000	-0.73500000	2.30010000
C	-1.50670000	-4.15800000	1.63050000
H	-0.99720000	-4.81170000	0.91190000
H	-1.20700000	-4.47750000	2.63420000
H	-2.58510000	-4.33480000	1.54660000
C	0.37680000	-2.50480000	1.68700000
H	0.96300000	-3.28660000	1.19010000
H	0.74530000	-1.54150000	1.31640000
H	0.59290000	-2.56290000	2.75860000

Structure **ts15d-*syn*-II-*Re*-Λ**

C	3.24380000	-1.96270000	0.78050000
C	2.76480000	-1.02860000	-0.35010000
N	1.31500000	-0.88220000	-0.03700000
C	1.00910000	-1.86310000	0.75230000
O	2.01500000	-2.60430000	1.23830000
N	-0.24950000	-2.24720000	1.14600000
C	-0.35370000	-3.09430000	2.34920000
Cu	-0.14030000	0.35130000	-0.46330000
C	-0.85960000	2.01800000	-0.46510000
C	-1.95580000	2.31570000	0.48640000
O	-3.06220000	1.87200000	0.21720000
C	3.53710000	0.30220000	-0.51380000
N	-1.40410000	-1.19260000	-0.65220000
C	-1.34570000	-2.19960000	0.24530000
C	-2.32080000	-3.20100000	0.30170000
C	-3.36480000	-3.16400000	-0.61350000
C	-3.40010000	-2.15570000	-1.57090000
C	-2.40380000	-1.18220000	-1.57210000
O	-1.65430000	2.95650000	1.61820000
C	-2.75450000	3.14110000	2.54300000
C	0.87550000	3.74380000	0.12760000
C	0.03400000	4.64610000	-0.40990000
C	-2.42220000	-0.06280000	-2.57330000
H	-2.25060000	-4.00880000	1.01690000
H	2.83150000	-1.56220000	-1.30890000
H	-4.19010000	-2.11370000	-2.31190000
H	-4.12940000	-3.93450000	-0.59340000
H	3.91750000	-2.75360000	0.45340000
H	3.67560000	-1.43530000	1.63500000
H	-1.04300000	2.53660000	-1.40760000
H	-3.55580000	3.71190000	2.06930000
H	-3.14060000	2.17240000	2.86720000
H	-2.33150000	3.69070000	3.38260000
H	-1.32560000	-2.92010000	2.81320000
H	-0.23590000	-4.15790000	2.11770000
H	0.42790000	-2.80260000	3.04840000
H	-0.75650000	5.10490000	0.17580000
H	0.11580000	4.95490000	-1.44920000
H	1.69600000	3.33000000	-0.44760000
H	0.83190000	3.48820000	1.18070000
H	-3.07900000	-0.30350000	-3.41300000
H	-2.79910000	0.84920000	-2.09710000
H	-1.42120000	0.13810000	-2.96880000
C	3.42750000	1.18290000	0.74440000
H	3.91810000	0.72940000	1.61280000
H	3.91750000	2.14710000	0.57160000
H	2.38270000	1.37460000	1.00920000
C	2.94250000	1.03800000	-1.73090000
H	3.07700000	0.45700000	-2.65120000
H	1.86840000	1.20410000	-1.59050000
H	3.42570000	2.01010000	-1.87740000
C	5.01720000	-0.02800000	-0.79430000
H	5.12640000	-0.67460000	-1.67340000
H	5.57920000	0.89150000	-0.98940000
H	5.49650000	-0.52610000	0.05710000

Structure **ts15d-*syn*-II-*Re*-V**

C	-2.13860000	3.06330000	0.62510000
C	-0.77250000	2.52660000	0.11890000
N	-0.88530000	1.07080000	0.37050000
C	-2.10330000	0.82130000	0.72980000
O	-2.92290000	1.86650000	0.90380000
N	-2.66360000	-0.40960000	0.96730000
C	-3.92010000	-0.43870000	1.74190000
Cu	0.40980000	-0.38110000	0.37970000
C	2.07070000	-0.70680000	1.06390000
C	3.29300000	-1.04700000	0.29990000
O	3.53490000	-2.22290000	0.08330000
C	-0.40510000	2.85410000	-1.35910000
N	-1.00200000	-1.69380000	-0.18110000
C	-2.27640000	-1.57290000	0.25460000
C	-3.23820000	-2.56290000	0.01410000
C	-2.87260000	-3.68850000	-0.71040000
C	-1.57620000	-3.79200000	-1.20370000
C	-0.66360000	-2.77540000	-0.93620000
O	3.99900000	-0.02650000	-0.20700000
C	5.13250000	-0.40370000	-1.02600000
C	2.47390000	1.43810000	1.94260000
C	3.40130000	0.82050000	2.70690000
H	0.03300000	2.92080000	0.74910000
H	2.09210000	-1.21730000	2.02870000
H	5.82650000	-1.02140000	-0.45200000
H	4.79490000	-0.95810000	-1.90400000
H	5.60010000	0.53580000	-1.31740000
H	1.48720000	1.65960000	2.33630000
H	2.73230000	1.86820000	0.98200000
H	4.41270000	0.66000000	2.34850000
H	3.16950000	0.45940000	3.70540000
C	0.73890000	-2.84060000	-1.46580000
H	-2.06450000	3.63240000	1.55430000
H	-2.69770000	3.64150000	-0.11070000
H	-1.26790000	-4.64600000	-1.79580000
H	-3.60540000	-4.46410000	-0.91120000
H	-4.80180000	-0.35570000	1.09840000
H	-3.95880000	-1.37020000	2.30850000
H	-3.91860000	0.39690000	2.43870000
H	-4.25800000	-2.44400000	0.35160000
H	0.84510000	-3.66470000	-2.17550000
H	1.00650000	-1.91320000	-1.98510000
H	1.46960000	-2.99200000	-0.66470000
C	-1.40630000	2.21490000	-2.33830000
H	-1.38470000	1.12100000	-2.28200000
H	-2.43590000	2.54460000	-2.15250000
H	-1.15940000	2.49910000	-3.36660000
C	1.01240000	2.30660000	-1.62210000
H	1.76960000	2.90450000	-1.10030000
H	1.11040000	1.27380000	-1.26660000
H	1.25180000	2.32730000	-2.69010000
C	-0.38860000	4.38430000	-1.54610000
H	0.26510000	4.87250000	-0.81290000
H	-0.01050000	4.63560000	-2.54270000
H	-1.38680000	4.82830000	-1.46030000

Structure **ts15d-*anti*-I-*Si*-Λ**

C	-3.43830000	-1.83650000	-0.29210000
C	-2.01800000	-1.77390000	-0.89310000
N	-1.41930000	-0.63270000	-0.14010000
C	-2.40910000	0.04250000	0.34660000
O	-3.63090000	-0.50200000	0.27350000
N	-2.34370000	1.29330000	0.91910000
C	-3.45030000	1.68450000	1.81140000
Cu	0.36100000	0.12750000	0.16560000
C	2.01990000	-0.06730000	0.88150000
C	3.24730000	-0.32590000	0.06840000
O	3.44940000	-1.31900000	-0.60090000
C	-1.19730000	-3.08470000	-0.87260000
C	-1.94380000	-4.13180000	-1.72420000
N	-0.37460000	1.95280000	-0.24570000
C	-1.54640000	2.30600000	0.32570000
C	-1.99980000	3.63020000	0.32600000
C	-1.23250000	4.59530000	-0.31290000
C	-0.05770000	4.22120000	-0.95900000
C	0.34610000	2.88930000	-0.91550000
C	1.60610000	2.43380000	-1.59390000
O	4.08410000	0.73410000	0.11690000
C	5.24930000	0.64970000	-0.73690000
C	0.17230000	-2.78940000	-1.51470000
C	-1.01160000	-3.62050000	0.55860000
C	3.16070000	-1.85340000	2.64690000
C	1.99260000	-2.21480000	2.07880000
H	2.27130000	0.44090000	1.81380000
H	4.95120000	0.49970000	-1.77720000
H	5.88290000	-0.18210000	-0.42140000
H	5.76820000	1.59920000	-0.61210000
H	1.05170000	-2.07970000	2.60320000
H	1.96890000	-2.76880000	1.14750000
H	4.11030000	-2.04840000	2.15730000
H	3.19970000	-1.35670000	3.61300000
H	-3.54060000	-2.55530000	0.52480000
H	-4.22920000	-1.99140000	-1.02480000
H	0.54450000	4.94780000	-1.49240000
H	-1.56820000	5.62760000	-0.33140000
H	-2.94360000	3.89830000	0.78040000
H	-4.30100000	2.09900000	1.26060000
H	-3.07730000	2.41790000	2.52830000
H	-3.78500000	0.80220000	2.35450000
H	-2.08720000	-1.45360000	-1.94260000
H	2.38910000	2.21020000	-0.86110000
H	1.43070000	1.52970000	-2.18760000
H	1.98750000	3.20900000	-2.26310000
H	0.06030000	-2.48910000	-2.56380000

H	0.69150000	-1.98190000	-0.98830000
H	0.81830000	-3.67280000	-1.49040000
H	-1.95100000	-3.97950000	0.99380000
H	-0.31850000	-4.46820000	0.55550000
H	-0.60470000	-2.85370000	1.22390000
H	-2.10040000	-3.77920000	-2.75070000
H	-1.36160000	-5.05770000	-1.77840000
H	-2.92180000	-4.38740000	-1.29800000

Structure **ts15d-*anti*-I-*Si*-V**

C	1.33410000	2.19870000	1.43250000
N	0.52610000	1.67040000	0.47110000
C	-0.19310000	2.50420000	-0.31470000
C	-0.09560000	3.89740000	-0.19610000
C	0.75300000	4.43020000	0.76270000
C	1.47090000	3.57410000	1.59270000
Cu	0.47760000	-0.30960000	0.22870000
C	1.85840000	-1.46070000	0.34660000
C	2.96950000	-1.39580000	-0.64460000
O	4.05840000	-0.86030000	-0.04750000
C	5.17560000	-0.57610000	-0.92190000
N	-1.07100000	1.96690000	-1.28560000
C	-1.51730000	2.83390000	-2.39560000
C	2.09710000	1.24530000	2.31020000
C	-1.72590000	0.77370000	-1.11630000
N	-1.33860000	-0.24260000	-0.41300000
C	-2.43110000	-1.24460000	-0.41790000
C	-3.39410000	-0.67720000	-1.49400000
O	-2.89430000	0.66760000	-1.75880000
C	-3.04180000	-1.47610000	0.99750000
O	2.91220000	-1.68710000	-1.82120000
C	0.84740000	-3.66400000	-0.60470000
C	1.89460000	-4.24530000	0.00630000
H	2.16570000	-1.96720000	1.26330000
H	4.86990000	0.09960000	-1.72430000
H	5.55510000	-1.50350000	-1.35600000
H	5.92800000	-0.11080000	-0.28640000
H	-0.13220000	-3.64310000	-0.13730000
H	0.93230000	-3.26950000	-1.61140000
H	2.86400000	-4.31300000	-0.47910000
H	1.81040000	-4.68450000	0.99730000
H	-4.42790000	-0.56910000	-1.16750000
H	-3.36330000	-1.22940000	-2.43590000
H	2.12900000	3.96160000	2.36180000
H	0.83510000	5.50700000	0.87450000
H	-0.69420000	4.55100000	-0.81500000
H	-0.65850000	3.39510000	-2.76600000
H	-2.30930000	3.52240000	-2.08450000
H	-1.89840000	2.20430000	-3.19670000
H	-2.01560000	-2.19780000	-0.76160000
C	-1.95510000	-2.10550000	1.89260000
C	-4.21730000	-2.46730000	0.87830000
C	-3.52810000	-0.15350000	1.61770000
H	2.59870000	1.78430000	3.11750000
H	1.43320000	0.50010000	2.76100000
H	2.86080000	0.70970000	1.73440000
H	-4.00590000	-0.34490000	2.58420000
H	-2.69780000	0.54000000	1.79100000
H	-4.26930000	0.35280000	0.98720000
H	-2.27150000	-2.12010000	2.94050000
H	-1.74770000	-3.14050000	1.59500000
H	-1.01250000	-1.54950000	1.82610000
H	-4.58160000	-2.73810000	1.87490000
H	-5.06780000	-2.04730000	0.32950000
H	-3.91290000	-3.39370000	0.37590000

Structure **ts15d-*anti*-II-*Si*-Λ**

C	1.90920000	3.33500000	-0.30810000
C	0.73090000	2.52120000	-0.88730000
N	0.85120000	1.23510000	-0.14360000
C	2.05250000	1.19700000	0.33390000
O	2.78920000	2.31450000	0.25670000
N	2.67120000	0.10610000	0.90190000
C	3.81100000	0.37120000	1.79830000
Cu	-0.22080000	-0.38270000	0.15570000
C	-1.68650000	-1.13480000	0.94260000
C	-2.81900000	-1.75040000	0.20740000
O	-2.77380000	-2.93760000	-0.07150000
C	-0.66530000	3.18650000	-0.83020000
N	1.39260000	-1.50020000	-0.30580000
C	2.55950000	-1.17210000	0.28980000
C	3.65760000	-2.03860000	0.29660000
C	3.54550000	-3.25570000	-0.36430000
C	2.37040000	-3.56260000	-1.04270000
C	1.30880000	-2.66090000	-1.00680000
O	-3.77960000	-0.91640000	-0.21180000
C	-4.82640000	-1.52280000	-1.00800000
C	-2.70380000	0.65470000	2.18170000
C	-3.42170000	-0.28780000	2.82730000
C	0.02410000	-2.93750000	-1.73040000
H	4.58850000	-1.76120000	0.77140000
H	0.93610000	2.29440000	-1.94340000
H	2.26830000	-4.48830000	-1.59760000
H	4.38590000	-3.94300000	-0.37650000
H	1.62430000	4.00780000	0.50460000
H	2.48650000	3.87940000	-1.05440000
H	-1.51050000	-1.69570000	1.86170000
H	-5.31880000	-2.31900000	-0.44540000
H	-4.40830000	-1.93500000	-1.92860000
H	-5.52340000	-0.71510000	-1.22680000
H	4.75320000	0.48080000	1.25110000
H	3.88970000	-0.44900000	2.51380000
H	3.61620000	1.29390000	2.34270000
H	-4.36710000	-0.64800000	2.43410000
H	-3.08050000	-0.72620000	3.76150000
H	-1.79670000	1.05870000	2.61910000
H	-3.08500000	1.14580000	1.29390000
H	0.14650000	-3.76490000	-2.43370000
H	-0.77860000	-3.20600000	-1.03520000
H	-0.30130000	-2.05760000	-2.29740000
C	-1.07420000	3.53880000	0.61140000
H	-0.46020000	4.34270000	1.03220000
H	-2.11200000	3.88800000	0.63350000
H	-0.99340000	2.67320000	1.27480000
C	-0.62280000	4.47070000	-1.68350000
H	-0.32200000	4.25830000	-2.71630000
H	-1.61410000	4.93500000	-1.71660000
H	0.07050000	5.21450000	-1.27240000
C	-1.67850000	2.20080000	-1.44570000
H	-1.45500000	2.01310000	-2.50320000
H	-1.65550000	1.23900000	-0.92130000
H	-2.69740000	2.59730000	-1.38570000

Structure **ts15d-*anti*-II-*Si*-V**

C	-1.02140000	2.34810000	-1.51870000
N	-0.33900000	1.72740000	-0.51660000
C	0.37720000	2.47750000	0.35150000
C	0.38920000	3.87690000	0.28570000
C	-0.34460000	4.50580000	-0.71000000
C	-1.04870000	3.73570000	-1.62950000
Cu	-0.49060000	-0.25850000	-0.30320000
C	-1.99940000	-1.23820000	-0.53480000
C	-3.24010000	-0.89560000	0.19710000
O	-3.46930000	-1.49410000	1.37000000
C	-4.65220000	-1.04520000	2.07650000
N	1.14680000	1.84050000	1.35730000
C	1.59890000	2.63990000	2.51390000
C	-1.76880000	1.48880000	-2.49900000
C	1.72050000	0.60610000	1.18620000
N	1.28730000	-0.36750000	0.45060000
C	2.29410000	-1.45400000	0.49000000
C	3.27780000	-0.96070000	1.58480000
O	2.85190000	0.40300000	1.87330000
C	2.91480000	-1.75140000	-0.90830000
O	-3.94050000	-0.01260000	-0.27390000
C	-1.35120000	-3.41070000	0.41960000
C	-2.37990000	-3.88790000	-0.30840000
H	-2.24860000	-1.65130000	-1.51390000
H	-5.54140000	-1.19640000	1.46100000
H	-4.56040000	0.01330000	2.32890000
H	-4.69540000	-1.65630000	2.97690000
H	-0.33320000	-3.46010000	0.04860000
H	-1.49170000	-3.07160000	1.43980000
H	-3.39350000	-3.89270000	0.07970000
H	-2.23400000	-4.29160000	-1.30710000
H	4.31840000	-0.90410000	1.26550000
H	3.21250000	-1.52970000	2.51480000
H	-1.61300000	4.19750000	-2.43140000
H	-0.34330000	5.58920000	-0.78060000
H	0.98420000	4.46250000	0.97210000
H	0.76530000	3.25170000	2.86160000
H	2.45170000	3.27860000	2.26280000
H	1.89520000	1.96220000	3.31150000
H	1.79390000	-2.36800000	0.83030000
C	1.79680000	-2.30150000	-1.81740000
C	4.00480000	-2.83120000	-0.75380000
C	3.51900000	-0.48010000	-1.53190000
H	-2.65380000	1.04730000	-2.02660000
H	-2.09970000	2.08230000	-3.35480000
H	-1.13910000	0.67440000	-2.87310000
H	3.99440000	-0.72030000	-2.48870000
H	2.75360000	0.27970000	-1.72450000
H	4.29030000	-0.03200000	-0.89360000
H	2.12430000	-2.34590000	-2.86100000

H	1.50780000	-3.31630000	-1.51750000
H	0.89910000	-1.67370000	-1.76430000
H	4.36780000	-3.14180000	-1.73920000
H	4.87370000	-2.47150000	-0.19080000
H	3.61820000	-3.72440000	-0.24800000

Structure **ts15d-*syn*-I-*Si*-Λ**

C	2.24770000	-2.96470000	0.50690000
C	2.01110000	-1.92870000	-0.61600000
N	0.77470000	-1.23700000	-0.14820000
C	0.25380000	-1.98350000	0.77110000
O	0.96290000	-3.03670000	1.19710000
N	-0.98090000	-1.82760000	1.37030000
C	-1.18600000	-2.48810000	2.67230000
Cu	-0.20580000	0.42250000	-0.50910000
C	0.20020000	2.19920000	-0.52670000
C	1.00850000	2.85860000	0.52800000
O	2.20910000	2.96150000	0.34730000
C	3.21420000	-1.00700000	-0.94050000
N	-1.93100000	-0.62380000	-0.43690000
C	-2.11320000	-1.46720000	0.60050000
C	-3.37160000	-1.99690000	0.90920000
C	-4.44710000	-1.66730000	0.09280000
C	-4.24270000	-0.86470000	-1.02660000
C	-2.96440000	-0.37290000	-1.27880000
O	0.38420000	3.19450000	1.66650000
C	1.23720000	3.74650000	2.69830000
C	-2.00030000	3.12090000	-0.09190000
C	-1.44990000	4.19200000	-0.70170000
C	-2.65580000	0.41500000	-2.52250000
H	-3.50740000	-2.67210000	1.74290000
H	1.74590000	-2.45310000	-1.54460000
H	-5.05610000	-0.62840000	-1.70380000
H	-5.43290000	-2.06580000	0.31270000
H	2.99510000	-2.65400000	1.24050000
H	2.47620000	-3.96770000	0.14830000
H	0.39380000	2.69470000	-1.48060000
H	1.75390000	4.63480000	2.32880000
H	1.97370000	3.00450000	3.01390000
H	0.56690000	4.00120000	3.51820000
H	-1.50820000	-3.52900000	2.56250000
H	-1.93280000	-1.92470000	3.23440000
H	-0.24690000	-2.47180000	3.22230000
H	-0.87240000	4.92500000	-0.14690000
H	-1.57810000	4.37450000	-1.76540000
H	-2.64240000	2.43480000	-0.63200000
H	-1.92510000	2.98410000	0.98040000
H	-2.43640000	-0.26900000	-3.35250000
H	-3.49740000	1.04260000	-2.82900000
H	-1.77230000	1.04020000	-2.37140000
C	3.62340000	-0.14060000	0.26350000
H	4.45100000	0.51830000	-0.01840000
H	2.80510000	0.50070000	0.59960000
H	3.96660000	-0.74240000	1.11310000
C	4.39500000	-1.90660000	-1.36310000
H	4.12580000	-2.55940000	-2.20250000
H	5.24070000	-1.28900000	-1.68310000
H	4.74920000	-2.53860000	-0.53950000
C	2.82020000	-0.10410000	-2.12490000
H	2.59830000	-0.69640000	-3.02140000
H	1.93420000	0.48790000	-1.87570000
H	3.62910000	0.59150000	-2.36960000

Structure **ts15d-*syn*-I-*Si*-V**

C	0.99980000	-2.64910000	1.22330000
N	1.17770000	-1.63970000	0.33280000
C	2.42690000	-1.36640000	-0.11270000
C	3.52960000	-2.13880000	0.26710000
C	3.33210000	-3.20620000	1.13530000
C	2.05750000	-3.46060000	1.62830000
Cu	-0.39120000	-0.57020000	-0.30290000
C	-2.05920000	-0.57680000	-1.01040000
C	-3.16590000	0.20540000	-0.41420000
O	-4.06530000	-0.44840000	0.32720000
C	-5.07650000	0.37770000	0.95570000
N	2.62000000	-0.27320000	-0.99200000
C	3.83150000	-0.24900000	-1.83510000
C	-0.38580000	-2.85800000	1.77180000
C	1.87700000	0.87900000	-0.90780000
N	0.69380000	1.01370000	-0.39630000
C	0.35780000	2.46000000	-0.40530000
C	1.43240000	3.02460000	-1.36600000
O	2.44860000	1.97290000	-1.42420000
C	0.33350000	3.09130000	1.02010000
O	-3.14340000	1.41780000	-0.56290000
C	-2.82720000	-2.87840000	-0.99710000
C	-3.66340000	-2.50770000	-1.98750000
H	-2.10500000	-0.50290000	-2.09950000
H	-5.62230000	0.94810000	0.20150000
H	-4.61270000	1.06400000	1.66730000
H	-5.73730000	-0.32060000	1.46750000
H	-1.88110000	-3.36520000	-1.21260000
H	-3.13330000	-2.82910000	0.04170000
H	-4.63600000	-2.07640000	-1.77360000
H	-3.39620000	-2.62430000	-3.03470000
H	1.93340000	3.92660000	-1.01840000
H	1.06410000	3.17610000	-2.38410000
H	1.87700000	-4.26950000	2.32820000
H	4.17630000	-3.81520000	1.44360000
H	4.00140000	-1.25160000	-2.23020000
H	4.71160000	0.08590000	-1.27650000
H	3.66580000	0.43540000	-2.66430000
H	4.52490000	-1.89630000	-0.07940000
H	-0.64170000	2.56890000	-0.83580000
C	1.70740000	2.99980000	1.70970000
C	-0.71740000	2.36010000	1.87840000
C	-0.09050000	4.56800000	0.87780000
H	-0.38310000	-2.78890000	2.86520000
H	-1.06510000	-2.10010000	1.37630000
H	-0.77370000	-3.84820000	1.50730000
H	-0.16230000	5.03500000	1.86580000
H	0.62760000	5.15750000	0.29580000
H	-1.07110000	4.65650000	0.39540000
H	-0.81560000	2.85190000	2.85240000
H	-1.69990000	2.36570000	1.39420000
H	-0.42820000	1.31920000	2.06560000
H	1.65600000	3.44940000	2.70700000
H	2.02340000	1.95800000	1.83810000
H	2.49220000	3.53100000	1.15860000

Structure **ts15d-*syn*-II-*Si*-Λ**

C	1.88640000	-3.12240000	0.53770000
C	1.70550000	-2.14800000	-0.64630000
N	0.56750000	-1.30830000	-0.17920000
C	-0.01110000	-1.96200000	0.77750000
O	0.60360000	-3.06170000	1.23450000
N	-1.21200000	-1.66100000	1.37980000
C	-1.47570000	-2.24850000	2.70640000
Cu	-0.18990000	0.45590000	-0.52220000
C	0.47420000	2.14240000	-0.40450000
C	1.02990000	2.56630000	0.91830000
O	0.44100000	2.52170000	1.98250000
C	2.97020000	-1.37530000	-1.09840000
C	2.59630000	-0.52420000	-2.32780000
N	-2.02890000	-0.35410000	-0.42600000
C	-2.29910000	-1.15820000	0.62390000
C	-3.60980000	-1.51590000	0.95900000
C	-4.64800000	-1.05360000	0.15870000
C	-4.36190000	-0.29170000	-0.97090000
C	-3.03530000	0.02650000	-1.25110000
O	2.32320000	2.92340000	0.78860000
C	3.02650000	3.19580000	2.02160000
C	3.52840000	-0.46310000	0.00830000
C	4.03650000	-2.41380000	-1.50510000
C	-1.58250000	3.42440000	-0.15420000
C	-0.77000000	4.44230000	-0.51090000
H	0.90710000	2.71410000	-1.22660000
H	2.99000000	2.32590000	2.68170000
H	2.57500000	4.05140000	2.52880000
H	4.05130000	3.41720000	1.72640000
H	-2.23770000	2.95480000	-0.87880000
H	-1.69350000	3.12860000	0.88290000
H	-0.17190000	4.97520000	0.22240000
H	-0.69400000	4.78120000	-1.54080000
C	-2.64930000	0.76080000	-2.50570000
H	2.65830000	-2.81460000	1.24760000
H	2.04380000	-4.15940000	0.24460000
H	-5.15030000	0.04610000	-1.63470000
H	-5.67310000	-1.31750000	0.40020000
H	-1.93200000	-3.24130000	2.63370000
H	-2.13160000	-1.57530000	3.26060000
H	-0.53200000	-2.33740000	3.24120000
H	-3.81730000	-2.16070000	1.80200000
H	1.34520000	-2.70860000	-1.52070000
H	3.83010000	-1.02250000	0.90120000
H	4.41840000	0.05930000	-0.35820000
H	2.80120000	0.29670000	0.30770000
H	3.66300000	-3.09520000	-2.27910000
H	4.91960000	-1.90750000	-1.90870000
H	4.37090000	-3.01720000	-0.65240000
H	2.25110000	-1.15100000	-3.15890000
H	1.79640000	0.18060000	-2.07620000
H	3.45820000	0.05350000	-2.67740000
H	-3.40650000	1.49350000	-2.79920000
H	-1.68770000	1.26460000	-2.37720000
H	-2.54060000	0.05080000	-3.33580000

Structure **ts15d-*syn*-II-*Si*-V**

C	1.06270000	-2.48650000	1.29950000
N	1.22410000	-1.50770000	0.37230000
C	2.46460000	-1.23730000	-0.09460000
C	3.57500000	-2.00170000	0.27750000
C	3.39190000	-3.05270000	1.16940000
C	2.12900000	-3.29060000	1.69890000
Cu	-0.37420000	-0.52360000	-0.32390000
C	-2.04540000	-0.76770000	-0.97470000
C	-3.25120000	-0.50180000	-0.13790000
O	-3.80530000	0.67740000	-0.48630000
C	-4.91120000	1.11500000	0.33780000
N	2.63670000	-0.14540000	-0.98050000
C	3.85860000	-0.09100000	-1.80690000
C	-0.30050000	-2.65280000	1.91290000
C	1.86840000	0.99070000	-0.90310000
N	0.66380000	1.09730000	-0.43530000
C	0.28640000	2.53060000	-0.46590000
C	1.42690000	3.15080000	-1.31410000
O	2.44010000	2.10150000	-1.38220000
C	0.08140000	3.14610000	0.95030000
O	-3.64270000	-1.19590000	0.78030000
C	-2.22810000	-3.18550000	-1.13530000
C	-3.25370000	-2.93380000	-1.97510000
H	-2.24470000	-0.62140000	-2.03700000
H	-4.59770000	1.20700000	1.38020000
H	-5.73380000	0.39990000	0.26990000
H	-5.20660000	2.08230000	-0.06690000
H	-1.23570000	-3.41760000	-1.51050000
H	-2.39990000	-3.29430000	-0.07140000
H	-4.25980000	-2.77190000	-1.60020000
H	-3.11590000	-2.88770000	-3.05230000
H	1.90620000	4.02200000	-0.86910000
H	1.12720000	3.38160000	-2.33930000
H	1.96390000	-4.07920000	2.42520000
H	4.24100000	-3.65850000	1.47080000
H	4.04980000	-1.08620000	-2.21080000
H	4.72550000	0.25140000	-1.23250000
H	3.69300000	0.59910000	-2.63120000
H	4.56430000	-1.76740000	-0.09080000
H	-0.66540000	2.61400000	-1.00080000
C	1.36540000	3.06780000	1.79610000
C	-1.05030000	2.38330000	1.66670000
C	-0.34970000	4.61680000	0.77420000
H	-0.26550000	-2.40870000	2.98130000
H	-1.02800000	-1.99170000	1.43880000
H	-0.65530000	-3.68550000	1.83010000
H	1.18580000	3.49110000	2.79000000
H	1.69060000	2.03050000	1.93500000
H	2.19500000	3.63160000	1.35330000
H	-0.55190000	5.06920000	1.75060000
H	0.42340000	5.22610000	0.29190000
H	-1.26530000	4.69700000	0.17570000
H	-1.28690000	2.86530000	2.62130000
H	-1.96560000	2.36690000	1.06290000
H	-0.76610000	1.34780000	1.88520000

Structure **ts15d-*syn*-II-*Re*-V supported onto clay**
E(ONIOM(M05-2X:UFF)= -2737.841899
E+ZPE(ONIOM(M05-2X:UFF)= -2737.423105
Lowest freq (cm-1) ONIOM(PM6/UFF): -205.7

C	2.5077	4.0834	3.3251
C	1.1172	3.8713	3.9834
O	3.1007	2.7310	3.2634
H	2.4544	4.4360	2.2855
H	3.2314	4.6722	3.9111
N	0.8990	2.3905	3.8553
C	1.0797	4.3964	5.4646
H	0.3142	4.3861	3.3935
C	2.0593	1.8386	3.5178
Cu	-0.7925	1.3882	3.6850
C	2.2620	3.8470	6.2750
C	-0.2287	3.9815	6.1537
C	1.1530	5.9320	5.3948
N	2.4218	0.5020	3.3472
C	-2.6190	1.8718	3.7005
N	0.1544	-0.3768	3.4898
H	2.2617	2.7520	6.3071
H	3.2328	4.1657	5.8797
H	2.2228	4.1949	7.3160
H	-1.1225	4.3187	5.6101
H	-0.2922	2.8951	6.2822
H	-0.2918	4.4185	7.1598
H	0.3116	6.3674	4.8457
H	1.1277	6.3706	6.4024
H	2.0764	6.2931	4.9305
C	3.8494	0.2362	2.9917
C	1.5223	-0.6043	3.4364
C	-3.2627	1.7458	5.0249
H	-3.3232	1.7764	2.8721
C	-2.3452	4.1747	3.4177
C	-3.5293	4.2033	2.7986
C	-0.6599	-1.4982	3.4985
H	3.9238	-0.2830	2.0194
H	4.4257	1.1804	2.9033
H	4.3387	-0.3691	3.7762
C	2.0766	-1.9061	3.4349
O	-3.4315	0.6812	5.5888
O	-3.6130	2.9462	5.5787
H	-1.3922	4.1881	2.8956
H	-2.2343	4.3083	4.5025
H	-4.4774	4.2745	3.3263
H	-3.6360	4.1889	1.7193
C	-0.1525	-2.8053	3.4840
C	-2.1367	-1.2955	3.5147
C	1.2276	-3.0080	3.4577
H	3.1545	-2.0705	3.4190
C	-4.2005	2.9127	6.9162
H	-0.8323	-3.6596	3.4880
H	-2.6824	-2.2463	3.3644
H	-2.5026	-0.9212	4.4960
H	-2.4976	-0.6359	2.7155
H	1.6400	-4.0223	3.4484
H	-3.3875	2.8347	7.6442
H	-4.7161	3.8790	6.9715
H	-4.8968	2.0710	7.0123
O	0.2983	1.8986	0.3917
Si	1.6254	1.3766	-0.1676
Si	-0.9218	2.8126	-0.2879
O	1.7897	-0.1192	0.2889
O	2.9067	2.2072	0.4658
O	1.6928	1.5903	-1.7942
O	-2.2493	2.2431	0.4531
O	-0.7412	4.3545	0.3286
O	-0.9299	2.7041	-1.8108
Si	1.6090	-1.6610	-0.3276
Si	4.2341	2.7767	-0.2751
Al	2.6616	2.8533	-2.8718
Al	0.0657	1.3979	-3.0220
Si	-3.5306	1.4125	-0.1805
Si	-0.9054	5.8501	-0.1278
Al	-2.4943	2.8894	-2.8846
O	0.2815	-2.2304	0.4132
O	2.8291	-2.5750	0.3520
O	1.6011	-1.7694	-1.8506
O	5.4543	1.8625	0.4044
O	4.4148	4.3184	0.3414
O	4.2261	2.6681	-1.7981
O	3.6428	1.6237	-3.8680
O	2.0549	4.3472	-1.8934
O	1.1067	2.6752	-3.8636
O	3.2946	4.3467	-3.9265
O	-0.5703	-0.0904	-1.9460
O	0.6694	-0.0910	-3.9789
O	-1.5132	1.6597	-3.8808
O	-3.3662	-0.0831	0.2761
O	-4.8576	1.9345	0.3789
O	-3.4632	1.6263	-1.8070
O	0.3758	6.6808	0.5055
O	-2.2325	6.3721	0.4314
O	-0.8380	6.0638	-1.7545
O	-3.1010	4.3833	-1.9062
O	-4.0494	2.7112	-3.8764
O	-1.8615	4.3827	-3.9394
Si	-0.9998	-3.0609	-0.2202
Si	4.1562	-3.0970	-0.2074
Mg	0.0364	-1.5842	-2.9243
Si	6.7814	1.3405	-0.1549
Si	4.2506	5.8140	-0.1151
Al	5.2217	1.3618	-3.0093
Al	2.6909	5.8354	-2.9696
Si	-3.5469	-1.6249	-0.3404
Si	-6.0778	2.8486	-0.3006
Si	1.7034	7.2502	-0.2355
Si	-3.4526	7.2862	-0.2482
Al	0.1307	7.3270	-2.8321
Al	-2.4651	5.8715	-2.9824
Al	-5.0903	1.4340	-3.0348
O	-0.8355	-4.5567	0.2364
O	-2.3268	-2.5390	0.3391
O	-0.9323	-2.8473	-1.8468
O	4.3206	-4.5927	0.2492
O	5.4375	-2.2664	0.4260
O	4.2237	-2.8833	-1.8340
O	1.0176	-2.8138	-3.9206
O	-1.5185	-1.7623	-3.9162
O	6.9457	-0.1551	0.3017
O	8.0626	2.1712	0.4786
O	6.8487	1.5542	-1.7815
O	5.5318	6.6448	0.5183
O	2.9235	6.3361	0.4441
O	4.3180	6.0277	-1.7417
O	4.5857	-0.1263	-1.9332
O	5.8254	-0.1269	-3.9662
O	6.2627	2.6392	-3.8508
O	1.1119	6.0973	-3.8283
O	3.7318	7.1127	-3.8111
O	-4.8745	-2.1944	0.4004
O	-3.5550	-1.7334	-1.8633
O	-7.4054	2.2792	0.4403
O	-5.8971	4.3905	0.3159
O	-6.0858	2.7402	-1.8236
O	1.8840	8.7920	0.3812
O	1.6953	7.1417	-1.7584
O	-4.7802	6.7167	0.4927
O	-3.2720	8.8280	0.3684
O	-3.4607	7.1777	-1.7711
O	-0.4760	8.8207	-1.8538
O	-1.4241	7.1487	-3.8239
O	0.7638	8.8202	-3.8867
O	-4.0441	6.1333	-3.8410
O	-5.7262	-0.0543	-1.9588
O	-4.4866	-0.0550	-3.9918
O	-6.6691	1.6958	-3.8935
Si	-1.0161	-6.0985	-0.3802
Si	4.1400	-6.1345	-0.3674
Si	6.7651	-1.6969	-0.3149
Al	5.1924	-1.6202	-2.9116
Al	2.5966	-3.0756	-3.0618

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Si -6.0615  5.8861 -0.1406
Al -7.6505  2.9254 -2.8974
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Si -3.4363 10.3237 -0.0882
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Al  0.1600 10.3091 -2.9298
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Mg 12.9736  2.7814 -2.8464
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Al -0.0578 -10.4953 -3.0166
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Structure **ts15d-*anti*-II-*Si*-V supported onto clay**
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E+ZPE(ONIOM(M05-2X:UFF)= -2737.405779
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C -6.4480 0.7355 3.8338
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H -6.5271 0.1371 4.7484
H -6.3006 0.0950 2.9588
C -4.1442 1.1425 4.3713
C -3.0185 2.0970 4.3861
O -4.0222 -0.0304 4.6817
Cu -1.3600 1.4441 3.6930
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N -0.0363 2.9287 3.9894
C -0.5065 -1.3287 3.5786
C 1.3548 0.1244 3.5813
C 1.2229 2.6381 3.6749
C -0.1687 4.4311 3.9675
C -1.9772 -1.5344 3.6302
C 0.3341 -2.4492 3.5219
N 1.9270 1.4315 3.5973
C 2.2367 -0.9813 3.5200
O 2.0226 3.7300 3.3284
C 1.1116 4.8835 3.2150
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C 3.4072 1.5513 3.4040
H 3.3195 -0.8554 3.4960
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Si  2.9875 -9.7621 -0.8436
Al  1.3115 -9.7904 -3.3758
Al 10.3548  0.4373 -3.1595
Al  8.3856 -4.3240 -3.3528
```

```
Mg  6.4164 -9.0854 -3.5461
Mg 12.3239  5.1988 -2.9663
Mg  9.1881  9.2552 -2.6026
Mg -11.2314  6.4354 -1.9216
Mg -13.2006  1.6739 -2.1148
Si -10.7658 -4.1182  0.1792
Al -10.0648 -2.3825 -2.4784
Si -7.6302 -8.1746 -0.1843
Al -6.9291 -6.4389 -2.8420
H -0.9152 -11.1365 -0.1561
H -3.2048 -11.1811  0.0113
O -2.1743 -10.5040 -2.1987
O -4.5639 -9.1519 -2.1293
O -5.8264 -7.4665 -3.9352
O -3.4237 -8.8788 -4.2019
H  4.1896 -10.4316 -0.3263
H  1.9001 -10.4762 -0.1589
O  2.9305 -9.7990 -2.3690
O 11.9737  0.4287 -2.1525
O 11.4574 -0.5903 -4.2527
O 10.0046 -4.3327 -2.3459
O  9.4882 -5.3516 -4.4460
H -12.0737 -3.8314  0.7859
H -10.3976 -5.4984  0.5263
O -10.7983 -3.8210 -1.4352
O -11.6192 -2.7355 -3.4229
H -7.2619 -9.5548  0.1627
H -8.9380 -7.8877  0.4224
O -7.6625 -7.8774 -1.7988
O -8.4836 -6.7919 -3.7865
Al -3.7934 -10.4953 -3.2055
Mg 13.0924 -0.6625 -3.4650
Mg 11.1232 -5.4239 -3.6583
Mg -12.4320 -4.1873 -2.6136
Mg -9.2963 -8.2437 -2.9772

Structure ts15d-Syn-II-Si-V supported onto clay
E(ONIOM(M05-2X:UFF)= -2737.821581
E+ZPE(ONIOM(M05-2X:UFF)= -2737.403525
Lowest freq (cm-1) ONIOM(PM6/UFF): -59.4
H -2.3585  2.7968  4.8545
C -1.4070  2.4034  5.2335
O -1.5950  0.9546  5.1588
H -0.5596  2.7326  4.6193
H -1.2523  2.6460  6.2894
C -0.5286  0.2041  4.7644
C -0.8271 -1.2466  4.7432
O  0.5519  0.6759  4.4653
Cu  0.2770 -2.5284  5.5367
H -1.4935 -1.5156  3.9168
N  2.1202 -3.2493  5.4226
N -0.5855 -4.3020  6.0658
C  3.1079 -2.4756  4.8352
C  2.4487 -4.5726  5.6815
C  0.2248 -5.1848  6.6426
C -1.9921 -4.7499  6.3553
C  2.8580 -1.0172  4.6946
C  4.3314 -3.0169  4.4099
N  1.6048 -5.3413  6.5425
C  3.6247 -5.1771  5.1893
O -0.3764 -6.0997  7.5041
C -1.8140 -5.7443  7.5353
C -2.6863 -5.4288  5.1180
H -2.5850 -3.8468  6.6612
H  2.0362 -0.7601  4.0049
H  3.7344 -0.4772  4.2919
H  2.6265 -0.5249  5.6557
C  4.5687 -4.3848  4.5389
H  5.0940 -2.3673  3.9752
C  2.2239 -6.4345  7.3492
H  3.8012 -6.2475  5.3050
H -2.3357 -6.7087  7.4244
H -1.9937 -5.3094  8.5299
C -4.1418 -5.7421  5.5004
C -2.6753 -4.4523  3.9352
C -1.9603 -6.7204  4.7151
H  5.4883 -4.8299  4.1446
H  2.2910 -7.3691  6.7637
H  1.6099 -6.6436  8.2505
H  3.2299 -6.1411  7.6978
H -4.6887 -4.8560  5.8387
H -4.2194 -6.5022  6.2846
H -4.6947 -6.1368  4.6353
H -3.2940 -3.5655  4.1246
H -1.6558 -4.1307  3.7066
H -3.0647 -4.9284  3.0276
H -2.5355 -7.2765  3.9648
H -0.9761 -6.5173  4.2800
H -1.8135 -7.4083  5.5547
H -2.8059 -2.2369  6.6599
C -3.0626 -1.3004  6.1676
H -2.7509 -0.4184  6.7193
C -3.7643 -1.2401  5.0387
H -4.0629 -0.3086  4.5684
H -4.1086 -2.1249  4.5052
O  0.0449  2.2595  1.8511
Si  1.4078  1.9606  1.2189
Si -1.3201  3.0196  1.2638
O  1.8017  0.4842  1.5902
O  2.5840  2.9361  1.8497
O  1.3754  2.2579 -0.3956
O -1.3341  4.5407  1.9537
O -2.5209  2.2310  2.0200
O -1.3771  2.9827 -0.2615
Si  1.8156 -1.0369  0.9003
Si  3.7847  3.7246  1.0935
Al -0.2584  1.8915 -1.5739
Al  2.1088  3.6963 -1.4387
Si -1.7279  6.0170  1.5825
Si -3.6971  1.2555  1.3891
Al -2.9960  2.9914 -1.2684
O  0.6148 -1.8254  1.6563
O  3.1806 -1.7969  1.4876
O  1.7587 -1.0737 -0.6251
O  5.1498  2.9644  1.6808
O  3.7708  5.2456  1.7834
O  3.7278  3.6877 -0.4318
O -0.6309  0.2784 -0.5558
O -1.8934  1.9637 -2.3617
O  0.5093  0.5515 -2.6283
O  0.5544  3.3433 -2.3832
O  1.3383  5.0398 -0.3625
O  2.4785  5.3130 -2.4351
O  3.2115  2.6687 -2.5320
O -0.5518  6.9925  2.2132
O -3.0907  6.3159  2.2147
O -1.7603  6.3143 -0.0320
O -5.0599  1.5545  2.0214
O -3.3031 -0.2207  1.7604
O -3.7295  1.5529 -0.2253
O -3.7665  4.3349 -0.1922
O -2.6265  4.6080 -2.2649
O -4.5506  2.6383 -2.2130
Si -0.5614 -2.8008  1.0256
Si  4.5435 -2.0959  0.8553
Al  2.8773 -2.1649 -1.9375
Mg  0.1396 -1.0651 -1.6320
Si  6.5127  2.6655  1.0486
Si  3.3770  6.7219  1.4122
Al  4.8465  2.5964 -1.7442
Al  1.7108  6.6529 -1.3807
Si  0.6491  7.7810  1.4570
Si -4.4558  7.0760  1.6273
Al -1.0269  7.7528 -1.0752
Al -3.3941  5.9480 -1.2104
Si -6.4250  2.3146  1.4341
Si -3.2892 -1.7418  1.0705
Al -5.3633  1.1866 -1.4036
O -0.1675 -4.2772  1.3969
O -1.9242 -2.5019  1.6578
O -0.5937 -2.5035 -0.5889
O  5.7196 -1.1204  1.4861
```

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O  4.9375 -3.5722  1.2266
O  4.5111 -1.7986 -0.7592
O  1.2423 -2.0927 -2.7253
O  2.5049 -3.7780 -0.9194
O  3.6901 -0.7131 -2.7469
O  3.6451 -3.5049 -2.9920
O -1.4148 -1.4181 -2.5766
O  6.9066  1.1893  1.4199
O  7.6888  3.6410  1.6794
O  6.4802  2.9628 -0.5659
O  4.5531  7.6975  2.0430
O  2.0141  7.0209  2.0443
O  3.3446  7.0192 -0.2023
O  4.4740  0.9834 -0.7261
O  5.6593  4.0483 -2.5535
O  5.6142  1.2565 -2.7986
O  0.0757  6.7251 -2.1684
O  2.5235  8.1046 -2.1900
O  0.5921  7.7441 -0.0683
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O -4.5128  7.0392  0.1020
O -5.6567  6.2875  2.3835
O -4.4697  8.5971  2.3173
O -2.5813  7.3997 -2.0197
O -0.6572  9.3694 -2.0715
O -1.7974  9.0962  0.0010
O -5.0291  6.0201 -1.9981
O -7.6259  1.5261  2.1903
O -6.4389  3.8358  2.1240
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O -6.9982  1.2588 -2.1914
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Si -0.1536 -5.7983  0.7069
Al -2.2276 -2.8699 -1.7673
Si  6.9205 -0.3318  0.7299
Si  4.9514 -5.0933  0.5366
Al  5.2445 -0.3601 -1.8023
Al  3.2754 -5.1215 -1.9956
Si  8.8897  4.4295  0.9232
Al  7.2137  4.4013 -1.6091
Si  5.7539  8.4860  1.2868
Al  4.0779  8.4577 -1.2454
Si  0.2412 10.7784  1.7758
Al -6.1318  7.0478 -0.9049
Si -6.8328  5.3120  1.7528
Si -4.8636 10.0734  1.9460
Al -1.4250 10.7094 -1.0171
Si -8.8019  0.5506  1.5594
Al -8.1010  2.2864 -1.0982
Si -5.6663 -3.5058  1.1958
Al -4.9652 -1.7700 -1.4618
O -1.3544 -6.5868  1.4631
O  1.2115 -6.5583  1.2942
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O -2.6000 -4.4830 -0.7492
O -3.8626 -2.7977 -2.5551
O -1.4598 -4.2099 -2.8217
O  8.2855 -1.0920  1.3173
O  6.8636 -0.3688 -0.7954
O  3.7505 -5.8818  1.2928
O  6.3164 -5.8534  1.1239
O  4.8943 -5.1301 -0.9887
O  6.3472 -1.3877 -2.8955
O  2.5419 -6.5600 -0.9525
O  4.3781 -6.1491 -3.0889
O  1.7209 -5.4745 -2.9402
H 10.0918  3.7601  1.4405
H  8.8774  5.7682  1.5304
O  8.8327  4.3927 -0.6021
O  8.3164  3.3736 -2.7023
O  6.4432  5.7447 -0.5328
O  7.5834  6.0179 -2.6054
H  5.7417  9.8246  1.8940
H  6.9560  7.8165  1.8041
O  5.6970  8.4491 -0.2386
O  3.3074  9.8012 -0.1692
O  4.4476 10.0744 -2.2418
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O  0.2088 11.0757  0.1613
H  1.2871 11.6458  2.3367
H -1.0667 11.0653  2.3825
O -7.6862  6.6948 -1.8494
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O -6.9023  8.3912  0.1713
O -6.8653  5.6093  0.1382
O -8.1957  5.6109  2.3850
O -4.8960 10.3707  0.3315
H -6.1715 10.3603  2.5527
H -3.8178 10.9409  2.5070
O -10.1648  0.8496  2.1917
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O -8.8344  0.8480 -0.0550
O -9.6554  1.9334 -2.0427
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Si  9.6483 -1.3909  0.6851
Al  7.9822 -1.4599 -2.1078
Si  7.6792 -6.1523  0.4917
Al  6.0131 -6.2213 -2.3011
Al  9.9514  3.3015 -1.9146
Al  6.8156  7.3579 -1.5510
Mg  3.6800 11.4143 -1.1873
Al -8.4990  5.2430 -1.0401
Al -6.5299 10.0044 -0.8468
Si -9.5607  6.3711  1.7976
Si -11.5299  1.6097  1.6044
Si -8.3941 -2.4468  1.2408
Al -10.4682  0.4816 -1.2334
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Al -7.3324 -3.5748 -1.5970
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O -2.5629 -7.2649 -0.7822
O  2.9683 -8.3336  1.0333
O -0.7268 -6.8541 -2.9186
O -3.3840 -6.1794 -2.7699
O  0.5357 -8.5394 -1.1126
O  1.6759 -8.2662 -3.1853
H 10.6942 -0.5235  1.2460
H 10.0166 -2.7711  1.0321
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O  8.7950 -0.0081 -2.9171
O  8.7499 -2.8000 -3.1623
H  8.0474 -7.5325  0.8388
H  8.7251 -5.2849  1.0526
O  7.6468 -5.8550 -1.1228
O  5.6405 -7.8344 -1.2830
O  6.8258 -4.7696 -3.1105
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O 11.5852  3.6677 -0.7362
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O 10.7190  1.9614 -2.9689
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O -11.5868  1.5728  0.0790
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H -12.6172  0.8957  2.2891
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O -8.9674 -3.5026 -2.3848
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Al -4.1968 -7.6313 -1.9606
Si  2.9822 -9.8546  0.3433
Al  1.3062 -9.8829 -2.1889
Al 10.3495  0.3448 -1.9726
Al  8.3803 -4.4165 -2.1659
Mg  6.4111 -9.1779 -2.3592
Mg 12.3186  5.1063 -1.7794
Mg  9.1828  9.1627 -1.4157
Mg -11.2367  6.3429 -0.7347
Mg -13.2059  1.5814 -0.9279
Si -10.7711 -4.2107  1.3661
Al -10.0701 -2.4750 -1.2915
Si -7.6355 -8.2671  1.0026
Al -6.9344 -6.5314 -1.6551
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H -3.2101 -11.2736  1.1982
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O -5.8317 -7.5590 -2.7483
O -3.4290 -8.9713 -3.0150
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H  1.8948 -10.5687  1.0280
O  2.9252 -9.8915 -1.1821
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O 11.4521 -0.6828 -3.0658
O  9.9993 -4.4252 -1.1590
O  9.4829 -5.4441 -3.2591
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H -7.2672 -9.6473  1.3496
H -8.9433 -7.9802  1.6093
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O -8.4889 -6.8844 -2.5996
Al -3.7987 -10.5878 -2.0186
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Mg 11.1179 -5.5164 -2.4714
Mg -12.4373 -4.2798 -1.4267
Mg -9.3016 -8.3362 -1.7903
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