

Reactivities of phosphalkynes towards diverse bis-silylenes

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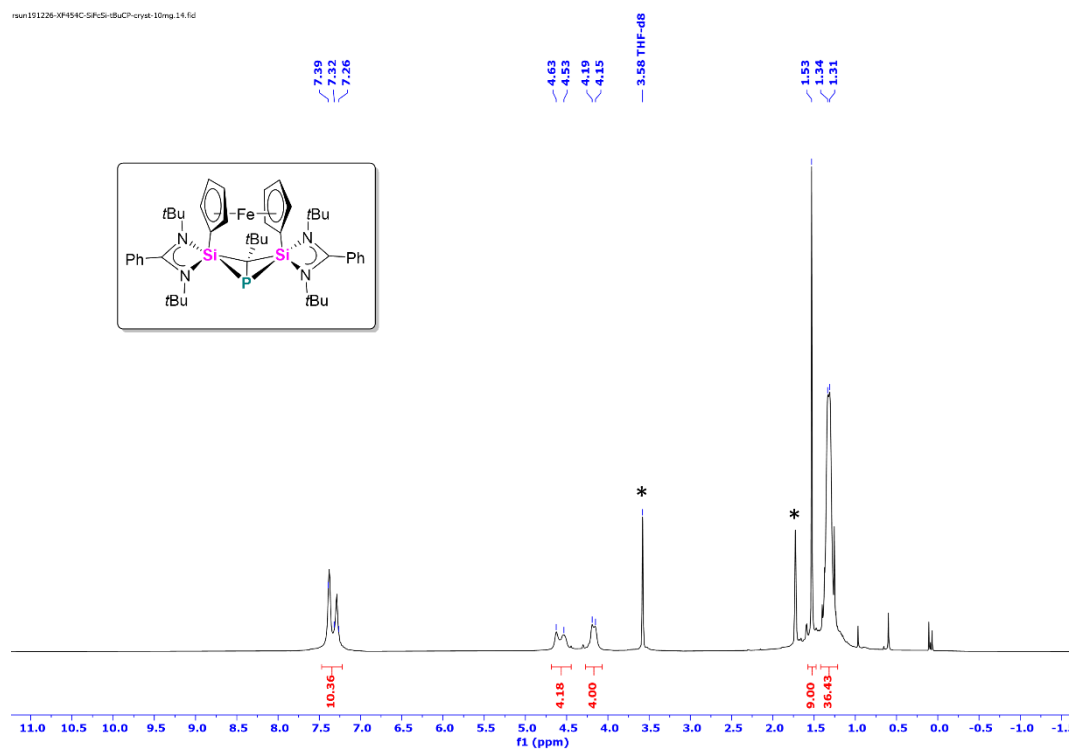
[b] Institute for Nanotechnology, Karlsruhe Institute of Technology (KIT), Kaiserstr. 12, 76131, Karlsruhe, Germany..

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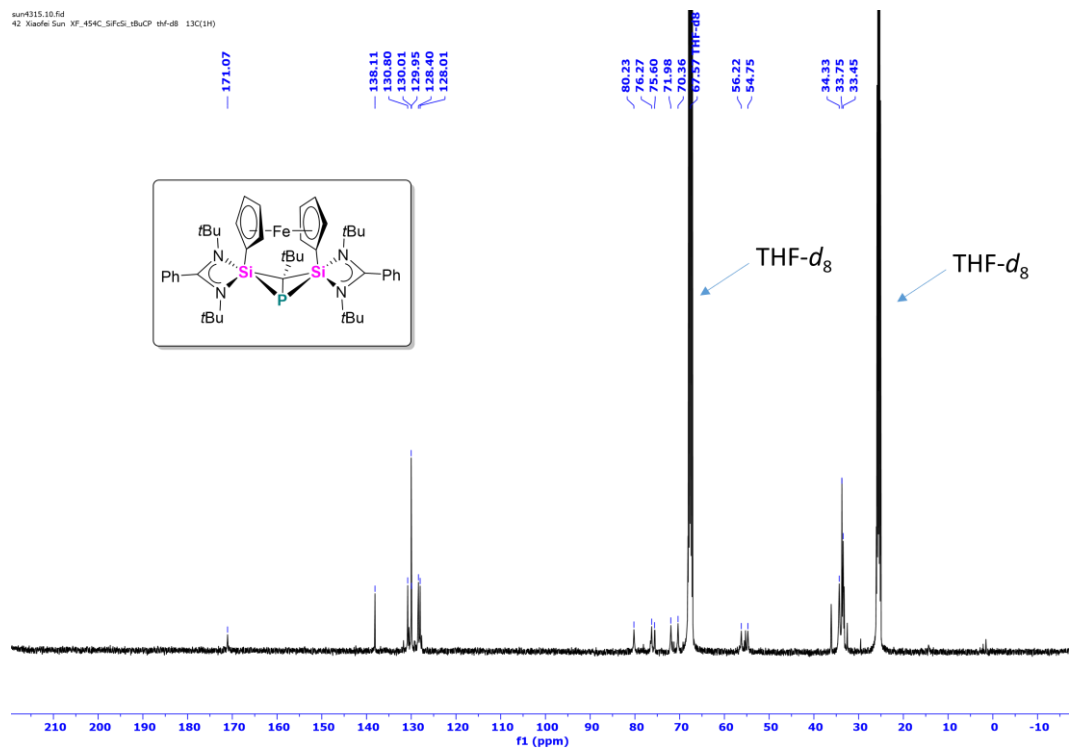
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I. NMR spectra

rsun191226_XF454C_SiFeSi_tBuCP-cryst-10mg-1.4.fid



sun4315_10.fid
42 Xiaofei Sun_XF_454C_SiFeSi_tBuCP_ThF-d8_13C(1H)



-76.09
-76.65

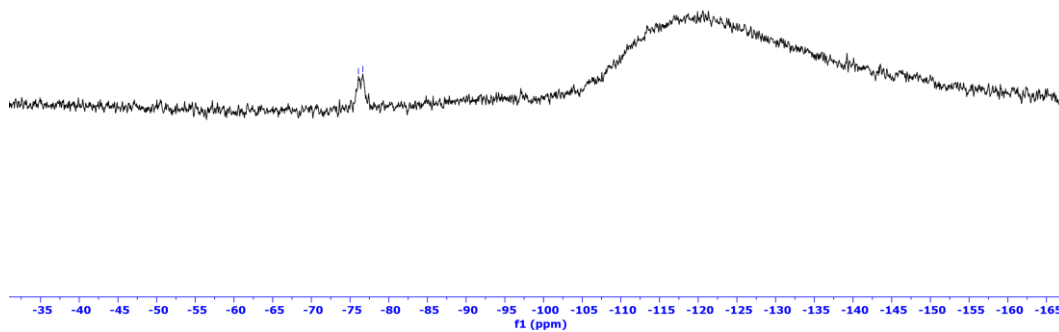
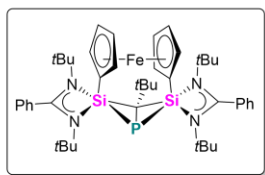


Figure S3. $^{29}\text{Si}\{^1\text{H}\}$ NMR spectrum of **1** in $\text{THF-}d_8$.

-294.19

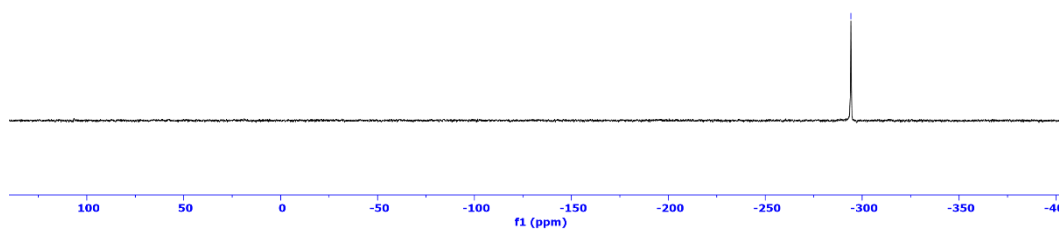
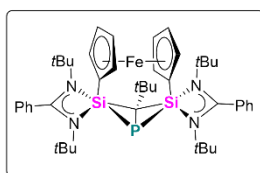


Figure S4. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of **1** in $\text{THF-}d_8$.

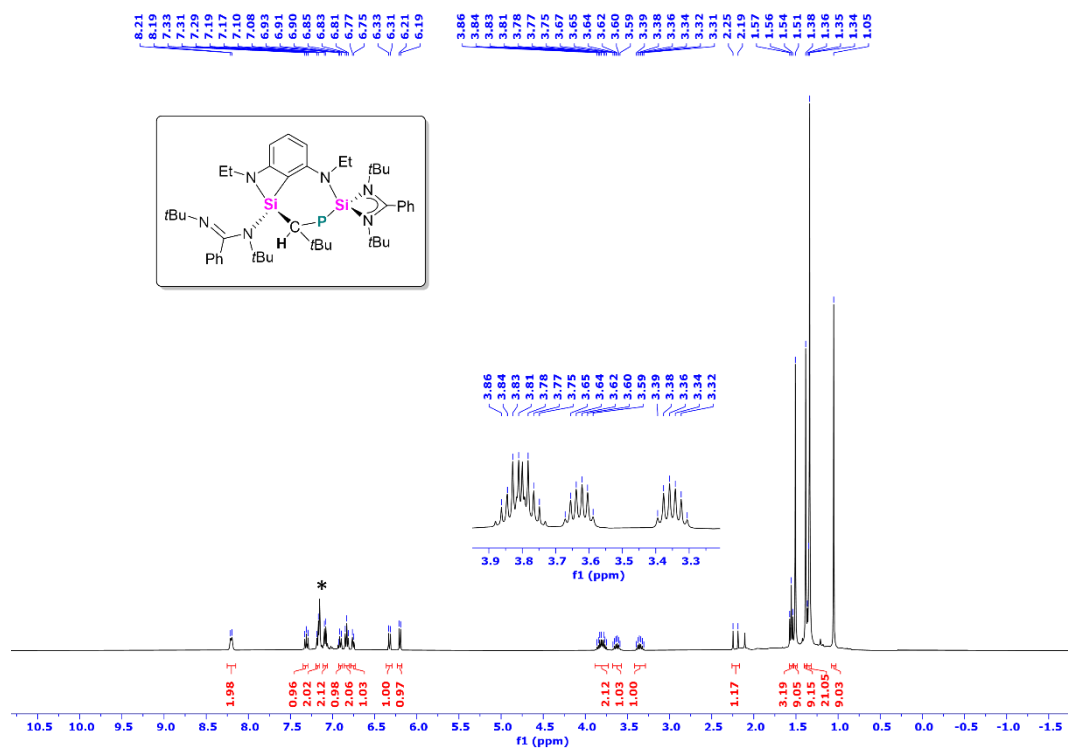


Figure S5. ^1H NMR spectrum of **2** in C_6D_6 . *, residual protio solvent signal.

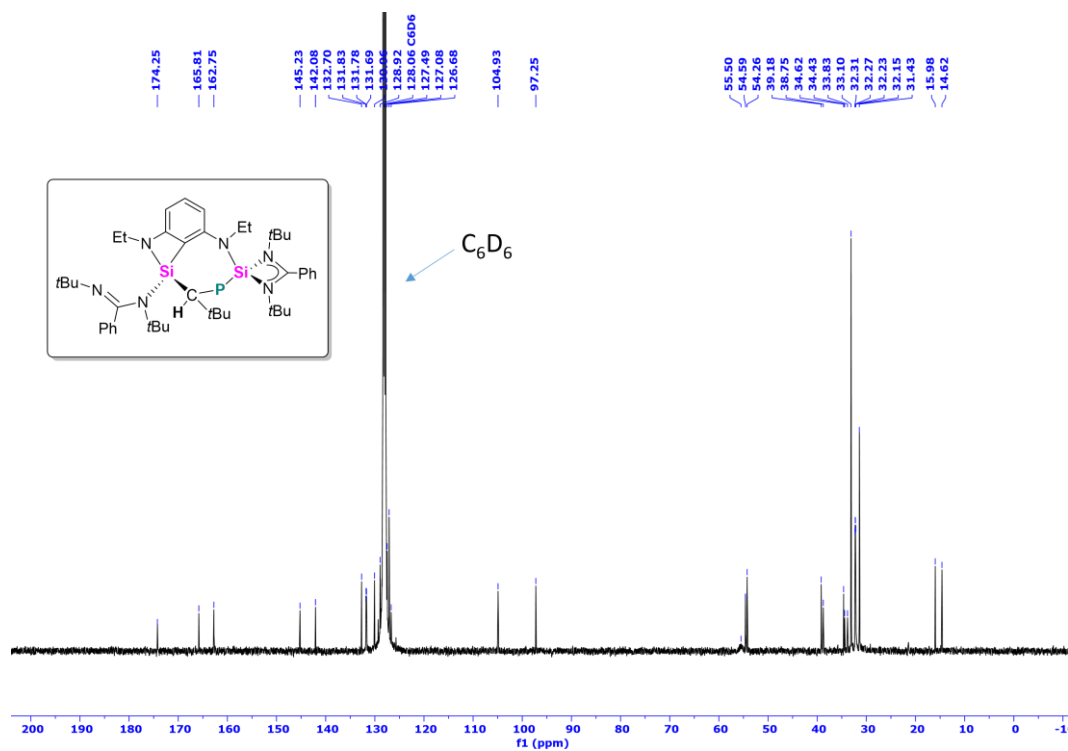


Figure S6. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **2** in C_6D_6 .

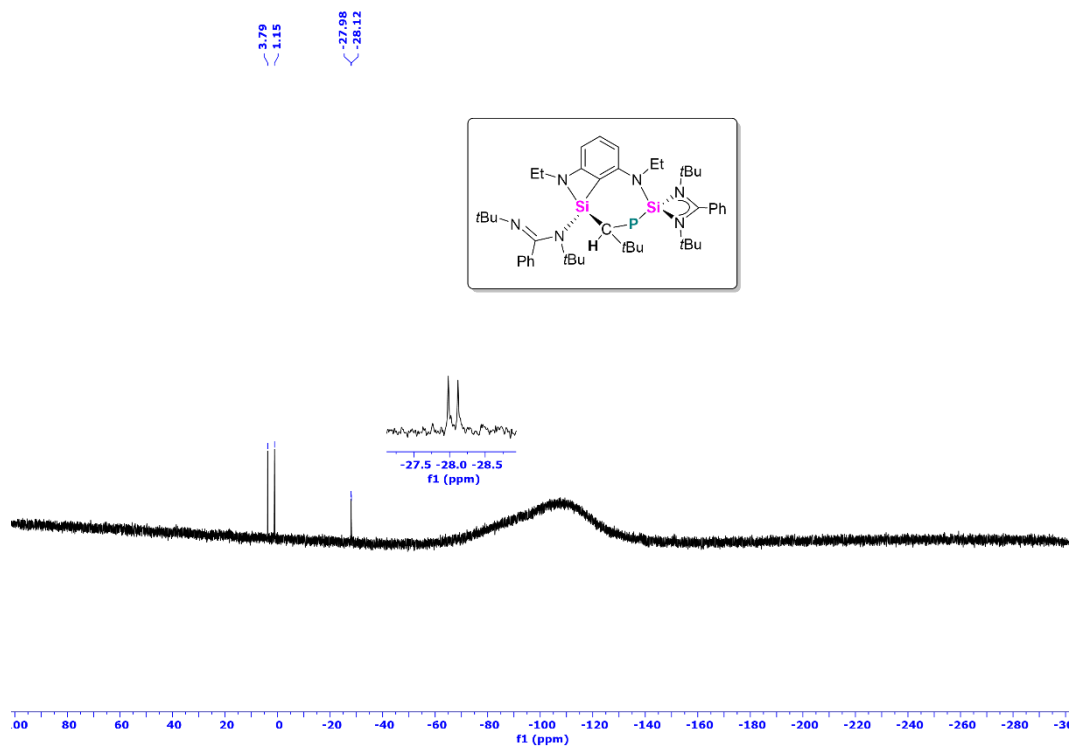


Figure S7. $^{29}\text{Si}\{^1\text{H}\}$ NMR spectrum of **2** in C_6D_6 .

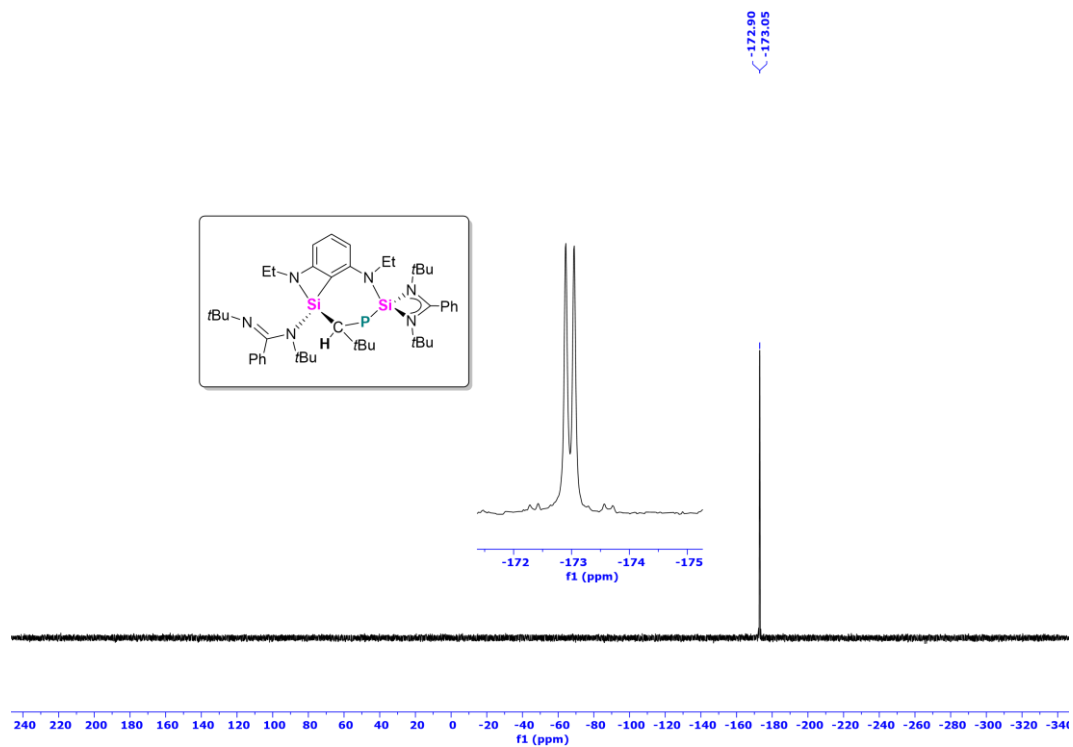


Figure S8. ^{31}P NMR spectrum of **2** in C_6D_6 .

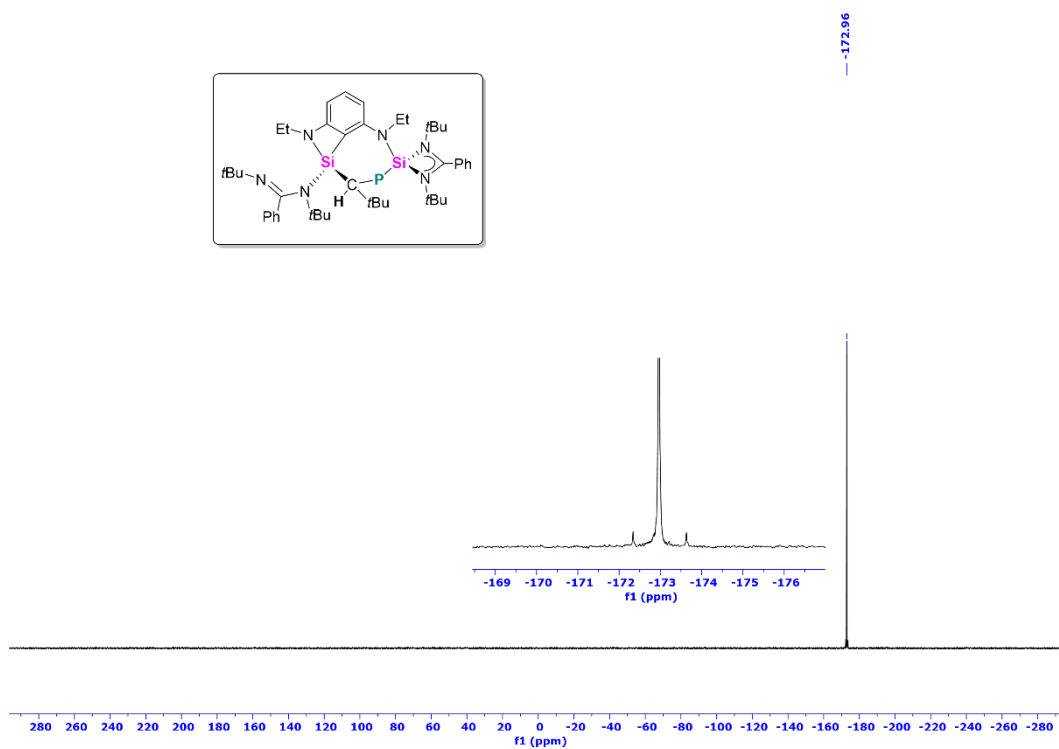


Figure S9. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of **2** in C_6D_6 .

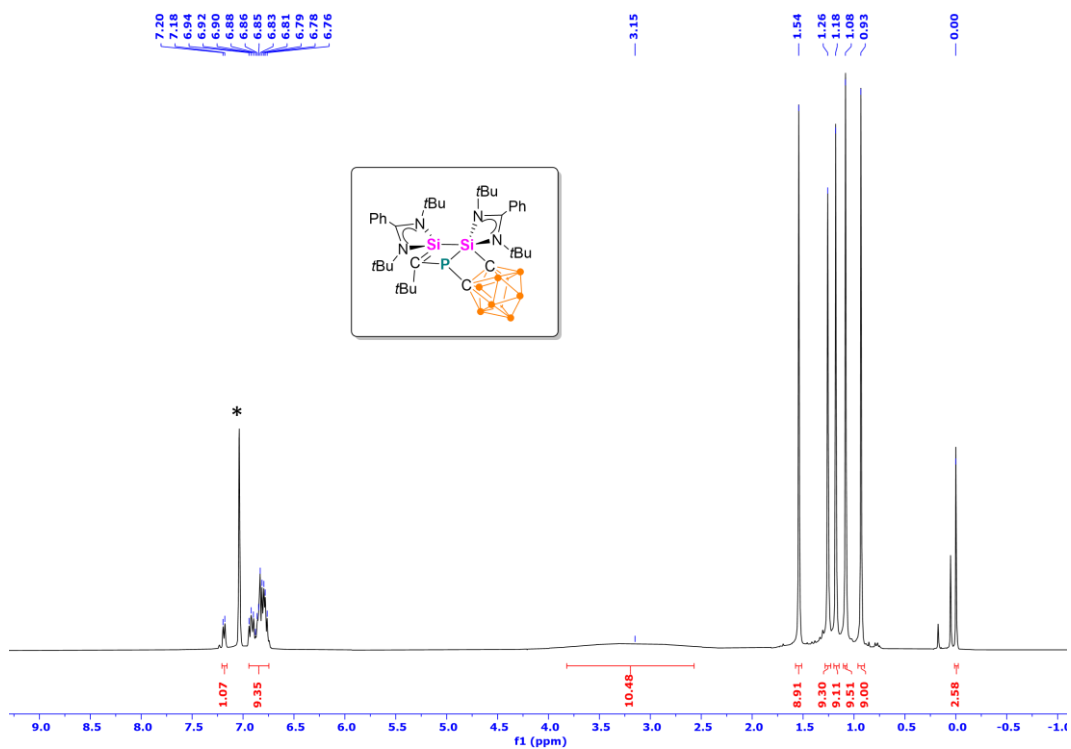


Figure S10. ^1H NMR spectrum of **3** in C_6D_6 . *, residual protio solvent signal.

run0729_20.fid
04 Xiaofei Sun SBiSiBuCP-cryst 11B(1H)

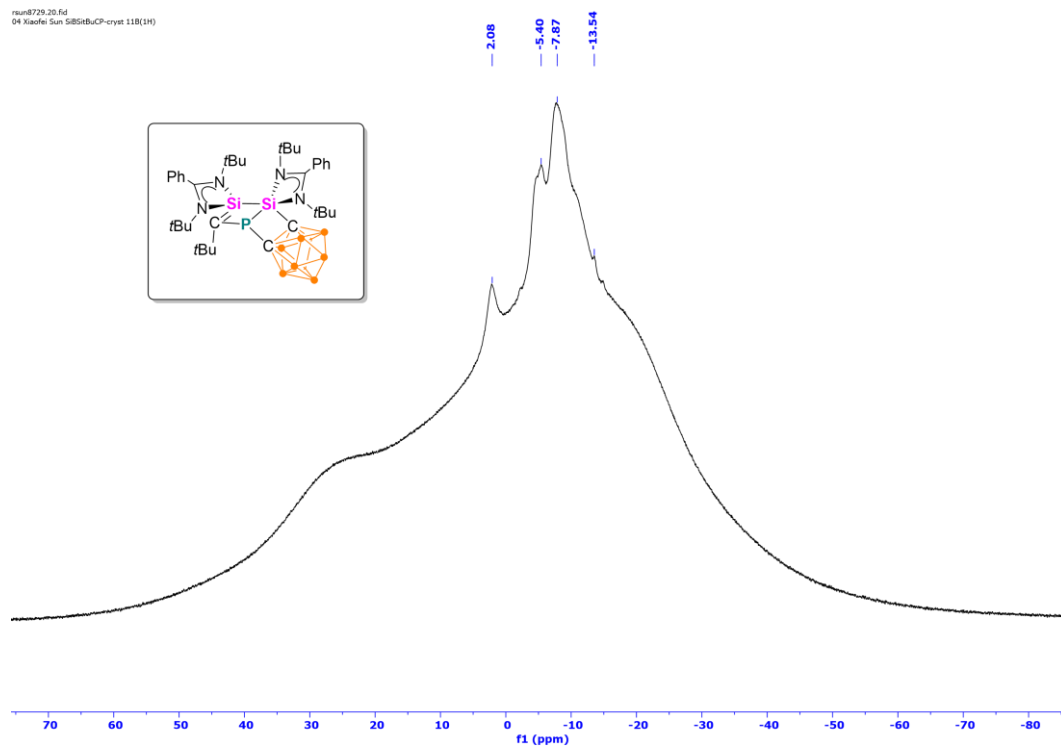


Figure S11. $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of **3** in C_6D_6 .

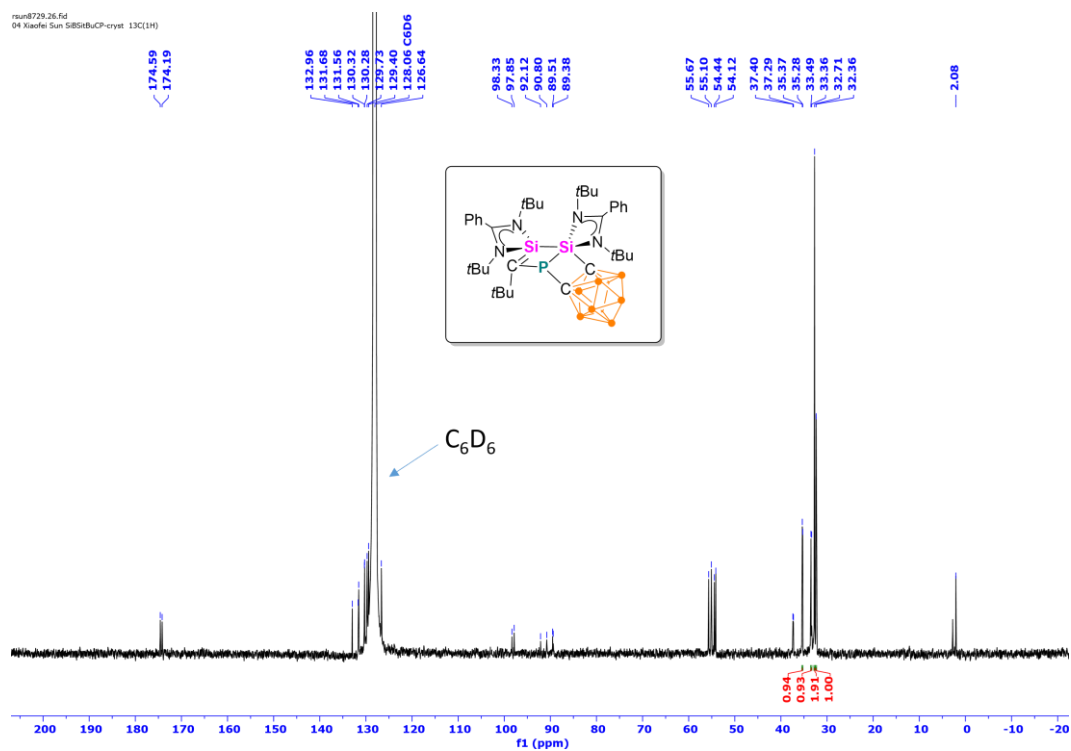


Figure S12. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **3** in C_6D_6 .

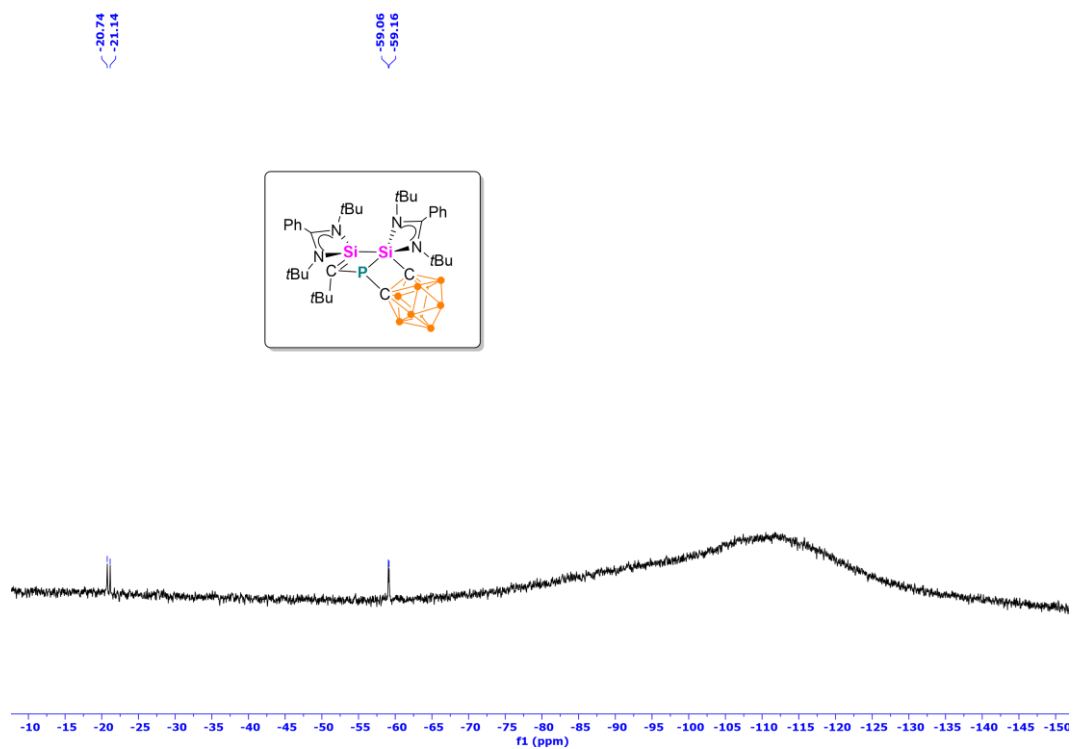


Figure S13. $^{29}\text{Si}\{^1\text{H}\}$ NMR spectrum of **3** in C_6D_6 .

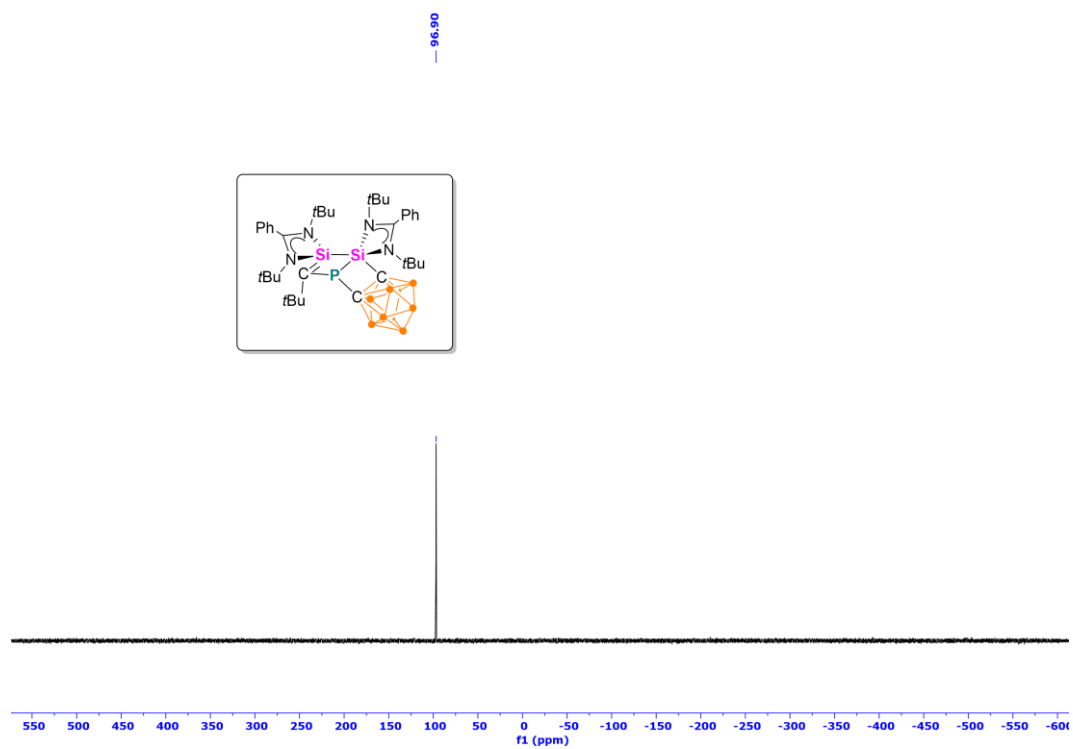


Figure S14. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of **3** in C_6D_6 .

II. IR spectra

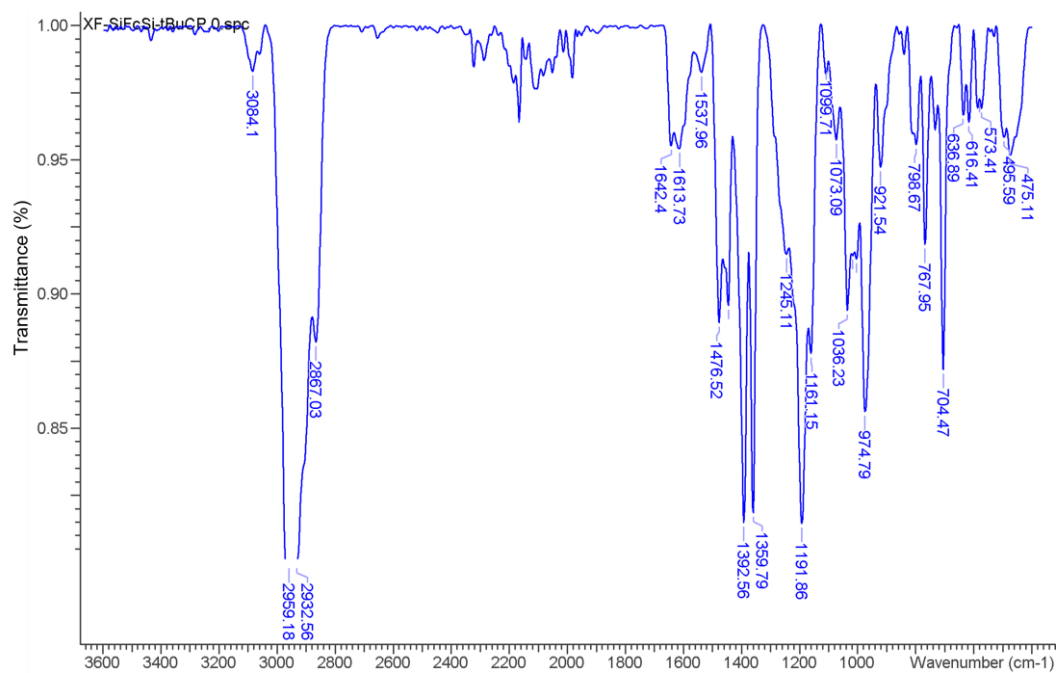


Figure S15. IR spectrum of compound 1.

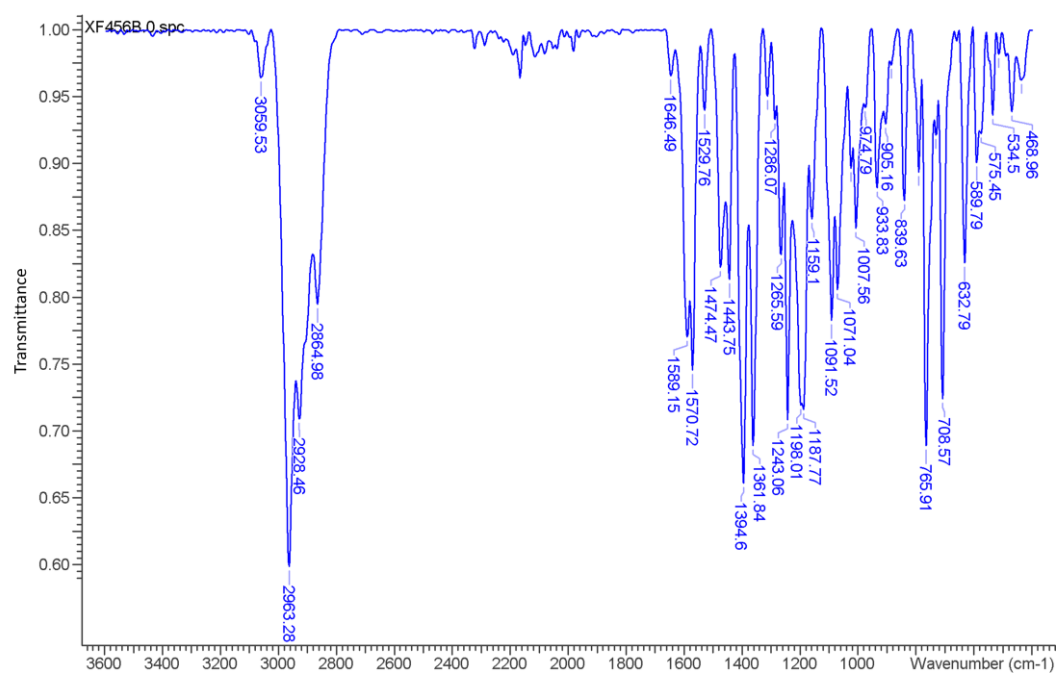


Figure S16. IR spectrum of compound 2.

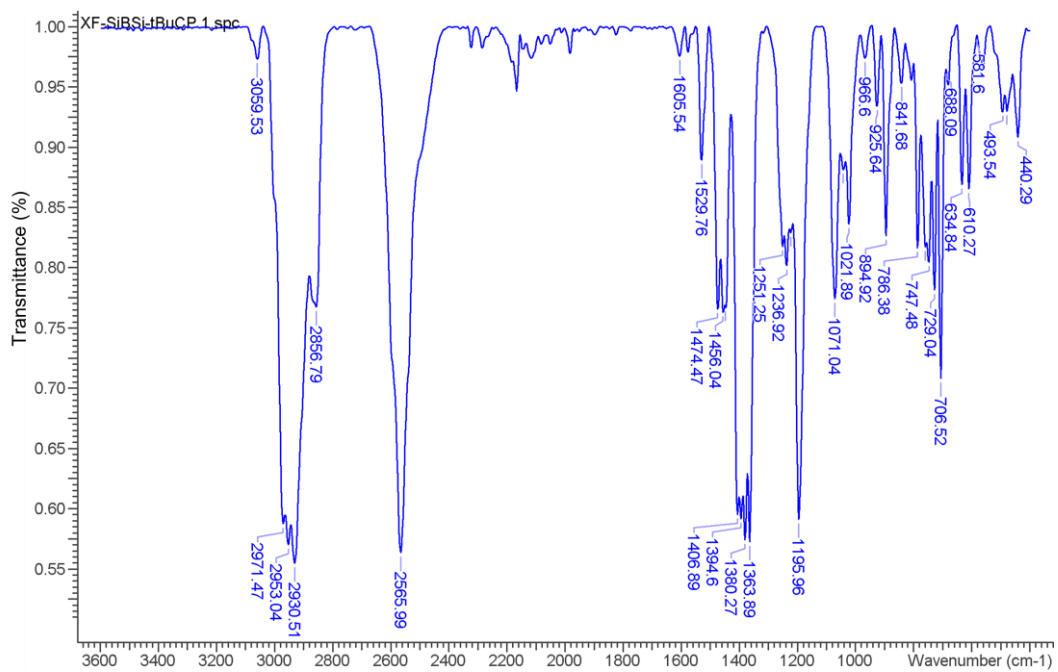


Figure S17. IR spectrum of compound 3.

III. X-ray crystallography

III.1 General methods

Suitable crystals for the X-ray analysis of all compounds were obtained as described above. A suitable crystal was covered in mineral oil (Aldrich) and mounted on a glass fibre. The crystal was transferred directly to the cold stream of a STOE StadiVari (100 K or 110 K) diffractometer. All structures were solved by using the program SHELXS/T^[1,2] and Olex2.^[3] The remaining non-hydrogen atoms were located from successive difference Fourier map calculations. The refinements were carried out by using full-matrix least-squares techniques on F_o^2 by using the program SHELXL.^[1,2] The H-atoms were introduced into the geometrically calculated positions (SHELXL procedures) unless otherwise stated and refined riding on the corresponding parent atoms. In each case, the locations of the largest peaks in the final difference Fourier map calculations, as well as the magnitude of the residual electron densities, were of no chemical significance. Specific comments for each data set are given below. Summary of the crystal data, data collection and refinement for compounds are given in Table S1.

Crystallographic data for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as a supplementary publication no. CCDC 2345640-2345642. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB21EZ, UK (fax: +(44)1223-336-033; email: deposit@ccdc.cam.ac.uk).

III.2 Summary of crystal data

Table S1. Crystal data, data collection and refinement for compounds **1-3**.

Compound	1	2	3
Chemical formula	C ₅₁ H ₅₇ FeN ₄ PSi ₂ (C ₆ D ₆)	C ₄₅ H ₆₉ N ₆ PSi ₂	C ₄₀ H ₇₁ B ₁₀ N ₄ P 0.5·(C ₆ H ₁₈ OSi ₂)
CCDC Number	2345640	2345641	2345642
$D_{calc.}/g\text{ cm}^{-3}$	1.279	1.141	1.158
m/mm^{-1}	0.454	0.150	0.166
Formula Weight	887.13	781.21	842.37
T/K	100	100	100
Crystal System	orthorhombic	triclinic	monoclinic
Space Group	<i>Pbca</i>	<i>P</i> $\bar{1}$	<i>P2</i> ₁ / <i>n</i>
$a/\text{Å}$	9.2620(4)	10.5917(5)	11.501(2)
$b/\text{Å}$	17.7607(6)	12.9028(6)	19.956(3)
$c/\text{Å}$	56.0109(19)	18.5962(9)	21.117(3)
$a/^\circ$	90	78.204(4)	90
$b/^\circ$	90	74.953(4)	94.297(11)
$g/^\circ$	90	69.055(4)	90
$V/\text{Å}^3$	9213.8(6)	2274.5(2)	4832.8(12)
Z	8	2	4
Z'	1	1	1
Wavelength/Å	0.71073	0.71073	0.71073
Radiation type	MoK α	MoK α	MoK α
$Q_{min}/^\circ$	2.316	3.015	1.934
$Q_{max}/^\circ$	26.000	25.499	25.250
Measured Refl's.	25451	28140	23166
Indep't Refl's	8869	8474	8735
Refl's $I \geq 2\sigma(I)$	6433	7312	5069
R_{int}	0.0360	0.0730	0.0817
Parameters	535	544	583
Restraints	0	106	58
Largest Peak	0.348	0.925	0.589
Deepest Hole	-0.421	-0.829	-0.936
Goof	1.024	1.043	1.012
wR_2 (all data)	0.1003	0.1957	0.2178
wR_2	0.0889	0.1848	0.1776
R_1 (all data)	0.0667	0.0771	0.1517
R_1	0.0399	0.0705	0.0803

III.3 Crystal structures

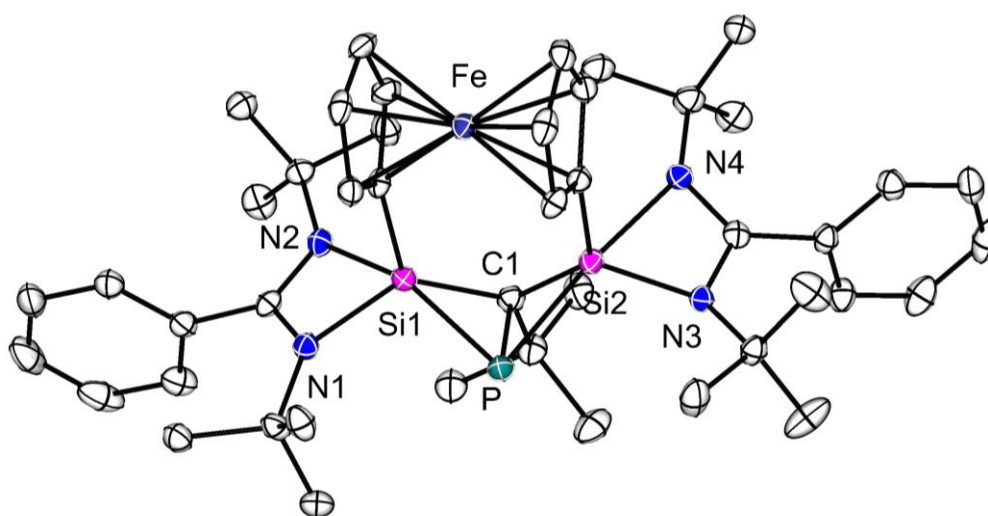


Figure S18. Molecular structure of the compound **1** in the solid state with thermal ellipsoids at 50% level. Hydrogen atoms and non-coordinating solvent molecules are omitted for clarity. Selected bond distances [Å] and angles [°]: P–C1 2.056(2), P–Si1 2.2716(9), P–Si2 2.2310(9), Si1–C1 1.867(2), Si2–C1 1.875(2), Si1–N1 1.858(2), Si1–N2 2.080(2), Si2–N3 1.817(2), Si2–N4 2.221(2); N1–Si1–N2 66.49(8), N3–Si2–N4 65.22(8), Si1–C1–Si2 105.07(11), Si1–P–Si2 82.54(3), Si1–C1–P 70.58(8), Si2–C1–P 68.97(8), Si1–P–C1 50.81(7), Si2–P–C1 51.68(7).

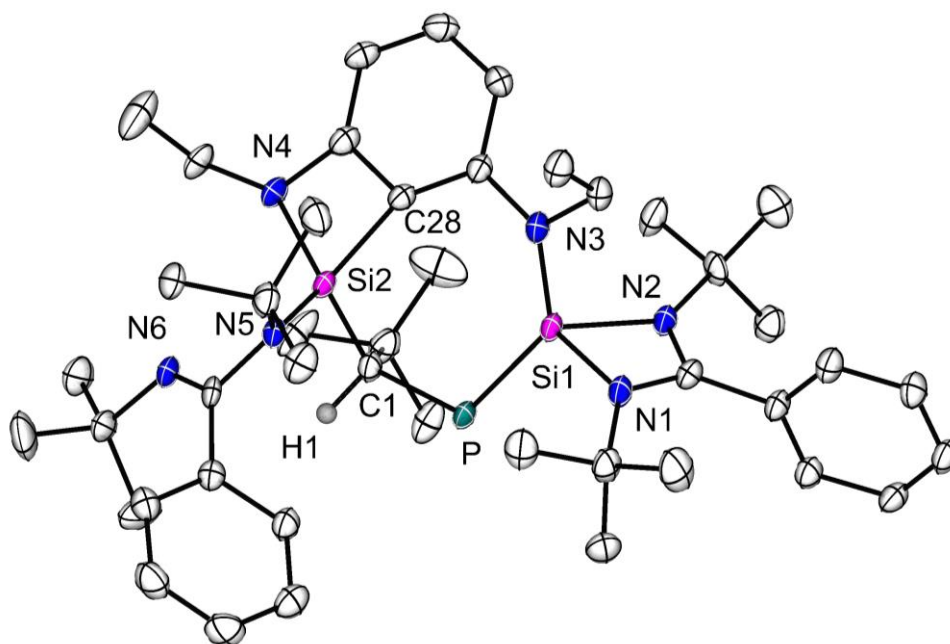


Figure S19. Molecular structure of the compound **2** in the solid state with thermal ellipsoids at 50% level. Hydrogen atoms are omitted for clarity. Selected bond distances [Å] and angles [°]: Si1–P 2.1322(8), Si1–N1 1.835(2), Si1–N2 1.889(2), Si1–N3 1.728(2), P–C1 1.897(2), Si2–C1 1.881(2), Si2–C28 1.855(2), Si2–N4 1.777(2), Si2–N5 1.748(2); N1–Si1–N2 70.42(8), Si1–P–C1 116.28(7), P–C1–Si2 106.15(10), N4–Si2–C28 75.40(9).

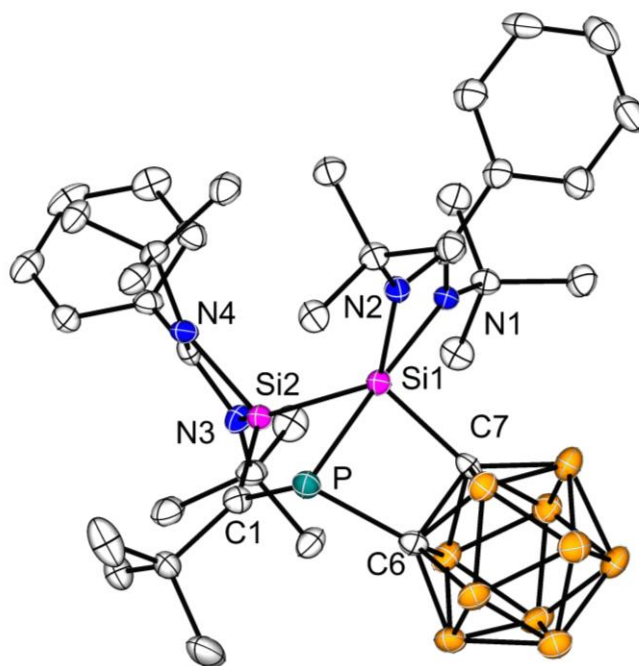


Figure S20. Molecular structure of the compound **3** in the solid state with thermal ellipsoids at 50% level. Hydrogen atoms and non-coordinating solvent molecules are omitted for clarity. Selected bond distances [Å] and angles [°]: Si1–Si2 2.352(2), Si2–C1 1.761(5), C1–P 1.780(5), P–Si1 2.343(2), P–C6 1.964(5), Si1–C7 1.969(5), Si1–N1 1.956(4), Si1–N2 1.857(4), Si2–N3 1.894(4), Si2–N4 1.884(4); N1–Si1–N2 68.7(2), N3–Si2–N4 69.2(2), Si1–P–C1 89.5(2), Si1–P–C6 79.93(14), Si1–Si2–C1 89.7(2), Si2–Si1–P 73.84(6), Si2–Si1–C7 118.53(14), Si2–C1–P 105.6(3), C1–P–C6 110.9(2), C7–Si1–P 80.64(14).

IV. Quantum chemical calculations

All computations were performed using Gaussian16^[4] utilizing the PBE0 level of theory, Def2SVP basis sets and empirical dispersion correction (GD3BJ). No solvent corrections were applied. All optimized molecular structures were checked to be minima on the energy hypersurface and possess no imaginary vibrational frequencies. The transition states possess exactly one imaginary frequency.

IV.1 Reaction pathway

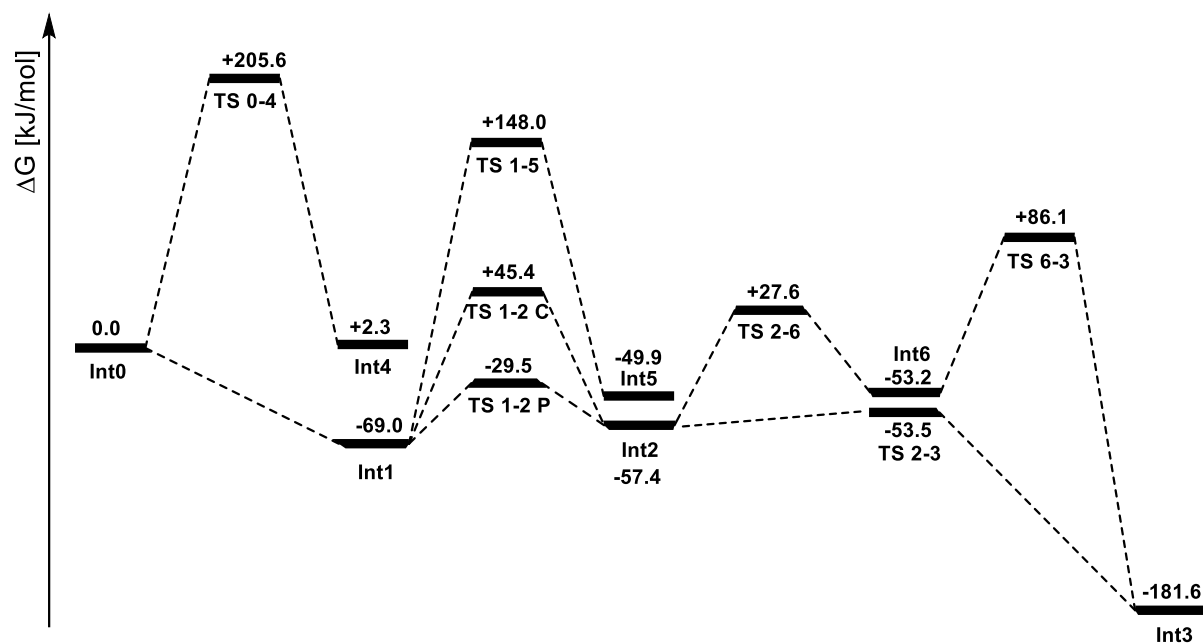


Figure S21. Computed reaction pathway for the reaction of [LSiSiL] and $t\text{BuC}\equiv\text{P}$.

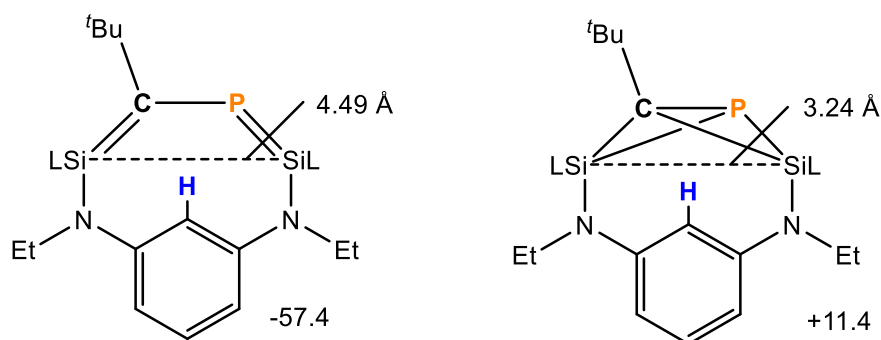


Figure S22. Computed isomers of Int2.

IV.2 Optimised Structures

IV.2 Int0

0 1

Si	-2.57600600	0.58375400	0.66372900
N	-3.39591000	-0.81868200	-0.38091900
N	-4.47786400	0.49729200	0.91162600
N	-2.47052700	1.90103800	-0.54033400
Si	2.35138600	0.29640400	0.32479000
C	-2.86068600	-1.93167000	-1.15855900
C	-4.56248500	-0.64842200	0.23524700
C	-5.39209800	1.15962800	1.83592900
C	-3.54559300	2.26509900	-1.44358200
C	-1.28789800	2.65592200	-0.60625400
N	2.36682600	1.96406400	-0.34701600
N	3.69016700	-0.54581100	-0.76656000
C	-0.05733900	2.00098300	-0.49732800
C	-1.44417700	-1.52042700	-1.56819500
C	-3.70129700	-2.16393700	-2.41667100
C	-2.78337500	-3.21441100	-0.32425400
C	-5.70950000	-1.59521200	0.24676600
C	-4.81074100	2.55551700	2.07164100
C	-6.79312500	1.29623100	1.23604300
C	-5.45628200	0.40855100	3.17023900
C	-3.17859600	2.11883700	-2.91221700
C	-1.29244400	4.05096500	-0.79127800
C	1.17344200	2.68176600	-0.48898000
C	3.60323000	2.62906000	-0.71137900
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C	4.55563500	-0.55800400	0.24763300
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C	4.82742100	-1.24726700	-2.84019400
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C	-7.76816800	-2.39830200	-0.74209400
C	4.51829900	0.61392700	2.51979800
C	6.98956600	-0.90798500	-0.19302300
C	5.77229800	-2.61192400	1.01256200
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C	3.63718700	1.78567000	2.95833300
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C	8.15437400	-1.66310500	-0.08298600
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H	2.94125600	3.45992800	-2.61720400
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H	4.67480600	-1.78231100	-3.78974400
H	3.75514600	2.64143200	2.27816500
H	2.57453900	1.49603500	2.95709500
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H	6.26471800	1.45829200	3.48221400
H	6.66151300	0.23663700	2.25501400
H	6.12622100	1.86366600	1.75258400
H	3.29305300	-0.90088500	3.47911900
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H	7.00383500	0.05780300	-0.70316700
H	9.08645900	-1.28781200	-0.51151500
H	9.04479100	-3.48580100	0.65827100
H	6.91470000	-4.33165300	1.63049800
H	4.83654100	-2.98222900	1.43700100
H	-0.98115300	-2.30526700	-2.18431300
H	-1.45857600	-0.58444800	-2.14547400
H	-0.81037100	-1.36313500	-0.68030800
H	-4.71100700	-2.51958400	-2.16862000
H	-3.79110000	-1.23212600	-2.99498400
H	-3.22514200	-2.92302000	-3.05592300
H	-2.22123900	-3.02802600	0.60337200
H	-3.78361400	-3.58653700	-0.06152500
H	-2.26705600	-4.00673100	-0.88809800
H	-4.76740700	3.12467600	1.13195100
H	-5.42807300	3.11220200	2.79187000
H	-3.78783100	2.48790600	2.47394000
H	-7.28974800	0.32307800	1.12288200
H	-7.41993200	1.91869600	1.89246700

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H	-6.59414100	-0.76784300	-1.53739200
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IV.2 Int0 - PC^fBu

O 1

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H	2.32904800	-1.20320000	0.84727800
H	0.86998700	-1.11831000	1.87330600
H	0.87240000	-2.14159200	0.41506600
C	1.23074000	1.31767000	0.61251000
H	0.87585300	1.43033700	1.64728900
H	2.33219200	1.33126900	0.61832300
H	0.87535300	2.18165200	0.03226000
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H 2.33298600 -0.13195500 -1.46181000

IV.2 Int1
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N 3.82443600 1.15297500 -0.65883500

N 4.15820100 -0.54038200 0.63665400

N 2.14632500 -1.22353000 -1.27855300

Si -2.77513100 -0.37144100 0.10906300

C 3.89897500 2.44497700 -1.35989800

C 4.73819900 0.49256700 0.07715000

C 4.74932700 -1.68716200 1.33094700

C 3.21072500 -1.56332200 -2.20520700

C 1.04994200 -2.10445900 -1.21882800

N -2.64327500 -1.86461400 -0.87150400

N -4.05911100 0.63956000 -0.88315500

C -0.25541000 -1.60904500 -1.14308600

C 2.93169300 2.36833300 -2.54532500

C 5.28769500 2.74464900 -1.93028300

C 3.49713300 3.57417900 -0.40520500

C 6.15285400 0.90776900 0.25764300

C 3.59834900 -2.63672000 1.65992400

C 5.74299800 -2.43220600 0.43155700

C 5.45403500 -1.26707900 2.62521700

C 2.74567800 -1.57701800 -3.65271600

C 1.22555000 -3.49997500 -1.27218400

C -1.37841700 -2.44406600 -1.02823000

C -3.78991000 -2.56307000 -1.41913000

C -3.92304500 1.66396700 -1.91530900

C -4.99566100 0.42378600 0.03913800

C 6.47208700 1.75588900 1.32302500

C 7.16030600 0.48165300 -0.61239400

C	0.11443600	-4.33690400	-1.22332700
C	-1.17696300	-3.83452800	-1.08872700
C	-3.76296600	-2.68055400	-2.93519000
C	-2.60634700	1.36311300	-2.63473900
C	-3.83961100	3.06470000	-1.30071100
C	-5.08015000	1.57889100	-2.91251900
N	-4.53754500	-0.55174200	0.82521600
C	-6.25594300	1.18928600	0.22628100
C	7.78583800	2.17869700	1.51047400
C	8.47300200	0.90325500	-0.41993100
C	-5.03583900	-1.12883500	2.06918300
C	-7.41860100	0.79644000	-0.44499700
C	-6.29457400	2.29776400	1.07869400
C	8.78817800	1.75380000	0.63940500
C	-4.18572700	-2.37687200	2.31862000
C	-6.50521300	-1.53586500	1.94869200
C	-4.84529800	-0.15017100	3.23315600
C	-8.60577400	1.50129300	-0.26280400
C	-7.48334900	3.00161500	1.25847900
C	-8.64032000	2.60426100	0.58965700
H	2.22364600	-3.93063700	-1.36371400
H	0.26116600	-5.41947000	-1.27270000
H	-2.02144900	-4.52168700	-1.02591100
H	-3.89224700	-3.56968900	-0.96893700
H	-4.69070000	-2.01419200	-1.10731600
H	-3.75007700	-1.68185400	-3.39742600
H	-2.86896400	-3.22224300	-3.27914400
H	-4.65040900	-3.21924700	-3.30335700
H	-1.75752900	1.45399200	-1.93785800
H	-2.60534000	0.34337700	-3.04572100
H	-2.44802600	2.07591100	-3.45710300
H	-3.62488100	3.81129900	-2.08079800

H	-4.78301300	3.34934900	-0.81384500
H	-3.02871400	3.10070800	-0.55704600
H	-5.15961000	0.56023300	-3.32155600
H	-6.03869100	1.84314300	-2.44449300
H	-4.91086600	2.27455400	-3.74834100
H	-4.30527000	-3.10117200	1.50004400
H	-3.11846900	-2.11364500	2.38686400
H	-4.47966700	-2.86036900	3.26174400
H	-6.81197800	-2.09119800	2.84788600
H	-7.16724600	-0.66495400	1.85007300
H	-6.65482100	-2.18825900	1.07488700
H	-3.79363600	0.16942000	3.29092900
H	-5.47629700	0.74142600	3.10856200
H	-5.11855500	-0.62609100	4.18769400
H	-7.38790200	-0.07099600	-1.10821500
H	-9.50974400	1.18644600	-0.78912700
H	-9.57192900	3.15667200	0.73247100
H	-7.50491800	3.86703600	1.92481100
H	-5.38553500	2.61096300	1.59690600
H	2.90294700	3.33537600	-3.06907700
H	3.26433900	1.59855100	-3.25792000
H	1.91652000	2.11481700	-2.21460900
H	6.03318900	2.97254300	-1.15856700
H	5.65854800	1.90802800	-2.54043000
H	5.20701500	3.62614900	-2.58369600
H	2.48470800	3.41403500	-0.00756800
H	4.19552400	3.62436900	0.44443200
H	3.51804100	4.54555800	-0.92293900
H	3.04196800	-2.91162300	0.75290400
H	3.98481200	-3.55386200	2.12771600
H	2.89024200	-2.17113100	2.35560300
H	6.63873000	-1.83081900	0.22843700

H	6.07091000	-3.35881500	0.92666500
H	5.27414600	-2.70344100	-0.52485300
H	4.78419600	-0.66999400	3.25990600
H	5.75781700	-2.16045600	3.19200800
H	6.35698400	-0.67492600	2.42304400
H	5.68362200	2.08148300	2.00545600
H	8.02767300	2.84286000	2.34331100
H	9.81845600	2.08563500	0.78673500
H	9.25511400	0.56856000	-1.10511500
H	6.91068600	-0.17135300	-1.45121000
H	4.00896600	-0.81591200	-2.09154800
H	3.67471600	-2.53725200	-1.95673900
H	2.34077300	-0.59331900	-3.93459400
H	3.57804300	-1.82303100	-4.33080000
H	1.95044800	-2.32200500	-3.80453200
H	-0.40709700	-0.53328300	-1.20788100
P	0.60934100	1.50002400	0.07719000
C	1.24003000	0.43427900	1.25523100
C	0.76061100	0.16238200	2.66261600
C	0.15757000	-1.25038100	2.68455700
H	-0.19591400	-1.50397300	3.69805700
H	-0.69742300	-1.30087200	1.99236300
H	0.88271900	-2.01232700	2.36777400
C	-0.32419500	1.16444000	3.06017500
H	-1.17109700	1.10870400	2.35767400
H	-0.69365800	0.94961000	4.07622600
H	0.06360500	2.19536700	3.04290400
C	1.93343400	0.26707000	3.64085200
H	2.72862800	-0.44626900	3.38840700
H	2.36977100	1.27839300	3.61670700
H	1.60169600	0.06143000	4.67185200

IV.2 Int2

0 1

Si	2.38716200	0.49798800	0.33413400
N	4.03996600	0.13280800	1.10080000
N	3.57981300	-0.13516900	-0.97890900
N	2.37762800	2.24418800	-0.00741200
Si	-2.08509000	0.07358400	0.41111000
C	4.47506000	-0.08004600	2.48781000
C	4.50025800	-0.37488400	-0.05233800
C	3.57759000	-0.25557800	-2.43703500
C	3.58071000	2.96268900	-0.37145700
C	1.13911900	2.86979800	-0.18864800
N	-2.21406600	1.79855000	0.82426400
N	-3.72345800	-0.56304500	1.11656600
C	0.06615800	2.35818800	0.54086400
C	3.58644600	0.82075300	3.34623300
C	5.93599500	0.33246600	2.67208800
C	4.26519200	-1.54199900	2.89045800
C	5.75591100	-1.13689300	-0.24871000
C	2.25925700	0.37205800	-2.89760400
C	4.75085500	0.51941700	-3.04276900
C	3.64121300	-1.71927100	-2.88050600
C	3.86431500	4.14500100	0.54179000
C	0.87727800	3.92021500	-1.08475200
C	-1.25140700	2.65344800	0.24825400
C	-3.43440300	2.42859100	1.29578200
C	-4.14414300	-1.13227900	2.39936200
C	-4.31838600	-0.48570800	-0.07387800
C	5.71446800	-2.53518200	-0.25910100
C	6.97402800	-0.47664800	-0.43788200
C	-0.44367400	4.34907200	-1.25650800
C	-1.52016900	3.71712100	-0.63439000

C	-3.18117400	3.40236000	2.43473300
C	-3.02983000	-0.78378300	3.38903200
C	-4.28033600	-2.65370000	2.29891500
C	-5.46512000	-0.53120900	2.88794500
N	-3.41982600	-0.05755900	-0.95007000
C	-5.73210500	-0.82773500	-0.36138500
C	6.88551400	-3.26445200	-0.45068400
C	8.14096600	-1.21007400	-0.63638100
C	-3.55055400	0.41770600	-2.32983700
C	-6.73672200	0.13307200	-0.20755800
C	-6.06446800	-2.11786400	-0.78725500
C	8.09860700	-2.60395500	-0.64111100
C	-2.12833200	0.67285000	-2.83434700
C	-4.33859700	1.73006100	-2.36655200
C	-4.23375400	-0.61513600	-3.23052900
C	-8.06225600	-0.19488500	-0.48064900
C	-7.39243200	-2.44265100	-1.05257900
C	-8.39252000	-1.48273300	-0.90152900
H	1.67713800	4.40234600	-1.64878900
H	-0.64061700	5.18157300	-1.93769300
H	-2.53964600	4.04381800	-0.84594000
H	-3.96196000	2.94946100	0.47199300
H	-4.11801100	1.64102300	1.63276900
H	-2.72067900	2.88422700	3.28973300
H	-2.49672100	4.20625800	2.12487100
H	-4.12215300	3.86599700	2.77024800
H	-2.06092600	-1.16657000	3.03333100
H	-2.93555100	0.30652900	3.50549600
H	-3.24619100	-1.21924400	4.37537300
H	-4.54234600	-3.07625900	3.28086700
H	-5.07131400	-2.93632100	1.58928600
H	-3.33446800	-3.10618900	1.97119600

H	-5.41290300	0.56733400	2.92596000
H	-6.31100500	-0.81899500	2.24903300
H	-5.67601200	-0.89169900	3.90593600
H	-1.62031400	1.43178700	-2.22052100
H	-1.52440000	-0.24452000	-2.79943500
H	-2.16031300	1.03644000	-3.87202300
H	-4.37115500	2.12566400	-3.39306100
H	-5.37428700	1.58340000	-2.02802400
H	-3.85668100	2.48071300	-1.72633100
H	-3.72303900	-1.58721900	-3.17806500
H	-5.28857300	-0.76122000	-2.96200400
H	-4.19938200	-0.26752000	-4.27390600
H	-6.47578500	1.13669000	0.13528500
H	-8.84261900	0.55982500	-0.35996300
H	-9.43319900	-1.73901000	-1.11263800
H	-7.64642700	-3.45194300	-1.38411700
H	-5.27557000	-2.86143000	-0.91986300
H	3.85827400	0.71897200	4.40702900
H	3.70436900	1.87547900	3.05486200
H	2.52573400	0.54482800	3.22702600
H	6.62689500	-0.33940300	2.14569000
H	6.09811700	1.35972100	2.31039000
H	6.19203700	0.30234900	3.74170700
H	3.22249000	-1.83478800	2.68924500
H	4.93749100	-2.20753100	2.32898300
H	4.47565300	-1.67661600	3.96247500
H	2.22504900	1.44433200	-2.65499100
H	2.14062200	0.25817400	-3.98477800
H	1.40387900	-0.11280500	-2.40292700
H	5.71570300	0.07365000	-2.76166500
H	4.68155400	0.50359200	-4.14094500
H	4.73766400	1.56859300	-2.71398800

H	2.83576000	-2.30162900	-2.41387800
H	3.52613000	-1.78327300	-3.97313300
H	4.60588600	-2.17520000	-2.61763400
H	4.75955900	-3.04494900	-0.11251300
H	6.84886300	-4.35614700	-0.45225400
H	9.01540700	-3.17793800	-0.79413300
H	9.08947700	-0.68952400	-0.78618900
H	7.00378200	0.61511000	-0.42707700
H	4.42500200	2.26028600	-0.32309200
H	3.53152500	3.30210500	-1.42496200
H	3.99912400	3.80290400	1.57893300
H	4.77764300	4.67410400	0.22785100
H	3.03216500	4.86449400	0.53229400
H	0.25701800	1.61562000	1.31454700
P	0.87605400	-0.68675500	1.35368600
C	-0.64974300	-0.94593800	0.34686700
C	-0.70532000	-2.38939200	-0.25162200
C	-2.02263200	-2.75059300	-0.94160300
H	-1.97104600	-3.78382100	-1.32184300
H	-2.87293700	-2.70275700	-0.24572800
H	-2.23041700	-2.09174200	-1.79293300
C	-0.49114700	-3.43931700	0.85311700
H	-1.28218000	-3.36494200	1.61571600
H	-0.50366500	-4.46208200	0.43743200
H	0.47203800	-3.27619800	1.35863300
C	0.40286200	-2.56476900	-1.29406000
H	0.21766500	-1.91985900	-2.16768300
H	1.36740700	-2.27740700	-0.84833100
H	0.46967700	-3.60889100	-1.64647100

IV.2 Int3
0 1

P	0.35016800	0.69778400	1.06488700
Si	1.75282800	-0.29406400	-0.20827200
C	-1.06513700	-0.44542000	1.60403400
N	2.96215900	1.03493400	-0.67717700
N	3.49922500	-0.69804700	0.47778700
N	1.59583600	-1.42370500	-1.53662800
Si	-1.83463600	-1.01945200	-0.01716400
C	-0.76946600	-1.48228400	2.72625600
C	2.83278400	2.39736500	-1.21655700
C	3.93074900	0.48123200	0.07020000
C	4.13309600	-1.76979800	1.24959800
C	2.68234200	-1.54624900	-2.49553100
C	0.57787400	-2.39415900	-1.54080300
N	-2.70201600	-2.58805200	-0.18327900
N	-2.57329100	0.37480200	-0.86561700
C	-0.65218700	-2.14379900	-0.95031000
C	0.12981300	-2.60487900	2.22371800
C	-0.08892300	-0.77604600	3.90213100
C	-2.08024000	-2.09297500	3.22379600
C	1.58104000	2.37962500	-2.08811500
C	4.03430200	2.77193000	-2.08580400
C	2.65340700	3.40639300	-0.07961300
C	5.21654400	1.11617000	0.44252700
C	3.54189400	-3.08621300	0.73689900
C	5.64899300	-1.82672600	1.05189200
C	3.81207200	-1.57750100	2.73440500
C	2.23747300	-1.31429300	-3.93071800
C	0.77148300	-3.66841500	-2.13200900
C	-1.65150700	-3.14646500	-0.89524300
C	-3.99530500	-3.18056400	-0.02192900
C	-2.45895400	0.77390800	-2.29878900
C	-3.57130000	0.90709000	-0.05630000

C	5.31723500	1.73228300	1.69377500
C	6.32389800	1.07860200	-0.40911900
C	-0.24078500	-4.62411800	-2.09855700
C	-1.47685600	-4.40074800	-1.48132300
C	-4.96216400	-2.86542800	-1.15461200
C	-1.41077000	-0.08548100	-2.99877300
C	-2.03471300	2.23938700	-2.48745800
C	-3.80360600	0.52478000	-2.98898000
N	-4.11272300	0.09574200	0.78131200
C	-3.75436600	2.39546800	-0.09777300
C	6.52279000	2.30812200	2.08854300
C	7.52791300	1.64863700	-0.00654200
C	-5.03984600	0.42892100	1.86980700
C	-4.85630400	3.04207600	-0.66262200
C	-2.72045500	3.16289900	0.45389200
C	7.62911000	2.26384000	1.24149300
C	-5.50427300	-0.90741000	2.45661100
C	-6.30153300	1.16728000	1.40008900
C	-4.34462100	1.24592500	2.96462000
C	-4.92671800	4.43405800	-0.67409000
C	-2.80105800	4.55210600	0.45923800
C	-3.90283200	5.19226700	-0.10838000
H	-1.75966000	0.29501500	2.03548600
H	1.71443600	-3.92056500	-2.61607100
H	-0.05404100	-5.59279200	-2.57127500
H	-2.25225300	-5.16839100	-1.46760200
H	-3.87643700	-4.27457800	0.08283300
H	-4.42260400	-2.82692900	0.92646500
H	-5.14773400	-1.78174200	-1.19173500
H	-4.54940200	-3.18054500	-2.12597000
H	-5.92699200	-3.37765200	-1.00986000
H	-0.42158400	0.02265300	-2.53395800

H	-1.67583800	-1.15039000	-2.98937900
H	-1.33627800	0.23711600	-4.04765800
H	-1.68530000	2.38132900	-3.52143800
H	-2.84766000	2.95324100	-2.31493600
H	-1.21215200	2.48836400	-1.80697600
H	-4.07918500	-0.53729000	-2.91970500
H	-4.60916500	1.11882700	-2.53511900
H	-3.74593700	0.80167500	-4.05302700
H	-6.06991900	-1.47639000	1.70355300
H	-4.64853900	-1.51520500	2.77252600
H	-6.15856800	-0.74347000	3.32627900
H	-7.07072900	1.11139400	2.18558600
H	-6.11737400	2.22745900	1.19356400
H	-6.70938700	0.69318000	0.49404600
H	-3.46641800	0.71223100	3.35576800
H	-4.01432100	2.22378700	2.58748900
H	-5.03552600	1.42039000	3.80385400
H	-5.66055900	2.45636300	-1.11087000
H	-5.78817000	4.92860200	-1.12915300
H	-3.96120700	6.28335900	-0.11538900
H	-1.98911400	5.13848100	0.89603300
H	-1.83335600	2.65740900	0.84920600
H	1.02193000	-2.17792200	1.74518000
H	0.46500700	-3.24351200	3.05659200
H	-0.37411200	-3.24042000	1.48238300
H	-0.72902700	0.02770900	4.30156100
H	0.11385700	-1.48798600	4.71873200
H	0.85781200	-0.31269900	3.58589000
H	-2.62863400	-2.57540900	2.40222300
H	-1.88180500	-2.85326900	3.99629700
H	-2.72823100	-1.32635200	3.67328900
H	1.38144100	3.38201900	-2.49301000

H	1.69707200	1.68096800	-2.93004200
H	0.71607500	2.06098600	-1.49011200
H	4.94712100	2.92619700	-1.49647200
H	4.22596800	1.99447000	-2.84145100
H	3.81733300	3.71209900	-2.61439400
H	1.80281600	3.11331900	0.55443900
H	3.55670900	3.46480300	0.54498300
H	2.46142100	4.40961300	-0.48959000
H	3.83166800	-3.25883300	-0.30959000
H	3.91431000	-3.92607600	1.34117200
H	2.44549600	-3.09496300	0.78524500
H	6.17193600	-0.98184700	1.51743100
H	6.02798600	-2.74956500	1.51533100
H	5.90880000	-1.85474700	-0.01701700
H	2.72815000	-1.52980600	2.90100600
H	4.22023700	-2.41153500	3.32515800
H	4.25683100	-0.64310200	3.10730900
H	4.44509600	1.75860300	2.35141000
H	6.59780300	2.79169500	3.06501400
H	8.57529700	2.71096800	1.55462500
H	8.39392700	1.61181400	-0.67108400
H	6.24231600	0.59288700	-1.38365000
H	3.44815400	-0.80235000	-2.23301700
H	3.17683400	-2.53030400	-2.40338200
H	1.83620400	-0.29720800	-4.05187800
H	3.08286300	-1.43910300	-4.62513700
H	1.44741400	-2.02168200	-4.22144200

IV.2 Int4
0 1

Si	1.44881100	0.39085100	0.32392500
N	3.10280700	-0.24296900	1.06696600

N	2.77783400	0.12848700	-1.01772000
N	1.60171700	2.16153600	0.57604900
Si	-1.82204800	0.93811800	-0.60921900
C	3.40247200	-0.92783100	2.32725400
C	3.59678500	-0.46339300	-0.16005900
C	2.78555500	0.31108600	-2.46473000
C	2.89201500	2.81510200	0.68211300
C	0.46752800	2.96046600	0.39584100
N	-2.84046200	2.39768000	-0.79660100
N	-2.32667100	-0.21235600	0.75586000
C	-0.75406500	2.41103200	-0.00250500
C	2.42785200	-0.37274000	3.36673300
C	4.83431000	-0.63528600	2.78254700
C	3.17969300	-2.43908300	2.20428000
C	4.78189000	-1.28420100	-0.51799300
C	1.94470900	1.56154200	-2.73906200
C	4.19753000	0.52551200	-3.01039500
C	2.12718400	-0.89714800	-3.13965600
C	3.28121600	3.24426500	2.08951100
C	0.50374300	4.36934900	0.58669200
C	-1.85785100	3.24438000	-0.27790300
C	-4.22076300	2.74664000	-0.93079500
C	-2.11955000	-0.29574700	2.21561900
C	-3.20670500	-0.90742600	0.00189800
C	4.62143600	-2.57170200	-1.04111900
C	6.06845200	-0.75401000	-0.37700600
C	-0.62275000	5.15516100	0.36311000
C	-1.83886500	4.62435500	-0.08230500
C	-4.97599400	2.78263800	0.39317700
C	-1.39279300	0.96471100	2.68051000
C	-1.26218500	-1.51789500	2.55908800
C	-3.45575400	-0.35713500	2.96361200

N	-3.30679900	-0.33488900	-1.17112100
C	-3.89823900	-2.15700900	0.41934100
C	5.73519300	-3.31980200	-1.41519500
C	7.17997300	-1.50077600	-0.75910900
C	-3.82249900	-0.84451100	-2.44157100
C	-5.26503900	-2.14568000	0.71625900
C	-3.19131900	-3.36212800	0.48146600
C	7.01553100	-2.78461800	-1.27791400
C	-3.38794300	0.15547600	-3.51775200
C	-5.35221900	-0.92515800	-2.42911600
C	-3.22593000	-2.21440600	-2.78385400
C	-5.91330500	-3.32259500	1.08174400
C	-3.84433100	-4.54035800	0.83617000
C	-5.20472600	-4.52223600	1.14043500
H	1.41501800	4.86031400	0.92569900
H	-0.54432800	6.23298300	0.53434300
H	-2.70158100	5.26205500	-0.28431000
H	-4.30938500	3.72685300	-1.43687100
H	-4.69834200	2.01444200	-1.60056400
H	-4.97580300	1.78522000	0.86022300
H	-4.49754000	3.48176100	1.09661500
H	-6.02237900	3.09876400	0.25416100
H	-0.40036200	1.05155700	2.21995200
H	-1.95785900	1.87249100	2.42679100
H	-1.26589500	0.92307400	3.77253700
H	-0.96487500	-1.49019100	3.61859800
H	-1.80778900	-2.45625200	2.39102900
H	-0.35617700	-1.51251700	1.93424200
H	-4.10316300	0.48222700	2.66732000
H	-3.99447000	-1.29726300	2.79184200
H	-3.27081900	-0.27594000	4.04510000
H	-3.75419900	1.16635000	-3.29100700

H	-2.29220200	0.20529700	-3.58641800
H	-3.78351400	-0.14779800	-4.49837500
H	-5.72567100	-1.17353400	-3.43439200
H	-5.71065400	-1.69894800	-1.73719000
H	-5.78852700	0.03985600	-2.13014400
H	-2.12697300	-2.17288700	-2.73562300
H	-3.57747200	-2.99718800	-2.09798500
H	-3.51461600	-2.50843600	-3.80473700
H	-5.81490500	-1.20304500	0.67535100
H	-6.97875100	-3.30248100	1.32185000
H	-5.71481600	-5.44589800	1.42350100
H	-3.28608600	-5.47853500	0.87545100
H	-2.12737500	-3.37244500	0.23619800
H	2.59460400	-0.85607200	4.34044400
H	2.55320000	0.71129900	3.49123300
H	1.38766600	-0.55905200	3.06422100
H	5.57620800	-1.09871200	2.11854400
H	5.01518600	0.44979700	2.80706500
H	4.99573300	-1.03453400	3.79541400
H	2.15764500	-2.64267500	1.84929500
H	3.89224800	-2.89692600	1.50382600
H	3.30903800	-2.92772000	3.18230100
H	2.40034300	2.44983900	-2.27880800
H	1.85823300	1.73228100	-3.82230800
H	0.92893100	1.45625200	-2.32743800
H	4.81683800	-0.37864000	-2.93816200
H	4.13875300	0.80911100	-4.07185100
H	4.70371100	1.33871000	-2.46821000
H	1.11963400	-1.05586600	-2.72634800
H	2.03777000	-0.73277300	-4.22456300
H	2.72010700	-1.80988900	-2.98150900
H	3.61725600	-2.98783000	-1.14747200

H	5.60218100	-4.32641900	-1.81827100
H	7.88814900	-3.37002200	-1.57669400
H	8.18098200	-1.07651000	-0.65309800
H	6.19167000	0.25523300	0.02195000
H	3.65946100	2.12557100	0.29673600
H	2.91200600	3.68979100	0.00713800
H	3.39584300	2.36797200	2.74255900
H	4.24012100	3.78710300	2.08091200
H	2.52101800	3.89848600	2.54038500
H	-0.97813500	0.27127600	-1.65658400

IV.2 Int5

0 1

Si	-1.69992400	0.01520300	0.03415900
N	-3.04733500	-1.12518500	-0.58598400
N	-3.59099300	0.66006400	0.50482000
N	-1.34342300	1.23883000	-1.18893200
Si	2.35428500	1.10328300	0.16016500
C	-3.01340000	-2.45550700	-1.21688000
C	-4.06377000	-0.43960900	-0.02578100
C	-4.30594000	1.82964800	1.02621600
C	-2.29580700	1.37076600	-2.28460800
C	-0.42063300	2.29704000	-1.01619700
N	2.97026600	2.75917400	-0.01972200
N	2.87604600	-0.29640500	-0.90102600
C	0.88673100	2.12665500	-0.55785600
C	-1.90995800	-2.42378900	-2.27958600
C	-4.31685000	-2.81516900	-1.93536500
C	-2.71417300	-3.52463100	-0.16087000
C	-5.47357100	-0.90323300	0.03377800
C	-3.24647000	2.78819400	1.56601600
C	-5.07301700	2.54237200	-0.09358400

C	-5.28187300	1.47012800	2.15235700
C	-1.65076900	1.40495000	-3.66048500
C	-0.81633100	3.61511700	-1.37835200
C	1.75241200	3.24847800	-0.49236400
C	4.20646400	3.47683000	-0.06575000
C	2.63845100	-0.70745200	-2.30018800
C	3.93593500	-0.66731500	-0.13143700
C	-5.86316700	-1.71096600	1.10742800
C	-6.40842000	-0.55498200	-0.94449400
C	0.06053300	4.68890500	-1.30173500
C	1.37939700	4.53791300	-0.86036500
C	4.79397100	3.59077800	-1.46757300
C	1.46929900	0.10029200	-2.84621900
C	2.28275600	-2.19365800	-2.41806000
C	3.88445800	-0.39688700	-3.13580500
N	4.16453100	0.25234300	0.76245900
C	4.58720100	-1.99926200	-0.21717900
C	-7.17532000	-2.16768500	1.19805700
C	-7.72048900	-1.01157900	-0.84943100
C	4.94206800	0.18787700	2.00243600
C	5.90515200	-2.14954000	-0.65393900
C	3.86229500	-3.11930900	0.20906300
C	-8.10627400	-1.81886600	0.22004200
C	4.36018200	1.25134700	2.94060300
C	6.40344500	0.52954300	1.69435900
C	4.86199100	-1.16522300	2.71755100
C	6.49723400	-3.41184200	-0.66486800
C	4.46229900	-4.37395000	0.21125300
C	5.77941900	-4.52305900	-0.22680900
H	-1.82800100	3.79941100	-1.73921800
H	-0.29514500	5.67956300	-1.59957100
H	2.06851700	5.38336600	-0.81635100

H	4.06852700	4.48659800	0.36589600
H	4.92590200	2.96201000	0.58859100
H	5.02546500	2.59081300	-1.86613000
H	4.08063200	4.07035500	-2.15536800
H	5.72161000	4.18496300	-1.46703500
H	0.56162300	-0.05581700	-2.24749200
H	1.68342100	1.17777200	-2.84674200
H	1.26784800	-0.21361200	-3.88097400
H	1.93780400	-2.40399700	-3.44166300
H	3.13723000	-2.85045100	-2.21372100
H	1.47095100	-2.44820100	-1.72156900
H	4.13745000	0.67162400	-3.06292300
H	4.75155700	-0.98722300	-2.80605300
H	3.70241400	-0.63534400	-4.19478600
H	4.31792000	2.23465800	2.45282900
H	3.33794300	0.98676900	3.24582100
H	4.97927800	1.33533900	3.84602800
H	6.98804900	0.59011600	2.62510200
H	6.86050800	-0.23982100	1.05611000
H	6.47734800	1.49711300	1.17612100
H	3.81383800	-1.48099300	2.83140400
H	5.40754600	-1.95784600	2.18982500
H	5.29964100	-1.07055300	3.72304500
H	6.46629600	-1.27591300	-0.99271200
H	7.52583600	-3.52595500	-1.01457600
H	6.24683200	-5.51061000	-0.22852600
H	3.89730300	-5.24355600	0.55472700
H	2.82949200	-2.98809200	0.54497900
H	-1.79608600	-3.41996600	-2.73209800
H	-2.16566800	-1.71032300	-3.07731000
H	-0.94832800	-2.12215300	-1.84648700
H	-5.14658700	-3.02449700	-1.24935900

H	-4.62584400	-2.01710500	-2.62643200
H	-4.14105600	-3.72387500	-2.53013500
H	-1.75788100	-3.32590100	0.34419500
H	-3.50718200	-3.54300900	0.60230300
H	-2.66170900	-4.52206500	-0.62388100
H	-2.48135700	3.00376000	0.80572000
H	-3.71378400	3.73702600	1.86708300
H	-2.74781100	2.36379000	2.44575300
H	-5.87042600	1.90907200	-0.50444400
H	-5.54225600	3.45734300	0.29848700
H	-4.39484700	2.83025200	-0.90840600
H	-4.78392500	0.87889200	2.93411600
H	-5.66232000	2.39312800	2.61563900
H	-6.14560900	0.89967000	1.78600300
H	-5.13190300	-1.97262800	1.87572800
H	-7.47312500	-2.79760400	2.03931500
H	-9.13578700	-2.17697500	0.29167300
H	-8.44591100	-0.73821000	-1.61898800
H	-6.10219600	0.06116400	-1.79227300
H	-2.97821300	0.51115400	-2.23833800
H	-2.93938400	2.25978900	-2.16079400
H	-1.14484800	0.45476700	-3.88157500
H	-2.41437100	1.57875200	-4.43503800
H	-0.90528700	2.21042200	-3.73161600
P	0.02194500	-1.37964500	0.55088700
C	-0.80757400	-0.29710100	1.57728900
C	-0.68091600	-0.05808600	3.06465900
C	-0.21967100	1.38396600	3.31961900
H	-0.21405500	1.59866900	4.40088000
H	0.79595900	1.54156200	2.93110400
H	-0.87025900	2.11418000	2.82253900
C	0.33615500	-1.02055800	3.67789000

H	1.32505900	-0.89366000	3.21006100
H	0.43853400	-0.84039700	4.75978900
H	0.03323700	-2.06831200	3.52571600
C	-2.05286300	-0.29524800	3.70646600
H	-2.80879900	0.37146400	3.27129900
H	-2.38426100	-1.33255400	3.53875000
H	-2.01369400	-0.11742300	4.79375600
H	1.87890900	0.60567200	1.47123100

IV.2 Int6

0 1

P	0.38326200	0.74964400	1.06873700
Si	1.86883800	-0.43514200	-0.38668800
C	-0.99073100	-0.18045400	1.58772500
N	3.12636300	0.79846900	-0.97459700
N	3.49015800	-0.74121900	0.47063200
N	1.64699800	-1.67708400	-1.58020900
Si	-1.73449000	-0.97584900	0.12969300
C	-0.95950100	-0.80574500	2.98842900
C	3.03901400	2.06504700	-1.71124300
C	3.98341400	0.38999900	-0.02318300
C	3.97168900	-1.69107800	1.47440200
C	2.68443000	-1.97670900	-2.55364300
C	0.61435700	-2.61597700	-1.34089900
N	-2.57247200	-2.56185600	0.25062700
N	-2.50308700	0.25298200	-0.91660600
C	-0.56724400	-2.23719200	-0.70994400
C	-0.24021500	-2.16310900	2.99222900
C	-0.27022100	0.11914700	3.99682800
C	-2.39540500	-1.02895700	3.46468200
C	1.94680500	1.85310100	-2.75633300
C	4.35487200	2.37628800	-2.42503800

C	2.65215000	3.21437900	-0.77749400
C	5.16886000	1.12166400	0.48044500
C	3.17665100	-2.97653200	1.23685000
C	5.46050300	-1.98240900	1.28766500
C	3.70566300	-1.15162800	2.88151900
C	2.17047200	-2.01138000	-3.98382600
C	0.77090900	-3.97125300	-1.71808400
C	-1.55604900	-3.21497500	-0.42009900
C	-3.86192300	-3.12742700	0.51264500
C	-2.38146300	0.49333500	-2.38050900
C	-3.54711200	0.90045600	-0.22620500
C	5.02901000	1.93548900	1.60995000
C	6.41544900	0.99659300	-0.14013600
C	-0.23597600	-4.89730600	-1.45650900
C	-1.42103300	-4.55239000	-0.80300300
C	-4.80451700	-3.07197300	-0.68152000
C	-1.42538600	-0.51330100	-3.01251500
C	-1.83829500	1.89636900	-2.70163500
C	-3.75209500	0.29394200	-3.03645700
N	-4.31029700	0.18406600	0.50661200
C	-3.54345600	2.40239300	-0.28633600
C	6.13276300	2.62250600	2.11064500
C	7.51590000	1.68106600	0.36830400
C	-5.39672700	0.65722500	1.37312900
C	-4.47099400	3.17925600	-0.98516700
C	-2.52485100	3.04110900	0.43133500
C	7.37574900	2.49480300	1.49249600
C	-5.81970600	-0.54077300	2.23029900
C	-6.60634500	1.04346100	0.51202400
C	-5.01454500	1.81269800	2.30705400
C	-4.38314700	4.57094800	-0.96661700
C	-2.44495300	4.42949700	0.45992300

C	-3.37237200	5.20037700	-0.24248400
H	1.67954200	-4.30870300	-2.21624200
H	-0.08543400	-5.93377200	-1.77208200
H	-2.19908800	-5.29262500	-0.60979200
H	-3.73478300	-4.17208900	0.85268600
H	-4.31058300	-2.58338300	1.35407100
H	-4.99184200	-2.02055000	-0.94554200
H	-4.36765800	-3.58157400	-1.55492300
H	-5.76900500	-3.55304800	-0.45180900
H	-0.40581900	-0.42134300	-2.61482300
H	-1.75483700	-1.54837300	-2.85416500
H	-1.38489600	-0.32657800	-4.09620500
H	-1.50415900	1.93543200	-3.74992200
H	-2.57876300	2.69058900	-2.55818600
H	-0.98112600	2.12879700	-2.05497700
H	-4.11357400	-0.72872500	-2.85500500
H	-4.50254600	0.99150600	-2.63971900
H	-3.68752600	0.45635200	-4.12350200
H	-6.13635000	-1.37486400	1.58758300
H	-4.99093700	-0.88606900	2.86074500
H	-6.66238700	-0.26917000	2.88404900
H	-7.49272100	1.18582400	1.14942200
H	-6.43453800	1.97796900	-0.03520200
H	-6.82850500	0.24517400	-0.21257900
H	-4.05884400	1.60224700	2.80899800
H	-4.91729000	2.76942800	1.77939000
H	-5.78958400	1.93265700	3.07966900
H	-5.25714000	2.70006300	-1.57102500
H	-5.10973400	5.16607600	-1.52514000
H	-3.30740600	6.29107000	-0.22593900
H	-1.65231000	4.91382200	1.03589200
H	-1.81856400	2.41996800	0.99032700

H	0.80918400	-2.04350200	2.68697900
H	-0.24589100	-2.62538100	3.99479900
H	-0.71611200	-2.86232000	2.28839000
H	-0.77408200	1.09748500	4.03269500
H	-0.28780400	-0.32239500	5.00676000
H	0.78294600	0.30317900	3.72903900
H	-2.93154700	-1.69380300	2.77336800
H	-2.41425200	-1.49070500	4.46620100
H	-2.93809100	-0.07464500	3.51077800
H	1.77191800	2.77727700	-3.32497300
H	2.22640400	1.05683500	-3.46110200
H	0.99728800	1.56988900	-2.28056700
H	5.15644400	2.63535200	-1.72127600
H	4.68089800	1.51816900	-3.03235100
H	4.21030600	3.23476200	-3.09745400
H	1.72517900	2.98195400	-0.23236900
H	3.44461300	3.40903300	-0.04075400
H	2.49381400	4.13702100	-1.35577700
H	3.39349400	-3.39501300	0.24329300
H	3.43138300	-3.72930600	1.99630900
H	2.09182700	-2.79946400	1.29257200
H	6.08706600	-1.11410300	1.53138200
H	5.75582800	-2.80633500	1.95378300
H	5.66994300	-2.28949900	0.25158000
H	2.64663400	-0.88360100	3.00227400
H	3.95719900	-1.91152600	3.63630100
H	4.31418700	-0.25812200	3.08184000
H	4.05057300	2.02963700	2.08730200
H	6.01960900	3.26011700	2.99018600
H	8.24049100	3.03184500	1.88878400
H	8.48934400	1.57820700	-0.11618700
H	6.52105400	0.35679200	-1.01878500

H	3.45668200	-1.19737700	-2.46004500
H	3.18836600	-2.92921500	-2.30493200
H	1.74385700	-1.03766600	-4.26711500
H	2.98491100	-2.25226700	-4.68438600
H	1.38033200	-2.76650000	-4.10299600
H	-0.10542100	1.33732000	-0.14613900

IV.2 TS 1-2 C

0 1

Si	1.77604200	0.20636400	0.87386900
N	3.45711000	-0.61105000	1.13761100
N	2.87234900	-0.00284800	-0.85614500
N	2.23346600	1.97079000	1.00254200
Si	-1.82661500	0.47363200	-0.24909500
C	4.09893200	-1.22872700	2.31147700
C	3.82720300	-0.56784800	-0.15425400
C	2.90963100	0.54211500	-2.21770100
C	3.55347300	2.44062500	1.36026900
C	1.34787200	2.86841400	0.45291800
N	-2.07049300	2.20916400	-0.58064500
N	-3.26202800	0.07770100	0.92517000
C	0.00759500	2.47558700	0.46203800
C	3.66337900	-0.43559000	3.54827800
C	5.62850600	-1.18107100	2.25206500
C	3.64267500	-2.68115100	2.46665500
C	5.09029100	-1.13405900	-0.69667800
C	1.51985500	1.10278500	-2.53102400
C	3.90236500	1.70709400	-2.30701500
C	3.28010700	-0.52241700	-3.25671500
C	3.54329200	3.35282500	2.57778800
C	1.65868800	4.07954600	-0.20311000
C	-0.92947900	2.99439300	-0.41965900

C	-3.30578500	2.84363500	-0.99399300
C	-3.53935900	0.21765900	2.36264700
C	-3.98991000	-0.43383800	-0.06169000
C	5.10462700	-2.47387900	-1.09867400
C	6.25388000	-0.36810300	-0.81095700
C	0.66210900	4.71221100	-0.95026300
C	-0.61530700	4.17193600	-1.12071100
C	-3.84221200	3.85385500	0.00806000
C	-2.59981900	1.30779200	2.87720300
C	-3.25705100	-1.09342300	3.09748600
C	-4.98423800	0.65896600	2.61115700
N	-3.32856200	-0.22643600	-1.20430100
C	-5.26438500	-1.18441500	0.08896700
C	6.27052600	-3.03997200	-1.60801900
C	7.41711100	-0.93591100	-1.32374800
C	-3.67263000	-0.54406400	-2.59481800
C	-6.50037300	-0.54228700	-0.03917300
C	-5.22204300	-2.55211600	0.37603800
C	7.42883500	-2.27218700	-1.72262700
C	-2.68973000	0.23211400	-3.47559600
C	-5.08777700	-0.07574800	-2.95305300
C	-3.56177200	-2.04779500	-2.86372400
C	-7.68103000	-1.26186900	0.11609500
C	-6.40714400	-3.27014600	0.52709300
C	-7.63657800	-2.62744000	0.39808100
H	2.66349100	4.50240200	-0.17436500
H	0.91222000	5.64079200	-1.47132600
H	-1.32825100	4.64502800	-1.79720800
H	-3.16432500	3.33520000	-1.97589200
H	-4.05176600	2.05530100	-1.16142100
H	-4.08264800	3.36667400	0.96431900
H	-3.10394800	4.64414500	0.20979300

H	-4.75751100	4.33198400	-0.37446200
H	-1.54684400	0.99495400	2.75997400
H	-2.75588000	2.25570000	2.34324100
H	-2.77422000	1.47577600	3.94990800
H	-3.45930600	-0.97036200	4.17229600
H	-3.89802500	-1.90426600	2.72126900
H	-2.19873800	-1.37574000	2.98375800
H	-5.24162600	1.53544600	1.99668800
H	-5.71026500	-0.13873000	2.40919100
H	-5.09145000	0.94415200	3.66785100
H	-2.81302500	1.31548400	-3.33868700
H	-1.64494700	-0.01593400	-3.24499000
H	-2.86589300	-0.00620400	-4.53435500
H	-5.23256200	-0.16481300	-4.04000100
H	-5.86114600	-0.68186500	-2.46547900
H	-5.23864300	0.97917800	-2.67968100
H	-2.54829000	-2.41481800	-2.66101100
H	-4.26702800	-2.60902600	-2.23365700
H	-3.80297700	-2.26347000	-3.91577300
H	-6.53354600	0.52802300	-0.25211500
H	-8.64240600	-0.75268400	0.01880200
H	-8.56432200	-3.19113700	0.51987000
H	-6.36642000	-4.33850600	0.75052000
H	-4.25732700	-3.05246900	0.48203000
H	4.05390800	-0.92368800	4.45349000
H	4.05495500	0.59118700	3.52011300
H	2.56894900	-0.38633800	3.62447200
H	6.05188100	-1.86486300	1.50598000
H	5.99154700	-0.16436000	2.03914100
H	6.02257500	-1.47783800	3.23561100
H	2.55578700	-2.71731000	2.62097500
H	3.89489400	-3.27125100	1.57298500

H	4.13767700	-3.14491100	3.33396600
H	1.27510300	1.94115800	-1.86691400
H	1.49522500	1.47297400	-3.56653500
H	0.74076800	0.34311500	-2.41147700
H	4.93671500	1.37371400	-2.14949400
H	3.84795400	2.17159700	-3.30352500
H	3.65143600	2.47516700	-1.56269700
H	2.62155800	-1.39975200	-3.18093700
H	3.17170200	-0.10333100	-4.26865200
H	4.31789300	-0.86358400	-3.14537100
H	4.19270200	-3.06943700	-1.01513400
H	6.27312900	-4.08708500	-1.91930200
H	8.34320600	-2.71613300	-2.12290300
H	8.32303000	-0.33124300	-1.40777300
H	6.25107400	0.67216100	-0.47954500
H	4.18704200	1.56708600	1.55711000
H	4.02750400	2.96342200	0.50649000
H	3.13712600	2.82136700	3.45140900
H	4.56003900	3.70148100	2.81939100
H	2.91174500	4.23731800	2.40469500
H	-0.26077700	1.67466600	1.15880900
P	0.32709300	-0.62027200	2.26922200
C	0.10970700	-0.67016200	0.43806000
C	-0.07010900	-2.05945100	-0.24413000
C	-0.04766100	-1.97777200	-1.76380500
H	-0.29039400	-2.95246300	-2.21797700
H	-0.77348300	-1.24082500	-2.13063600
H	0.94631600	-1.67639000	-2.11430100
C	-1.35960200	-2.73350100	0.22839600
H	-2.24446300	-2.22977400	-0.18097100
H	-1.39732700	-3.78316100	-0.10693400
H	-1.41328800	-2.71789300	1.32778800

C	1.08293100	-2.98514100	0.16027500
H	2.05643900	-2.53607600	-0.07781900
H	1.05535100	-3.18438100	1.23867800
H	1.00329800	-3.94043800	-0.38554700

IV.2 TS 1-2 P
O 1

Si	-2.11834900	-0.62788300	-0.10863400
N	-2.65572700	1.12555800	0.50688600
N	-3.93810900	-0.20095500	-0.59260200
N	-2.30865200	-1.58510200	1.39708200
Si	2.09369300	-0.49773900	0.09949100
C	-2.04708300	2.23296700	1.24605100
C	-3.83405800	1.02365500	-0.08387000
C	-4.92464600	-0.79622100	-1.49537800
C	-3.53259500	-1.67728800	2.16396900
C	-1.23781800	-2.42148800	1.72529400
N	2.34224300	-2.03765500	0.96439900
N	3.32217000	0.69476100	0.94115600
C	0.03233300	-1.89322300	1.52720700
C	-0.91915900	1.63033600	2.07832300
C	-3.03428200	2.91636200	2.19602300
C	-1.45942900	3.25491900	0.26676000
C	-4.84323100	2.10499400	-0.19432700
C	-5.04175500	-2.26667700	-1.08838900
C	-6.32504500	-0.18737800	-1.40136100
C	-4.40699400	-0.63909900	-2.92983900
C	-3.37271200	-1.27378500	3.62161500
C	-1.32548200	-3.75668400	2.16300300
C	1.20028900	-2.65570100	1.48608100
C	3.63010800	-2.68271500	1.12065700
C	3.27013900	1.55927100	2.11795000

C	4.07973000	0.71839600	-0.14936400
C	-4.74204100	3.03046700	-1.23676600
C	-5.89339000	2.20379800	0.72305200
C	-0.14787900	-4.49741700	2.27332300
C	1.10669600	-3.99036300	1.91573000
C	4.18007000	-2.64681800	2.53892600
C	2.41317800	0.82193000	3.14907300
C	2.61888600	2.89799900	1.75492700
C	4.65977600	1.79388200	2.71329100
N	3.64753900	-0.26366700	-0.95066200
C	5.14868800	1.70299500	-0.45143000
C	-5.68878100	4.04563500	-1.36124300
C	-6.83477500	3.22003900	0.59703100
C	3.98041600	-0.55362800	-2.35172400
C	6.47630400	1.42390500	-0.10999500
C	4.83314700	2.91855400	-1.06607400
C	-6.73532600	4.14203500	-0.44573000
C	3.41917000	-1.94230500	-2.64311600
C	5.49211000	-0.57742600	-2.58381200
C	3.30788100	0.47003000	-3.27081900
C	7.47744900	2.35084100	-0.38334300
C	5.83888400	3.84379400	-1.33957200
C	7.16064700	3.56194900	-0.99914500
H	-2.28822000	-4.22037900	2.38463800
H	-0.21104600	-5.53555600	2.61151600
H	1.97992300	-4.64258300	1.94956400
H	3.56160500	-3.72913100	0.76867600
H	4.33621700	-2.18474500	0.43937200
H	4.38084500	-1.61089600	2.84912500
H	3.46823600	-3.08312300	3.25560100
H	5.12245600	-3.21276700	2.60694100
H	1.42985000	0.56010800	2.73568100

H	2.89742900	-0.11095600	3.46759300
H	2.25364000	1.45439500	4.03443000
H	2.46186400	3.50913100	2.65702900
H	3.25692200	3.47022800	1.06620200
H	1.64521500	2.73300800	1.27244100
H	5.17489700	0.83718400	2.88848500
H	5.29068900	2.41731000	2.06639600
H	4.55942700	2.30840100	3.68074300
H	3.86560500	-2.69833400	-1.98019600
H	2.33127300	-1.95520800	-2.50186000
H	3.62602600	-2.22547000	-3.68521600
H	5.69294500	-0.96857000	-3.59225900
H	5.94507000	0.41997100	-2.51923100
H	5.99127000	-1.23789700	-1.85799200
H	2.22638100	0.51383100	-3.05839600
H	3.73878300	1.47181300	-3.12605300
H	3.45088100	0.19097600	-4.32605600
H	6.71960300	0.47393300	0.37071200
H	8.51217100	2.12652700	-0.11473900
H	7.94765500	4.28832900	-1.21437900
H	5.58656000	4.79036500	-1.82282600
H	3.79680800	3.13576500	-1.33364500
H	-0.43158100	2.41190100	2.67816600
H	-1.29506900	0.84798600	2.75222400
H	-0.17286100	1.18163600	1.40756500
H	-3.79353400	3.50598000	1.66719300
H	-3.54414000	2.17558700	2.83099000
H	-2.47975500	3.60242500	2.85405700
H	-0.77136500	2.74792900	-0.42592600
H	-2.25324700	3.74480000	-0.31612700
H	-0.91055400	4.03752100	0.81407700
H	-5.54449200	-2.34955600	-0.11328000

H	-5.62816300	-2.83050200	-1.82906300
H	-4.05559700	-2.73370300	-1.00181000
H	-6.37383500	0.84430600	-1.77163300
H	-7.00164600	-0.79553100	-2.02066400
H	-6.70664900	-0.20711600	-0.37031100
H	-3.36809000	-0.98671200	-3.00586100
H	-5.03292700	-1.19837100	-3.64233200
H	-4.42366000	0.42381500	-3.21764000
H	-3.92376600	2.94469900	-1.95534500
H	-5.60811700	4.76419300	-2.18005100
H	-7.47673300	4.93828200	-0.54410500
H	-7.65287000	3.29386700	1.31709200
H	-5.96638400	1.48188500	1.53937500
H	-4.28349600	-1.03793200	1.67784500
H	-3.94708100	-2.70328500	2.10881600
H	-3.06249900	-0.22106200	3.70450200
H	-4.31869000	-1.39863800	4.17206500
H	-2.60739600	-1.88948000	4.11846500
H	0.10287000	-0.83108900	1.28573000
P	-0.07115100	0.06538600	-1.28312500
C	-1.12373800	-1.34084200	-1.39002100
C	-0.84922100	-2.59931900	-2.21747800
C	0.22018700	-3.44716100	-1.51868600
H	0.54639800	-4.28100400	-2.16371100
H	1.10381400	-2.85032900	-1.25884400
H	-0.16976600	-3.86778300	-0.58119000
C	-0.36423400	-2.18564000	-3.61040400
H	0.46604400	-1.46603800	-3.53416500
H	-0.02232400	-3.05662200	-4.19382800
H	-1.17166300	-1.68699900	-4.17009300
C	-2.07552300	-3.49815800	-2.36836900
H	-2.43491600	-3.82975000	-1.38200100

H	-2.89887600	-2.99858100	-2.89608200
H	-1.81348300	-4.40155600	-2.94352000

IV.2 TS 2-3

0 1

Si	1.98631800	-0.80403600	0.35156600
N	3.01243300	0.06559200	-0.95814000
N	3.55953800	0.03207800	1.12916900
N	2.53937400	-2.53608800	0.47730500
Si	-1.73166700	-0.22434100	0.07365200
C	2.85253300	0.33372900	-2.39249500
C	3.81488300	0.60706700	-0.03363700
C	4.00721500	0.38029300	2.48063400
C	3.80634500	-3.17601300	0.70685100
C	1.60690000	-3.00912800	-0.43305500
N	-1.32428600	-1.01952500	-1.48767300
N	-2.75459500	1.31093000	-0.23895500
C	0.55923800	-2.05283500	-0.46006600
C	2.65352100	-1.01249200	-3.08996800
C	4.06577100	1.00579000	-3.03751600
C	1.61356200	1.21172500	-2.56862300
C	4.75326000	1.73559900	-0.25927000
C	3.30710500	-0.59395600	3.42684900
C	5.52175800	0.20429600	2.61553400
C	3.59034100	1.80549200	2.85837600
C	4.84186300	-2.95935400	-0.39128700
C	1.65315000	-4.04947700	-1.36100900
C	-0.36953600	-2.01727400	-1.52225900
C	-2.16898600	-0.82789600	-2.65061900
C	-2.46596100	2.75596700	-0.17005200
C	-3.91669900	0.64702600	-0.09104900
C	4.25117300	3.04113500	-0.27308000

C	6.11551400	1.51278800	-0.46992600
C	0.66931600	-4.04427600	-2.36330000
C	-0.30095900	-3.04800400	-2.48799000
C	-1.45244600	-0.20732500	-3.83953700
C	-1.22793300	3.00320200	-1.03339000
C	-2.19147700	3.14260800	1.28588600
C	-3.59675700	3.62327200	-0.72680300
N	-3.64938300	-0.63647000	0.02716500
C	-5.26530700	1.26059300	-0.00995700
C	5.10893400	4.11413800	-0.49958500
C	6.96966000	2.58836700	-0.70201400
C	-4.53157900	-1.80880900	-0.05008200
C	-6.00938300	1.54942500	-1.15723900
C	-5.79213600	1.55555800	1.25128800
C	6.46824300	3.88919300	-0.71740400
C	-3.61904700	-3.03386700	-0.15418800
C	-5.42563700	-1.77017900	-1.29583400
C	-5.42706500	-1.92066100	1.18810500
C	-7.26677600	2.13493400	-1.04291000
C	-7.04865600	2.14685800	1.36143500
C	-7.78704800	2.43784700	0.21536200
H	2.44744600	-4.79820400	-1.36346100
H	0.68591400	-4.84101900	-3.11271800
H	-1.00352500	-3.09484900	-3.32059800
H	-2.62948100	-1.78776800	-2.95157600
H	-3.00250900	-0.17334600	-2.36413700
H	-1.11947500	0.81245100	-3.60195100
H	-0.56650200	-0.79230800	-4.12670400
H	-2.12659900	-0.15693800	-4.70896100
H	-0.38776900	2.38987000	-0.68103300
H	-1.43697100	2.74971700	-2.08414600
H	-0.94217300	4.06449300	-0.98264700

H	-1.94459100	4.21309300	1.35963300
H	-3.08016000	2.95291100	1.90799200
H	-1.34715100	2.56037000	1.68615400
H	-3.88815900	3.30391700	-1.73828700
H	-4.49036900	3.63391700	-0.09074300
H	-3.22810000	4.65739100	-0.79544100
H	-3.06067200	-3.03734700	-1.10014100
H	-2.88143700	-3.05573900	0.65849400
H	-4.21833400	-3.95449700	-0.10449500
H	-5.94716700	-2.73367800	-1.39896500
H	-6.19124000	-0.98631200	-1.22694700
H	-4.83277500	-1.60876500	-2.20660800
H	-4.83101900	-1.95225600	2.10750900
H	-6.12424000	-1.07337100	1.25090100
H	-6.02497400	-2.84295200	1.13169000
H	-5.59634400	1.32139100	-2.14206700
H	-7.84353400	2.35990500	-1.94282800
H	-8.77253000	2.90103700	0.30241600
H	-7.45277600	2.38022800	2.34901400
H	-5.20875000	1.32389000	2.14542300
H	2.49264700	-0.85755500	-4.16743000
H	3.54156700	-1.64745800	-2.95962800
H	1.78668300	-1.55101900	-2.69191900
H	4.22138100	2.03852000	-2.70340600
H	4.98758500	0.43575800	-2.85098000
H	3.90120100	1.02950700	-4.12488000
H	0.74294000	0.74239300	-2.08880800
H	1.76839800	2.19487900	-2.09894700
H	1.39346600	1.36734000	-3.63576900
H	3.57381900	-1.63606200	3.20061800
H	3.59002000	-0.38288800	4.46820400
H	2.21739600	-0.49072400	3.33765200

H	6.07401300	0.94833000	2.02605700
H	5.81907500	0.32441200	3.66842700
H	5.82519900	-0.80105300	2.28514800
H	2.51016900	1.93420600	2.68431900
H	3.80070500	1.98935800	3.92312700
H	4.13889300	2.55729700	2.27465800
H	3.18443100	3.20707500	-0.10467200
H	4.71315000	5.13224200	-0.50785100
H	7.13968900	4.73160100	-0.89901100
H	8.03345700	2.40892600	-0.87327600
H	6.50289900	0.49147600	-0.46379500
H	4.21198000	-2.80786200	1.66215200
H	3.63549000	-4.25831500	0.85111000
H	5.08251300	-1.89070100	-0.49018700
H	5.77286700	-3.50282700	-0.16499400
H	4.46972400	-3.30974500	-1.36545000
P	0.35449600	0.59649400	1.11100000
C	-0.88570100	-0.69607900	1.54183000
C	-1.03164100	-1.30610300	2.93733000
C	-2.46440500	-1.75996000	3.20251100
H	-2.56900500	-2.15370900	4.22727400
H	-3.16323400	-0.91772500	3.08350100
H	-2.76635900	-2.55803600	2.51157000
C	-0.67563800	-0.27018600	4.00855500
H	-1.36710200	0.58589200	3.96097400
H	-0.73202500	-0.71396000	5.01673900
H	0.33597900	0.13169400	3.85576600
C	-0.09760000	-2.51777300	3.06822200
H	-0.40139500	-3.31962100	2.37719200
H	0.93932300	-2.25228800	2.81394800
H	-0.10396400	-2.92503800	4.09338100
H	-0.09318700	-1.70682700	0.56653200

IV.2 TS 0-4

0 1

Si	-1.70980700	0.43562500	-0.15440300
N	-3.30154200	-0.26230100	-1.00046400
N	-3.09913100	0.04662700	1.10767300
N	-1.97588400	2.19355000	-0.35181900
Si	2.23759500	0.84382600	0.62842500
C	-3.48847500	-0.90128700	-2.30305100
C	-3.84151400	-0.55721200	0.18744000
C	-3.19808400	0.15965800	2.55675200
C	-3.28391300	2.80684800	-0.38081700
C	-0.83657700	3.01039300	-0.32805900
N	2.72324900	2.46693200	0.25612300
N	2.64393400	-0.41085400	-0.67777500
C	0.41548500	2.40454200	-0.14716400
C	-2.50453800	-0.22041200	-3.25688300
C	-4.91407000	-0.69444300	-2.82050800
C	-3.15821700	-2.39697600	-2.24188500
C	-4.99168600	-1.46256100	0.44746100
C	-2.26088800	1.30335500	2.95426500
C	-4.62368000	0.49766300	2.99645600
C	-2.72432900	-1.13287000	3.23085300
C	-3.76727400	3.21676100	-1.76581700
C	-0.90151200	4.41351400	-0.48520600
C	1.55735900	3.20478700	-0.03959200
C	4.04219700	3.02950700	0.13683200
C	2.14551700	-0.78116400	-2.01277500
C	3.67783500	-0.85983000	0.03449000
C	-4.78540800	-2.77780700	0.87754700
C	-6.29917400	-0.99140400	0.28514600
C	0.26301800	5.17834500	-0.40596100

C	1.51008100	4.60234300	-0.17233400
C	4.48988000	3.20720200	-1.30833400
C	1.52671200	0.47863600	-2.61775800
C	1.07529300	-1.86499600	-1.86306800
C	3.27037100	-1.26234400	-2.93139700
N	3.81488300	-0.04664000	1.09296800
C	4.47873100	-2.07261300	-0.24947200
C	-5.87193300	-3.60940700	1.13975600
C	-7.38402500	-1.82217300	0.55387300
C	4.48364400	-0.26593000	2.38028200
C	5.79173900	-1.95586100	-0.71654900
C	3.91647200	-3.34123600	-0.07163400
C	-7.17252400	-3.13264700	0.98109300
C	4.09969700	0.92201800	3.26455000
C	6.00413900	-0.29459300	2.21380600
C	3.99086200	-1.55842200	3.03706500
C	6.53089600	-3.09789500	-1.01275600
C	4.66311100	-4.48137600	-0.35784400
C	5.96866700	-4.36128800	-0.83274800
H	-1.84658600	4.91989500	-0.68873600
H	0.19010100	6.26294900	-0.52865800
H	2.40191000	5.22767400	-0.08664600
H	4.08509200	3.99935400	0.66613000
H	4.74920700	2.36526200	0.65744100
H	4.54095600	2.23184000	-1.81746600
H	3.77785700	3.83724500	-1.86215300
H	5.48377100	3.67900800	-1.36333900
H	0.76760800	0.90852500	-1.94280100
H	2.29330100	1.25184700	-2.77779500
H	1.06445600	0.24091300	-3.58738200
H	0.63548900	-2.10178400	-2.84414000
H	1.50411200	-2.79139500	-1.45260700

H	0.27359500	-1.50898900	-1.19598900
H	4.09713100	-0.53570200	-2.95633000
H	3.67333000	-2.24202900	-2.64355200
H	2.87246500	-1.35375700	-3.95267700
H	4.43908900	1.87125900	2.82571300
H	3.00691200	0.97597400	3.39127500
H	4.55714500	0.81782000	4.25902300
H	6.48776400	-0.31681000	3.20197600
H	6.33664200	-1.18165200	1.65842300
H	6.35208800	0.60375300	1.68182300
H	2.89366200	-1.54411800	3.12621700
H	4.28421900	-2.44381300	2.45547900
H	4.41853200	-1.66204200	4.04592300
H	6.22336900	-0.96386300	-0.86505600
H	7.55184500	-3.00065200	-1.38860000
H	6.55062200	-5.25638800	-1.06402600
H	4.22117700	-5.46959800	-0.21202500
H	2.89281600	-3.42955300	0.29811300
H	-2.57830600	-0.66088800	-4.26213600
H	-2.70483000	0.85733900	-3.33089000
H	-1.47149900	-0.34396700	-2.89772400
H	-5.65031000	-1.23773100	-2.21272700
H	-5.17544300	0.37422200	-2.81236300
H	-4.99625300	-1.06148100	-3.85500400
H	-2.14561000	-2.54293300	-1.83566600
H	-3.87259400	-2.94201800	-1.60880900
H	-3.19532700	-2.84109700	-3.24884900
H	-2.57389500	2.24906300	2.48995100
H	-2.25219600	1.43020900	4.04688300
H	-1.23018000	1.09555500	2.62476800
H	-5.32225100	-0.32630800	2.79566700
H	-4.64253100	0.69935600	4.07821800

H	-4.98501400	1.39658400	2.47421200
H	-1.71793800	-1.39545000	2.87139700
H	-2.68362200	-1.00626700	4.32393900
H	-3.40520800	-1.96787400	3.01269900
H	-3.76564800	-3.15002000	0.99741000
H	-5.70137600	-4.63664200	1.47042400
H	-8.02387600	-3.78442100	1.19067800
H	-8.40114200	-1.44342900	0.42968600
H	-6.45928600	0.03727400	-0.04553500
H	-4.00655400	2.09686600	0.05263700
H	-3.29044200	3.68665300	0.28997000
H	-3.88930600	2.33073500	-2.40466900
H	-4.74067600	3.73026800	-1.70657900
H	-3.05354700	3.89181800	-2.26032300
H	0.76428000	1.01695800	0.93559100

IV.2 TS 1-5

0 1

Si	-1.96683100	-0.03703900	0.04666600
N	-3.30157400	-1.30537200	-0.34292200
N	-3.85662900	0.65097200	0.38582000
N	-1.63947400	0.90404800	-1.40197200
Si	2.59434400	0.89081900	0.23471500
C	-3.24954200	-2.74415700	-0.64881300
C	-4.32526100	-0.52766000	0.05725700
C	-4.57017100	1.91303900	0.60256500
C	-2.50268000	0.75736100	-2.55948000
C	-0.68685700	1.95408600	-1.43218500
N	2.76176300	2.49929200	-0.41506800
N	3.26752300	-0.50647000	-0.78016000
C	0.58276500	1.79621100	-0.88129000
C	-2.11696000	-2.95224200	-1.66023800

C	-4.53214900	-3.27024300	-1.29950700
C	-2.98157300	-3.53885200	0.63395000
C	-5.74210600	-0.96314200	0.15786200
C	-3.51009900	2.98040100	0.86854800
C	-5.35366100	2.32201500	-0.65008300
C	-5.52364900	1.83441200	1.79953300
C	-1.74083400	0.40624100	-3.82833700
C	-1.00406500	3.17542600	-2.07705900
C	1.50808400	2.84797600	-0.95786000
C	3.94953000	3.26350700	-0.68842400
C	2.87337400	-1.32865600	-1.93665000
C	4.34850400	-0.58299700	0.00305200
C	-6.19262000	-1.49814500	1.36926100
C	-6.62450600	-0.85747100	-0.92083400
C	-0.07254700	4.20776600	-2.12305200
C	1.19944600	4.07315300	-1.56087100
C	4.46673800	3.08478700	-2.11082200
C	1.64501300	-0.67953300	-2.56663200
C	2.50243600	-2.74547600	-1.48715200
C	4.00196000	-1.36754100	-2.96969700
N	4.29111100	0.44585800	0.85956700
C	5.39560200	-1.63278300	-0.02173800
C	-7.51073200	-1.92923100	1.49651800
C	-7.94298400	-1.28464900	-0.78872700
C	4.98467600	0.67584700	2.13178100
C	6.62637600	-1.36964500	-0.63257700
C	5.17205900	-2.87806500	0.57519200
C	-8.38824800	-1.82326600	0.41810600
C	4.31441300	1.89463300	2.76988800
C	6.46555300	0.97597900	1.89313400
C	4.82310800	-0.51966000	3.07514800
C	7.61951800	-2.34569900	-0.65401100

C	6.17092200	-3.84864000	0.55892900
C	7.39347000	-3.58547900	-0.05753600
H	-1.97316200	3.31954700	-2.56000000
H	-0.34188200	5.14486800	-2.61864800
H	1.91786700	4.89455000	-1.61709700
H	3.75748100	4.33304000	-0.48726000
H	4.73267200	2.95811000	0.02210600
H	4.74176200	2.03301900	-2.28812200
H	3.69402400	3.35692900	-2.84530900
H	5.35425100	3.71055700	-2.29560700
H	0.80928400	-0.61444700	-1.85437900
H	1.85937400	0.34454900	-2.90247700
H	1.32549400	-1.27592300	-3.43423400
H	2.04869400	-3.29431500	-2.32598500
H	3.38139000	-3.31367800	-1.15427300
H	1.77080600	-2.70285700	-0.66595200
H	4.28723500	-0.34658800	-3.26590000
H	4.89301500	-1.88849800	-2.59339900
H	3.65910100	-1.89967400	-3.86947800
H	4.39267400	2.78075000	2.12442800
H	3.24620100	1.69947600	2.95352500
H	4.79155600	2.12587300	3.73312700
H	6.95037700	1.25386900	2.84106400
H	6.99486800	0.10264800	1.48809800
H	6.58303800	1.81315500	1.18858900
H	3.75788300	-0.77168400	3.19186500
H	5.35663600	-1.40559200	2.70523900
H	5.22980500	-0.27466000	4.06798200
H	6.79732200	-0.39695600	-1.09919300
H	8.57547600	-2.13582200	-1.13891100
H	8.17388600	-4.34975300	-0.07239700
H	5.99154700	-4.81725900	1.03085200

H	4.21446100	-3.07908100	1.05976900
H	-1.99366300	-4.02574200	-1.86742000
H	-2.35260100	-2.44314700	-2.60680200
H	-1.16701400	-2.55262900	-1.28327500
H	-5.38131100	-3.31748700	-0.60684800
H	-4.82047000	-2.65797200	-2.16656200
H	-4.34054100	-4.29221600	-1.65939300
H	-2.04097800	-3.22173900	1.10725500
H	-3.79753300	-3.38590500	1.35703400
H	-2.91540600	-4.61611900	0.41608400
H	-2.77297400	3.02011800	0.05349100
H	-3.98483600	3.96836500	0.95807400
H	-2.97412800	2.77703100	1.80326600
H	-6.18022800	1.62961100	-0.85713200
H	-5.78623200	3.32433100	-0.51057800
H	-4.69028400	2.35507100	-1.52566800
H	-4.99745400	1.47620000	2.69622400
H	-5.92830000	2.83449000	2.01795400
H	-6.37210300	1.16415600	1.60623200
H	-5.50300400	-1.57079800	2.21341200
H	-7.85491700	-2.34774700	2.44502500
H	-9.42244200	-2.16048600	0.51840800
H	-8.62672600	-1.20062300	-1.63648500
H	-6.27117800	-0.45263900	-1.87134500
H	-3.22859200	-0.03981700	-2.34443700
H	-3.10748300	1.66707800	-2.73522300
H	-1.21479200	-0.55245300	-3.70836000
H	-2.42508900	0.32629400	-4.68807800
H	-0.98849200	1.17483800	-4.05956500
P	-0.25885400	-1.28917400	0.90154000
C	-1.05013700	0.05190700	1.60557400
C	-0.82889500	0.70791700	2.95014300

C	-0.32388900	2.14042400	2.72222500
H	-0.19982900	2.66155200	3.68602500
H	0.64991100	2.13181300	2.20969100
H	-1.01014000	2.72294000	2.09474300
C	0.22103900	-0.06141100	3.75235300
H	1.16925800	-0.10978800	3.19295500
H	0.40802000	0.42946700	4.72089600
H	-0.10316100	-1.09664300	3.94145400
C	-2.15057100	0.72028700	3.72480000
H	-2.93385500	1.24438200	3.16173600
H	-2.50113500	-0.30830800	3.90527400
H	-2.02977100	1.21933400	4.70052700
H	1.11580900	0.79502600	0.49063200

IV.2 TS 2-6

0 1

P	0.18177300	0.66442900	0.74025200
Si	1.95433800	-0.32637700	-0.26833600
C	-0.88637900	-0.41852400	1.63855900
N	3.09216100	1.06338400	-0.79705100
N	3.68420700	-0.59359000	0.44221100
N	1.78725200	-1.44502600	-1.58517700
Si	-2.08451300	-0.90259400	0.35993000
C	-0.33865500	-1.30722000	2.76646800
C	2.87827000	2.41944400	-1.32715800
C	4.06157500	0.60292100	0.00509400
C	4.39941800	-1.63713400	1.18749900
C	2.85899200	-1.62404900	-2.54714900
C	0.66387700	-2.31348800	-1.61038300
N	-2.66100500	-2.47100000	-0.20062000
N	-2.67765300	0.45083400	-0.80109000
C	-0.53457800	-1.94555800	-0.97589100

C	0.55013100	-2.41015400	2.18487100
C	0.48094700	-0.44715200	3.73520400
C	-1.43351100	-2.01025500	3.56652200
C	1.62911000	2.33425000	-2.19679300
C	4.05316800	2.86381100	-2.20032900
C	2.64144800	3.41336100	-0.18738200
C	5.28711100	1.32563100	0.42022900
C	3.86151400	-2.98279100	0.69140200
C	5.90639900	-1.60907200	0.92386100
C	4.13361200	-1.47277900	2.68542400
C	2.44836300	-1.29847700	-3.97478900
C	0.76711400	-3.55604500	-2.27354300
C	-1.58034200	-2.90019300	-0.96581400
C	-3.95136200	-3.10034800	-0.26645400
C	-2.44223600	0.99855400	-2.16019300
C	-3.71841300	0.75697500	-0.00963500
C	5.33275100	1.90161900	1.69398200
C	6.40290800	1.40261200	-0.41845500
C	-0.31077700	-4.43250500	-2.29468300
C	-1.49938000	-4.12654900	-1.63701400
C	-4.73176300	-2.77497400	-1.53334300
C	-1.35467400	0.20869000	-2.88370500
C	-2.01065100	2.46797800	-2.07573100
C	-3.70578200	0.86542000	-3.01952100
N	-3.82104400	-0.13531100	0.95523500
C	-4.52963200	2.00072300	-0.11438200
C	6.48740000	2.55244800	2.12238500
C	7.55765600	2.04550500	0.01764300
C	-4.54788300	-0.00669300	2.23180400
C	-5.80181800	2.02252900	-0.69128000
C	-4.00130900	3.17027600	0.44082100
C	7.60150300	2.62170200	1.28722800

C	-4.73571400	-1.41984000	2.78625000
C	-5.95589700	0.58644000	2.09848300
C	-3.72285900	0.86099600	3.19091700
C	-6.53781100	3.20379500	-0.71501900
C	-4.74432400	4.34835700	0.42582300
C	-6.01252500	4.36735400	-0.15316000
H	1.68876200	-3.84409500	-2.77915500
H	-0.21627200	-5.38277600	-2.82733300
H	-2.33382600	-4.83030800	-1.63907500
H	-3.82975500	-4.19475900	-0.16951500
H	-4.53089800	-2.78414400	0.60909400
H	-4.96453100	-1.69997700	-1.57132600
H	-4.14955900	-3.02783300	-2.43287500
H	-5.68102800	-3.33268300	-1.57140200
H	-0.38808300	0.25964600	-2.37273500
H	-1.62265200	-0.85070900	-2.98363900
H	-1.23410200	0.63619900	-3.89033300
H	-1.61753700	2.80104100	-3.04823800
H	-2.84550700	3.12878300	-1.80987000
H	-1.22141300	2.58218000	-1.31952200
H	-4.04107700	-0.18158200	-3.04838000
H	-4.52808300	1.49550100	-2.66213100
H	-3.47979100	1.17760300	-4.05011800
H	-5.49940000	-1.96007400	2.20707700
H	-3.80715200	-1.99650800	2.75654400
H	-5.07713200	-1.37471700	3.83068400
H	-6.48632900	0.41985800	3.04846300
H	-5.95799100	1.66574500	1.90853400
H	-6.52685800	0.08438800	1.30301700
H	-2.66719100	0.55257900	3.16949000
H	-3.76272900	1.91450400	2.87580600
H	-4.12330800	0.79955300	4.21481400

H	-6.22116100	1.10570900	-1.11062300
H	-7.53156900	3.21421100	-1.16835400
H	-6.59416500	5.29205700	-0.16711300
H	-4.32808200	5.25709400	0.86652900
H	-3.00286500	3.14565500	0.88389300
H	1.29611000	-1.96773700	1.50425000
H	1.10044000	-2.96920300	2.96208800
H	-0.03998400	-3.11989500	1.58705000
H	-0.15586400	0.32287500	4.19722000
H	0.93161900	-1.05934600	4.53540300
H	1.29151600	0.07615500	3.20271000
H	-2.01698100	-2.67877500	2.91432400
H	-0.98812400	-2.63726900	4.35658500
H	-2.11561600	-1.29610300	4.04687200
H	1.38413400	3.32245600	-2.61142000
H	1.77552700	1.63202200	-3.02993100
H	0.77316300	1.99132000	-1.60029500
H	4.95563500	3.07302400	-1.61221500
H	4.28853700	2.09673900	-2.95405000
H	3.78066900	3.78891100	-2.72975900
H	1.80822800	3.06729700	0.44347400
H	3.53993200	3.52628200	0.43659000
H	2.38838900	4.40381100	-0.59522100
H	4.11006800	-3.13104300	-0.36908300
H	4.31428500	-3.80085400	1.27028400
H	2.77178100	-3.05712500	0.79603500
H	6.40305900	-0.74308600	1.37914300
H	6.35459000	-2.51541400	1.35686200
H	6.12001400	-1.61019200	-0.15578000
H	3.05735100	-1.48469900	2.89821900
H	4.60737300	-2.29051500	3.24916800
H	4.54857300	-0.52204800	3.05106500

H	4.45664800	1.84253100	2.34371400
H	6.51653600	3.00581400	3.11566000
H	8.50855100	3.12691300	1.62678300
H	8.43014800	2.09574700	-0.63748700
H	6.36813600	0.94370200	-1.40851800
H	3.68796500	-0.96315800	-2.25026900
H	3.26534200	-2.65080200	-2.49462400
H	2.13553300	-0.24695300	-4.05572300
H	3.28520300	-1.46604000	-4.67068100
H	1.60307000	-1.92384200	-4.29598700
H	-0.18180500	-0.38506100	-0.54729200

IV.2 TS 6-3

O 1

P	0.41111000	0.60332000	1.28528000
Si	1.86996500	-0.33058000	-0.26179100
C	-1.01890200	-0.46669000	1.64421300
N	3.01907600	1.06160900	-0.68855300
N	3.59079100	-0.70927100	0.37881000
N	1.63304200	-1.32756600	-1.66486300
Si	-1.77087400	-1.00836900	0.05701600
C	-0.87026600	-1.38604700	2.87792800
C	2.81428000	2.45477300	-1.10984900
C	4.00013700	0.50855400	0.04652300
C	4.24027200	-1.82941400	1.06312400
C	2.65125600	-1.39062600	-2.70085600
C	0.63560400	-2.33137500	-1.60544600
N	-2.58454400	-2.60486000	-0.12140700
N	-2.53004900	0.36677200	-0.83854800
C	-0.56671800	-2.10064400	-0.94910100
C	0.25585600	-2.37775300	2.57741700
C	-0.49712900	-0.56530300	4.11720400

C	-2.14564200	-2.16327300	3.19291400
C	1.47904600	2.46387200	-1.84720500
C	3.92223400	2.89911900	-2.06540700
C	2.73229200	3.38745900	0.10083300
C	5.25503800	1.15935200	0.48720400
C	3.44908900	-3.07957900	0.67236200
C	5.68807700	-1.99335700	0.59913000
C	4.18723900	-1.62626600	2.57948200
C	2.10032300	-1.14826500	-4.09649400
C	0.83630900	-3.59538700	-2.21014100
C	-1.53696000	-3.12928100	-0.85845300
C	-3.85950400	-3.23683300	0.03997100
C	-2.42638900	0.74180400	-2.28119400
C	-3.59700800	0.84995700	-0.07588300
C	5.34494800	1.65909700	1.79097900
C	6.35407600	1.25378000	-0.37235200
C	-0.15082500	-4.57577000	-2.13472400
C	-1.35949600	-4.37766400	-1.46068000
C	-4.82197300	-2.98142500	-1.11134300
C	-1.32267500	-0.05661900	-2.96535400
C	-2.08864700	2.22844700	-2.49024100
C	-3.74111100	0.39490000	-2.98720000
N	-4.13508700	0.02244800	0.74182900
C	-3.88593600	2.32178200	-0.15622300
C	6.52742900	2.25135900	2.22781800
C	7.53599900	1.84014800	0.07208400
C	-5.06685000	0.33266900	1.83254200
C	-5.00113400	2.85641000	-0.80808200
C	-2.97346600	3.19404200	0.44749400
C	7.62388700	2.33998000	1.37114900
C	-5.57538400	-1.01458400	2.35471200
C	-6.30890600	1.13620900	1.42136300

C	-4.31732000	1.07133700	2.94721900
C	-5.19239200	4.23472400	-0.86949900
C	-3.17180000	4.57123800	0.40119500
C	-4.27841400	5.09674000	-0.26477000
H	1.76039500	-3.81799800	-2.74367000
H	0.03293500	-5.53798500	-2.62148500
H	-2.12080600	-5.15858100	-1.42092400
H	-3.70585600	-4.32372100	0.17276500
H	-4.30925100	-2.87499900	0.97343100
H	-5.04539100	-1.90614500	-1.17354000
H	-4.38690900	-3.30291600	-2.07088200
H	-5.76954400	-3.52478800	-0.96616900
H	-0.34825400	0.09394100	-2.48368800
H	-1.53250200	-1.13288300	-2.97035800
H	-1.24391800	0.28004900	-4.00962700
H	-1.75052100	2.37752100	-3.52696200
H	-2.93862700	2.89854300	-2.32416400
H	-1.27901600	2.53611300	-1.81716000
H	-3.94889400	-0.68077900	-2.89670600
H	-4.59232900	0.94438500	-2.56402100
H	-3.68040800	0.64919300	-4.05673000
H	-6.13949200	-1.53783200	1.56757900
H	-4.74293300	-1.65731700	2.66267900
H	-6.24258900	-0.86962200	3.21773800
H	-7.05412800	1.08245400	2.22981400
H	-6.09325800	2.19539200	1.24347100
H	-6.76648800	0.70946200	0.51542500
H	-3.37679000	0.55449300	3.18271900
H	-4.06652800	2.09615700	2.63836400
H	-4.93656800	1.13017400	3.85589100
H	-5.72643400	2.18947500	-1.27707900
H	-6.06343000	4.63754200	-1.39177300

H	-4.42973500	6.17781700	-0.31169400
H	-2.45167100	5.23825800	0.88112000
H	-2.09290100	2.78214300	0.94726600
H	1.15420300	-1.82901700	2.24362000
H	0.54370300	-2.96301600	3.46732600
H	-0.03022800	-3.07597900	1.77558700
H	-1.28052800	0.17548500	4.34156700
H	-0.37495300	-1.21946100	4.99677300
H	0.44379800	-0.01600200	3.95898800
H	-2.48417300	-2.74548900	2.32546900
H	-1.97176800	-2.86128800	4.02818400
H	-2.95139100	-1.48087100	3.49216600
H	1.23420300	3.47926100	-2.18962500
H	1.50571600	1.79965400	-2.72374900
H	0.67383300	2.12435000	-1.17797000
H	4.89166300	2.98954100	-1.55761900
H	4.02318200	2.18791900	-2.89952600
H	3.67258800	3.88494000	-2.48517700
H	1.96375200	3.02959200	0.80360500
H	3.69464600	3.44705600	0.62865200
H	2.46345000	4.40383100	-0.22411800
H	3.50487600	-3.26007300	-0.41062100
H	3.85280100	-3.95981100	1.19265600
H	2.38716400	-2.98697200	0.94204900
H	6.32967900	-1.16856100	0.93654700
H	6.09775500	-2.92710300	1.01171300
H	5.74029300	-2.05405300	-0.49875100
H	3.15368600	-1.45929800	2.91428600
H	4.57875200	-2.51575400	3.09553100
H	4.79655700	-0.76316600	2.88282800
H	4.47943000	1.59212700	2.45397100
H	6.59148500	2.64607300	3.24421700

H	8.55173600	2.80098300	1.71727000
H	8.39445400	1.90567100	-0.59999000
H	6.28404900	0.85361900	-1.38597700
H	3.40602500	-0.62351300	-2.47005100
H	3.18611400	-2.35779600	-2.66441400
H	1.66604800	-0.14039700	-4.17353400
H	2.89712000	-1.24126700	-4.85057700
H	1.30979100	-1.87252800	-4.34108300
H	-0.99545300	1.05575600	1.00873700

IV.2 Int2 – isomer 2

0 1

Si	1.62024300	0.39639400	0.49101000
N	3.12828000	-0.54607800	1.07432000
N	3.03786500	0.04334000	-1.01049600
N	2.19150700	2.11352900	0.63891600
Si	-1.61989300	0.39595100	0.49154400
C	3.56648900	-0.99253400	2.41580900
C	3.77491300	-0.55331900	-0.10974700
C	3.33378500	0.39033700	-2.40513000
C	3.56642800	2.55476900	0.66337900
C	1.20606300	3.04393200	0.32473300
N	-2.19171400	2.11292400	0.63985200
N	-3.12804700	-0.54636200	1.07432700
C	-0.00013800	2.76666000	0.94690700
C	3.09923600	0.05109900	3.43677800
C	5.08697700	-1.09478600	2.56370000
C	2.94660400	-2.35447300	2.73570100
C	5.08296300	-1.21679400	-0.35824200
C	2.16014800	1.25260300	-2.87802100
C	4.61096100	1.22724500	-2.56297000
C	3.49419600	-0.86202000	-3.27689100

C	3.81171800	3.60272500	1.73784300
C	1.22737400	4.06678300	-0.64181700
C	-1.20667100	3.04359300	0.32520900
C	-3.56676500	2.55375300	0.66445400
C	-3.56592700	-0.99338300	2.41574600
C	-3.77466800	-0.55362300	-0.10978100
C	5.09206700	-2.59469000	-0.59882600
C	6.28923300	-0.51111700	-0.34878000
C	-0.00077800	4.60391700	-1.04896800
C	-1.22862500	4.06643500	-0.64134200
C	-3.81216400	3.60178800	1.73882500
C	-3.09899700	0.05020100	3.43691800
C	-2.94545500	-2.35514800	2.73524000
C	-5.08633800	-1.09637800	2.56382400
N	-3.03766000	0.04284100	-1.01064600
C	-5.08290300	-1.21676900	-0.35821200
C	6.29556400	-3.25735000	-0.82834100
C	7.49067300	-1.17705700	-0.57355900
C	-3.33400100	0.39019300	-2.40510100
C	-6.28902900	-0.51085100	-0.34798800
C	-5.09232900	-2.59449500	-0.59970100
C	7.49709600	-2.55069800	-0.81445800
C	-2.16032300	1.25228300	-2.87823000
C	-4.61104200	1.22739200	-2.56247700
C	-3.49503200	-0.86199300	-3.27701200
C	-7.49065900	-1.17642100	-0.57283600
C	-6.29602200	-3.25679400	-0.82925000
C	-7.49741200	-2.54991900	-0.81455500
H	2.15585400	4.40683900	-1.10477200
H	-0.00104200	5.40860300	-1.78984200
H	-2.15736900	4.40625600	-1.10393900
H	-3.87458300	2.96327900	-0.31707300

H	-4.21267400	1.68536000	0.85132900
H	-3.57588400	3.20152200	2.73607200
H	-3.17665800	4.48567200	1.57771700
H	-4.86264800	3.93256100	1.73214500
H	-2.01268400	0.19532800	3.39537700
H	-3.58446600	1.01860000	3.24987600
H	-3.36912200	-0.28110700	4.45057500
H	-3.24746000	-2.68421900	3.74142400
H	-3.28234100	-3.11271500	2.01146300
H	-1.84751200	-2.29204400	2.70186300
H	-5.58810300	-0.15903000	2.28294000
H	-5.52720900	-1.91711200	1.98558300
H	-5.30657700	-1.28456400	3.62491200
H	-2.12322600	2.19369600	-2.31218600
H	-1.19772800	0.75203200	-2.72143100
H	-2.26472700	1.49128700	-3.94677700
H	-4.66902500	1.60310300	-3.59526300
H	-5.51687300	0.63726400	-2.37625900
H	-4.60669500	2.09444800	-1.88927500
H	-2.63248900	-1.53455900	-3.19982500
H	-4.39265600	-1.42693200	-2.98784100
H	-3.60743200	-0.57031600	-4.33244100
H	-6.28739200	0.56171100	-0.14511300
H	-8.42956600	-0.61841400	-0.55568700
H	-8.44171900	-3.07015800	-0.99052200
H	-6.29421600	-4.33279900	-1.01743800
H	-4.14994100	-3.14625700	-0.60223400
H	3.36972300	-0.27980800	4.45046900
H	3.58420400	1.01967500	3.24936800
H	2.01285000	0.19569800	3.39539200
H	5.52813900	-1.91554500	1.98571700
H	5.58823100	-0.15730100	2.28234700

H	5.30749700	-1.28244200	3.62482300
H	1.84863400	-2.29184300	2.70222700
H	3.28385000	-3.11213500	2.01219100
H	3.24869000	-2.68312100	3.74200000
H	2.12351300	2.19419400	-2.31225200
H	2.26422500	1.49127500	-3.94667400
H	1.19747400	0.75264600	-2.72073900
H	5.51671000	0.63686800	-2.37714700
H	4.66867400	1.60301400	-3.59574900
H	4.60707500	2.09423200	-1.88967400
H	2.63138600	-1.53419800	-3.19944400
H	3.60650300	-0.57052300	-4.33238000
H	4.39166100	-1.42726500	-2.98781900
H	4.14959000	-3.14629100	-0.60070000
H	6.29349000	-4.33347400	-1.01584800
H	8.44125100	-3.07122400	-0.99039300
H	8.42968900	-0.61921600	-0.55698800
H	6.28789900	0.56155000	-0.14646500
H	4.21267500	1.68654300	0.84988600
H	3.87388000	2.96458800	-0.31815000
H	3.57572200	3.20228700	2.73508500
H	4.86210100	3.93381300	1.73102600
H	3.17591800	4.48643600	1.57693600
H	0.00011500	2.09830500	1.80034800
P	0.00035400	-0.42996000	1.87201200
C	0.00020800	-0.39614700	-0.18617300
C	0.00018800	-1.80118400	-0.88411400
C	-1.21871000	-2.63389500	-0.48290600
H	-1.13177900	-3.64995900	-0.89985500
H	-1.28741900	-2.71736800	0.60995600
H	-2.14255300	-2.19379400	-0.87202100
C	1.21975200	-2.63338000	-0.48385800

H	1.28959300	-2.71653000	0.60895800
H	1.13280200	-3.64958900	-0.90044900
H	2.14304700	-2.19303500	-0.87399400
C	-0.00045300	-1.66237000	-2.40307700
H	-0.88260900	-1.12126400	-2.75350700
H	0.88075900	-1.12016000	-2.75422700
H	-0.00003600	-2.65587000	-2.88169000

V. References

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