Steric C-N Bond Activation on the Dimeric Macrocycle $[\{P(\mu\text{-NR})\}_2(\mu\text{-NR})]_2$

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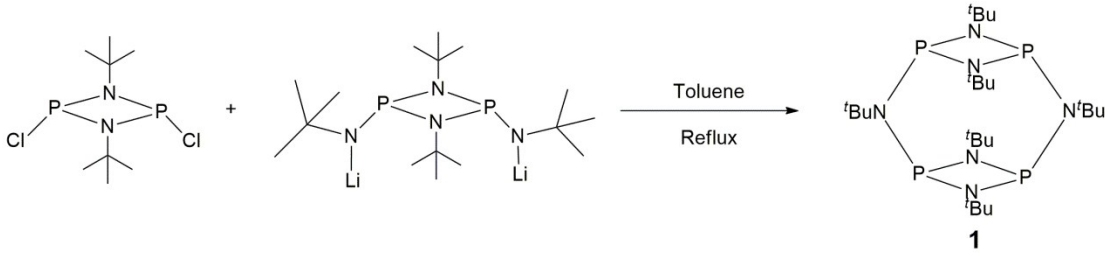
1 Experimental Section

Compounds **1-4** were prepared under dry, O_2-free Ar atmosphere on a double manifold (argon/vacuum) line. All solvents (toluene, THF, n-hexane, diethyl ether, n-pentane) were freshly distilled over appropriate drying agents (sodium/benzophenone) under nitrogen atmosphere, degassed and stored under molecular sieves. Starting material were either synthesized as described below or obtained commercially from Strem, Sigma-Aldrich, Alfa-Aesar and used without further purification. PCl_3, Et_3N were distilled from calcium hydride before use and stored under argon and molecular sieves. Starting material $[ClP(\mu\text{-}N^tBu)]_2$ was synthesized by the condensation of PCl_3 with primary amines in the presence of excess triethylamine as the Brønsted base as reported.[1] Compounds **1-4** were isolated and characterized with the aid of an Ar-filled innovative technology glove box. ^1H, ^{13}C and $^{31}P\{H\}$ NMR spectra were recorded on Bruker AV400 MHz spectrometer in the appropriate deuterated solvent (using the solvents resonances as the internal standard for ^1H and ^{13}C NMR and 85% $H_3PO_4 – D_2O$ as the external standard for ^{31}P NMR). In situ ^{31}P NMR spectroscopic studies on reaction mixtures in non-deuterated solvents were recorded using an internal d_6-acetone capillary to obtain a lock. Single crystal X-ray diffraction was carried out with Bruker X8 CCD diffractometer. Shimadzu IR Prestige-21 FTIR Spectrometer was used to record the IR data and elemental analysis data performed using Euro Vector Euro EA Elemental Analyzer (CHNS).

1.1 Synthesis of $P_4(\mu\text{-}N^tBu)_6$ (1)

The method was adopted from: Brask, J. K.; Chivers, T.; Krahn, M. L.; Parvez, M. *Inorg. Chem.* **1999**, *38*, 290-295. To a solution of $\{Li[P(N^tBu)_2]\}_2 \cdot 2THF$ (4.89 g, 9.74 mmol)[1] in toluene (50 mL) at 0 °C, a solution of $[ClP(\mu\text{-}N^tBu)]_2$ (2.67 g, 9.74 mmol) in toluene (20 mL) was dropwise added. The mixture was then set to reflux at 120 degree for 6 h. resulting suspension mixture was filtered through celite (P3). The residue was washed with toluene (3 x

10 mL). The solvent was removed under vacuum and the white solid obtained was dissolved in the minimum amount of THF. Storage at room temperature afforded colorless crystals. Yield: 1.96 g, 3.56 mmol (37 %).

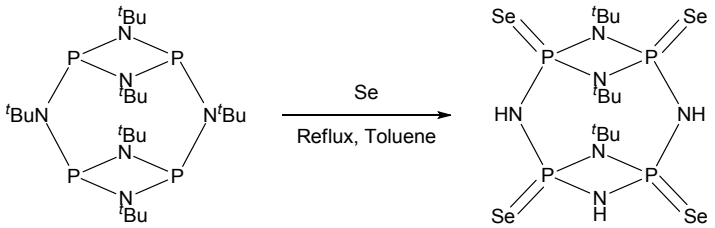


1

Scheme S1

1.2 Synthesis of $P_4(\mu\text{-}N^tBu)_3(\mu\text{-}NH)_3Se_4$ (2)

A suspension of Se (0.6 g, 7.5 mmol) and $P_4(\mu\text{-}N^tBu)_6$ (**1**) (1.0 g, 1.8 mmol) in toluene (20 mL) was refluxed for 96 hours. The resulting suspension mixture was filtered through celite (P3). The residue was washed with toluene (3 x 10 mL).The solvent was removed under vacuum and the white solid obtained was dissolved in the minimum amount of toluene. Storage in fridge at 7 °C afforded colourless crystals. Yield: 0.76 g, 1.08 mmol (60 %). Mp: 246 °C. $^{31}P\text{-}\{^1H\}$ NMR (162 MHz, $CDCl_3$, δ): 24.86 (dd, J = 59.9 Hz, J = 9.7 Hz), 22.26 (dd, J = 59.9 Hz, J = 9.7 Hz). ^1H NMR (400 MHz, C_6D_6, δ): 5.64 (s, 2H), 4.28 (s, 1H), 1.62 (s, 18H), 1.31 (s, 9H). ^{13}C NMR (101 MHz, $CDCl_3$, δ): 60.8 (s), 59.9 (s), 59.8 (s), 30.1 (t, J = 4.0 Hz), 29.9 (t, J = 5.0 Hz), 29.7 (t, J = 4.0 Hz). IR (Nujol, NaCl) ν (cm^{-1}): 3398 (s, N-H), 592 (s, P=Se) cm^{-1}. MS (EI) m/z: 702.82 $[M+1]^+$. Anal. Calcd for $C_{55}H_{128}N_{24}P_{16}Se_{16}$: C, 22.90; H, 4.47; N, 11.65. Found: C, 22.96; H, 4.71; N, 11.60 %.



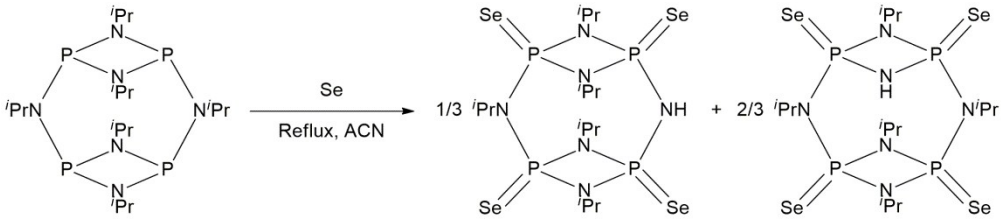
1 **2**

Scheme S2

1.3 Synthesis of $P_4(\mu\text{-}N^iPr)_6$ (3)

The method was adopted from:[2] Scherer, O. J.; Andres, K.; Krüger, C.; Tsay, Y.-H.; Wolmerhäser, G.; *Angew. Chem. Int. Ed. Engl.*, **1980**, *19*, 571-572. A solution of crude $\{SiMe_3(^iPr)\,N\{P(\mu\text{-}N^iPr)\}\}_2$ (7.25 g, 22.5 mmol) [obtained from 5.56 g (22.5 mmol) $\{ClP(\mu\text{-}N^iPr)\}_2$, and 22.5 mmol $LiN(^iPr)SiMe_3$ in 100 ml CH_3CN is heated under reflux for 15 h. After cooling to room temperature is filtered off and washed several times with CH_3CN. Filtrate and washings are again heated under reflux for 15 h; is isolated from the solution after cooling to -45 °C, washed, and recrystallized from CH_3CN. Yield 1.1 g, 2.4 mmol (21%).

1.4 Synthesis of $P_4(\mu\text{-}N^iPr)_6Se_4$ (4)



3 **4**

Scheme S3

A suspension of Se (0.7 g, 8.8 mmol) and $P_4(\mu\text{-}N^iPr)_6$ (1.0 g, 2.1 mmol) in ACN (10 mL) was refluxed for 24 hours. The resulting suspension mixture was filtered through celite (P3). The residue was washed with toluene (3 x 10 mL). The solvent was removed under vacuum and the white solid obtained was dissolved in the minimum amount of toluene. Storage at room temperature afforded colourless crystals. Yield: 0.18 g, 0.24 mmol (12 %). $^{31}P\text{-}\{^1H\}$ NMR (162 MHz, C_6D_6, δ): 55.25 (dd, J = 247.9 Hz, J = 32.4 Hz), 30.65 (dd, J = 212.2 Hz, J = 32.4 Hz). ^1H NMR (400 MHz, C_6D_6, δ): 1.68 (d, J = 4.0 Hz, 30H), 1.57 (d, J = 4.0 Hz, 36H), 1.53 (d, J = 8.0 Hz, 24H)). ^{13}C NMR (101 MHz, C_6D_6, δ): 50.4 (s), 49.2 (s), 46.5 (s), 24.3 (s), 23.1 (s), 22.1 (s). IR (Nujol, NaCl) ν (cm^{-1}): 3454 (s, N-H), 540 (s, P=Se) cm^{-1}. MS (EI) m/z: 741.87 [M+1].

2 NMR Spectra

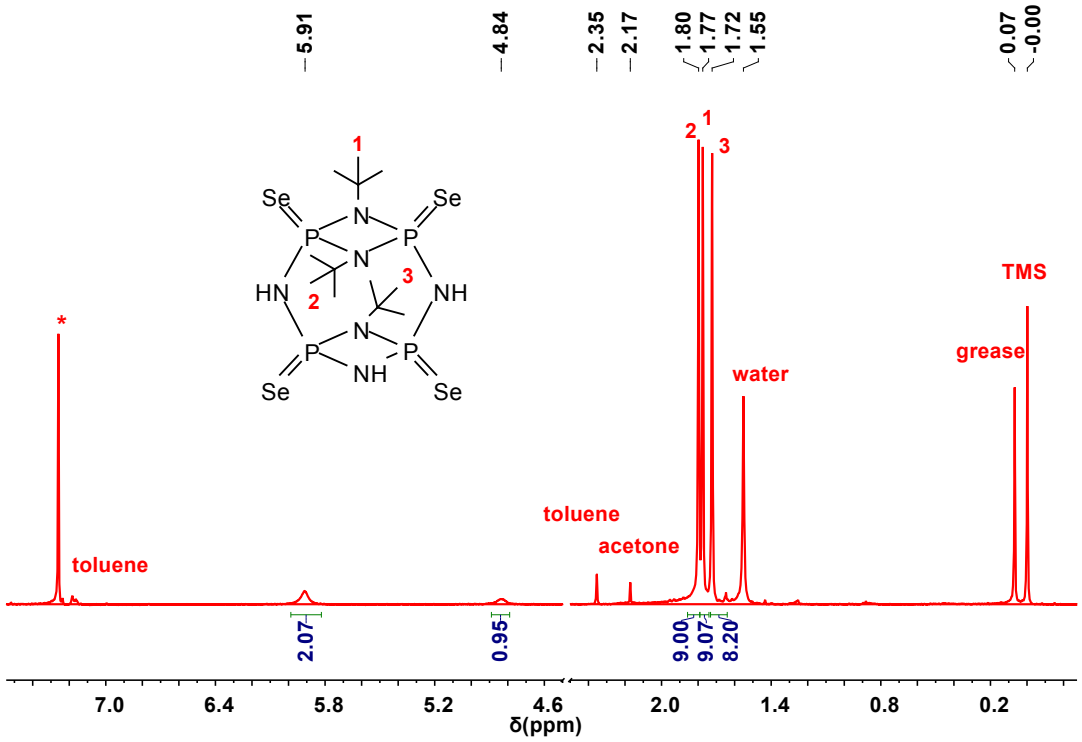


Figure S1: ^{1}H NMR spectrum of $P_4(\mu\text{-N}^t\text{Bu})_3(\mu\text{-NH})_3Se_4$ (**2**) in C_6D_6

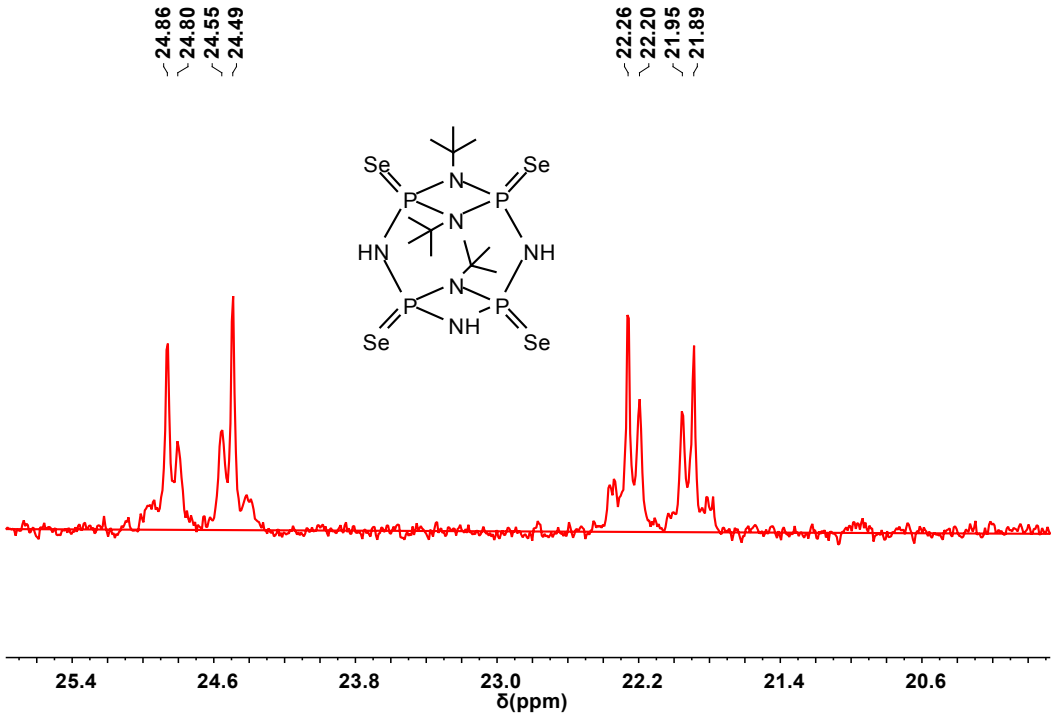


Figure S2: ^{31}P{^{1}H} NMR spectrum of $P_4(\mu\text{-N}^t\text{Bu})_3(\mu\text{-NH})_3Se_4$ (**2**) in $CDCl_3$

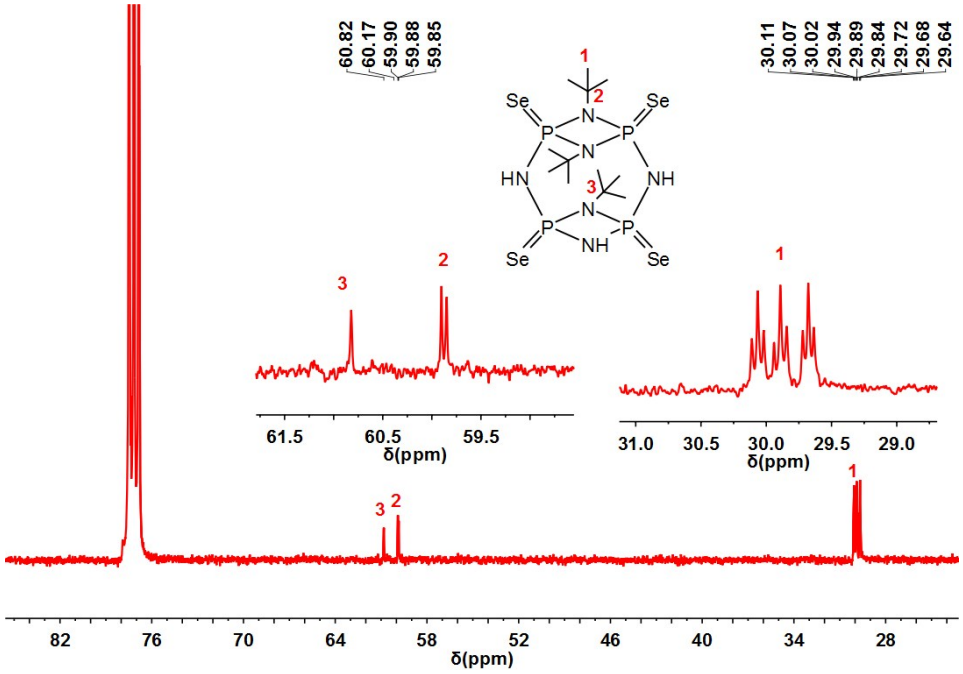


Figure S3: ^{13}C NMR spectrum of $P_4(\mu\text{-}N^tBu)_3(\mu\text{-}NH)_3Se_4$ (**2**) in C_6D_6

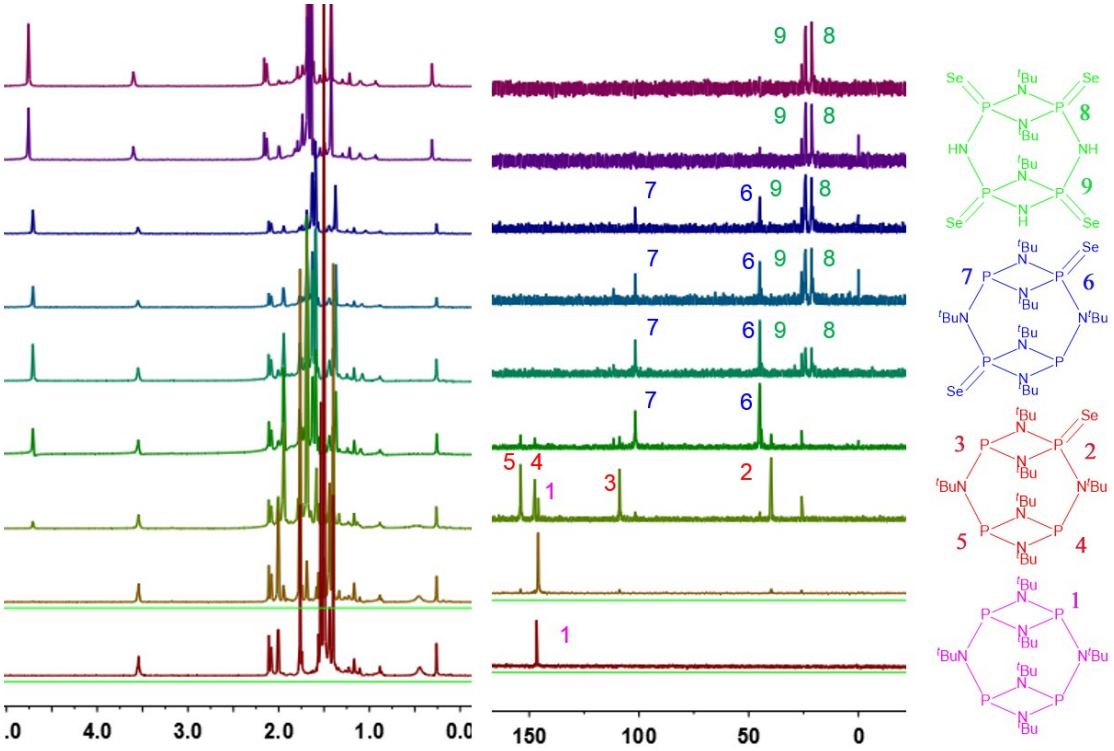


Figure S4: ^{1}H and $^{31}P\{^{1}H\}$ NMR spectrum of monitoring the reaction of $P_4(\mu\text{-}N^tBu)_6$ (**1**) with elemental Se in a sealed NMR tube in toluene-d_8

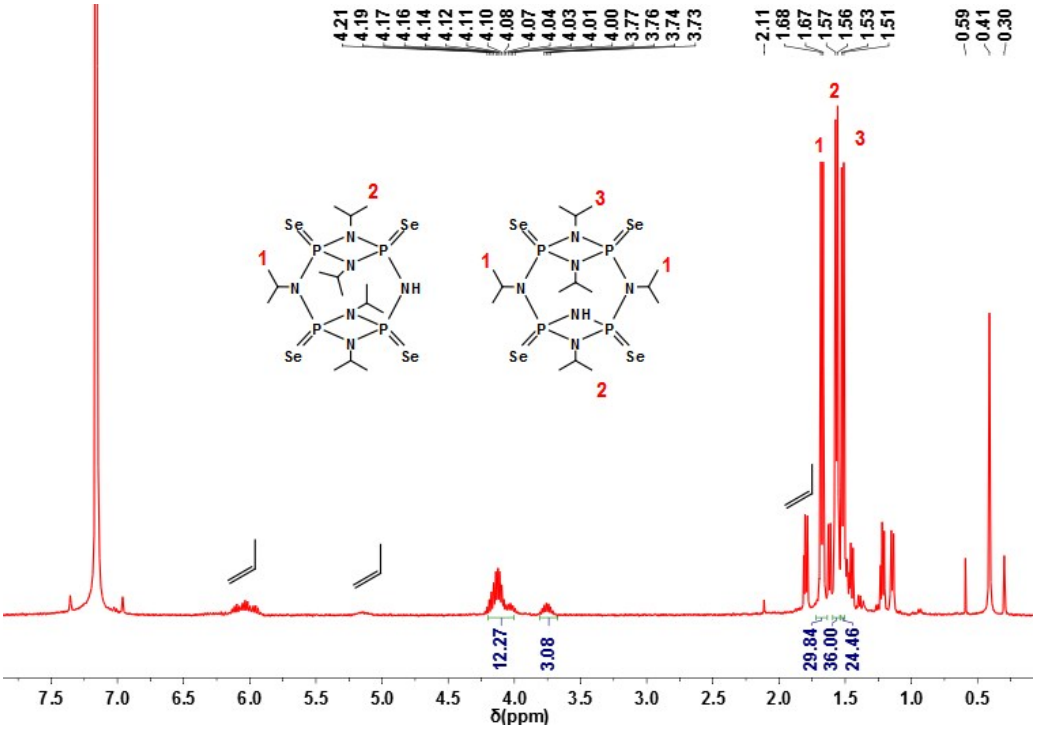


Figure S5: ^{1}H NMR spectrum of $P_4(\mu\text{-}N^iPr)_5(\mu\text{-}NH)Se_4$ (**4**) in C_6D_6

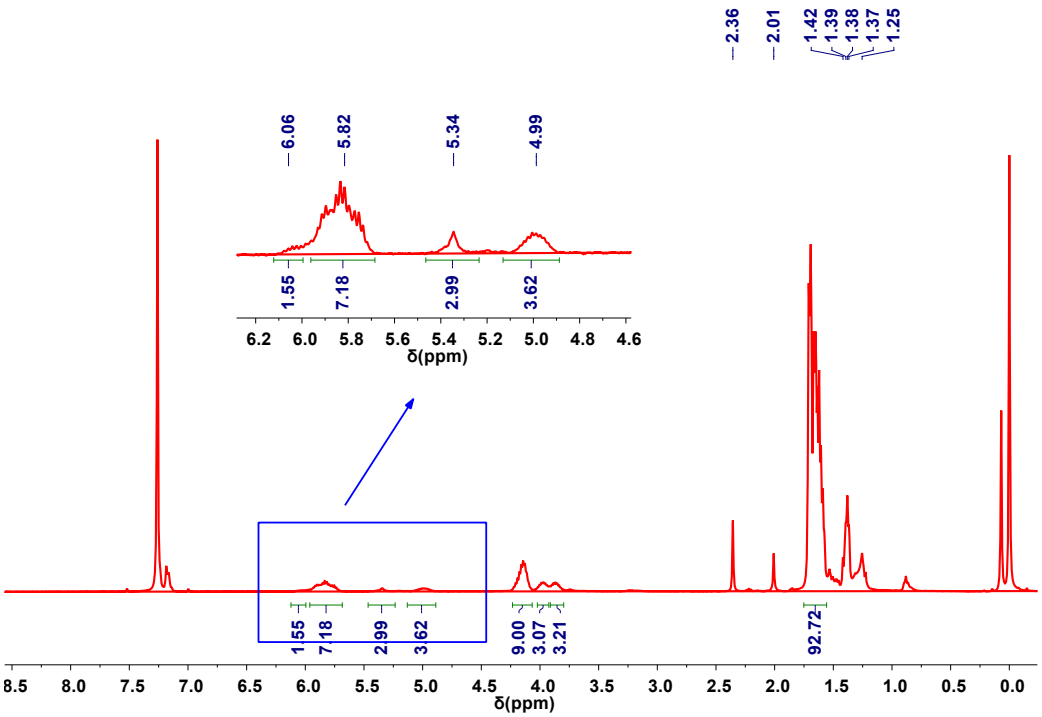


Figure S6: ^{1}H NMR spectrum of $P_4(\mu\text{-}N^iPr)_5(\mu\text{-}NH)Se_4$ (**4**) in $CDCl_3$

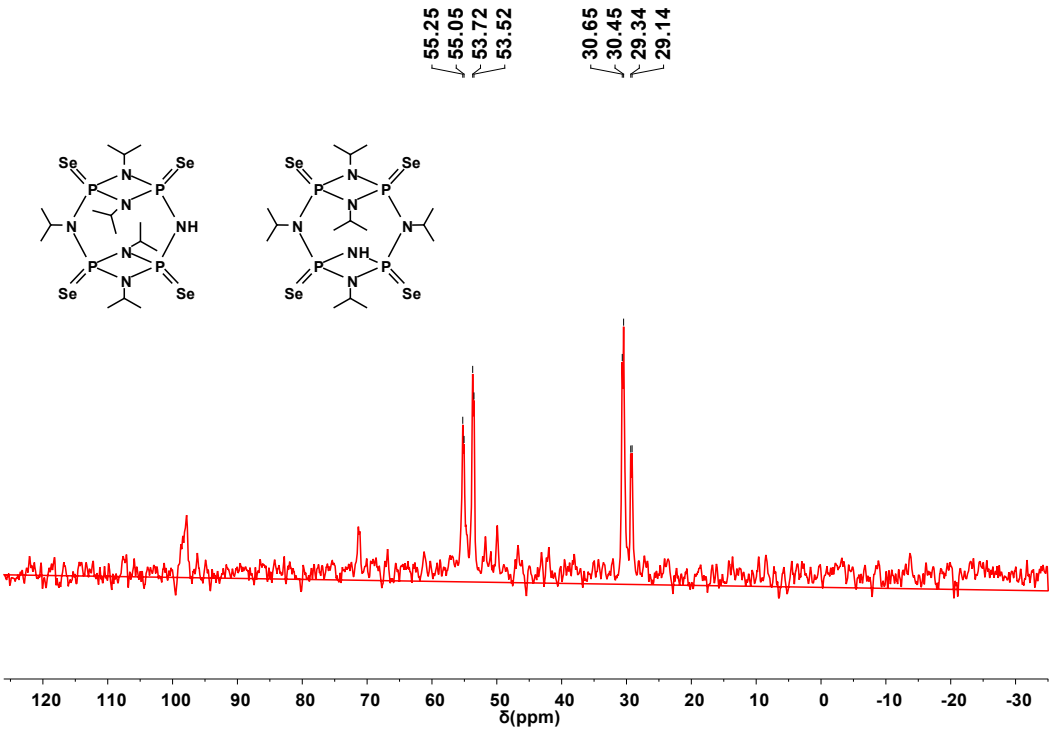


Figure S7: $^{31}P\{^{1}H\}$ spectrum of $P_4(\mu\text{-}N^iPr)_5(\mu\text{-}NH)Se_4$ (**4**) in C_6D_6

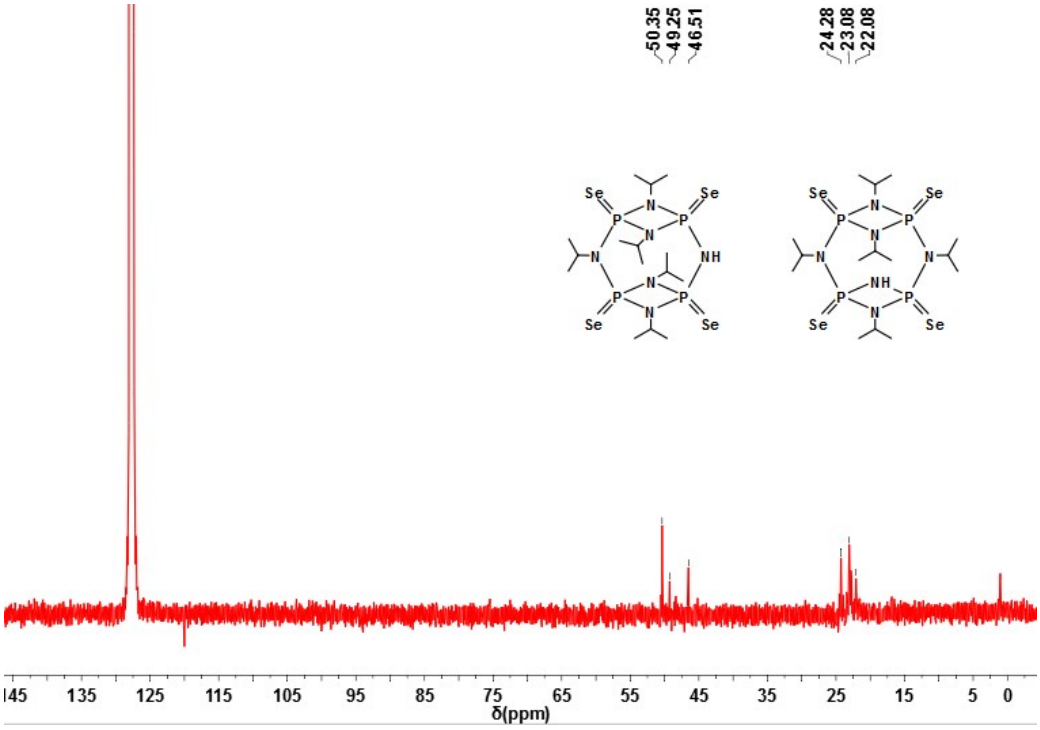
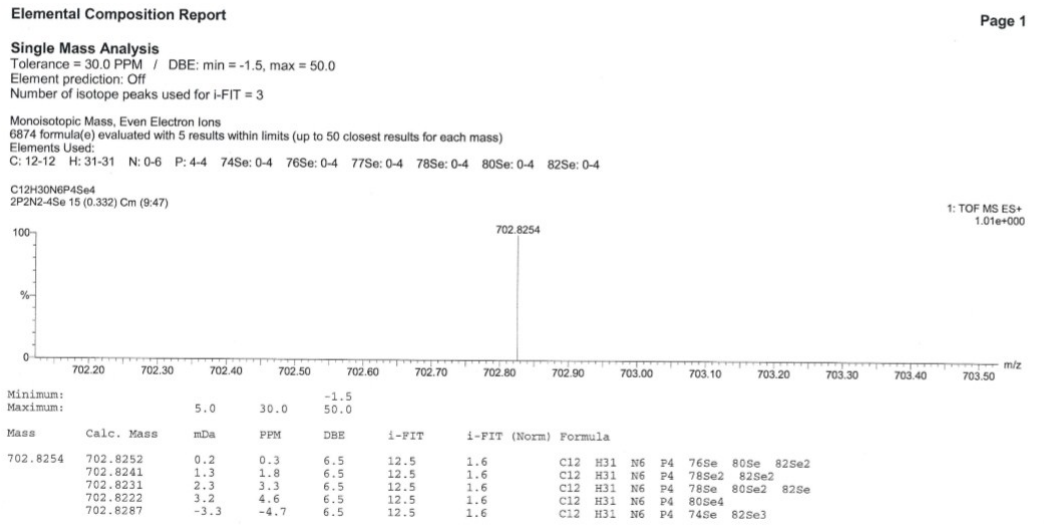


Figure S8: ^{13}C NMR spectrum of $P_4(\mu\text{-}N^iPr)_5(\mu\text{-}NH)Se_4$ (**4**) in C_6D_6

3 FTIR and HRMS spectra



Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 30.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
6874 formula(e) evaluated with 5 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 12-12 H: 31-31 N: 0-6 P: 4-4 74Se: 0-4 76Se: 0-4 77Se: 0-4 78Se: 0-4 80Se: 0-4 82Se: 0-4

C12H30N6P4Se4
2P2N2-4Se 15 (0.332) Cm (9:47)

1: TOF MS ES+
1.01e+000

Minimum:				-1.5			
Maximum:		5.0	30.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
702.8254	702.8252	0.2	0.3	6.5	12.5	1.6	C12 H31 N6 P4 76Se 80Se 82Se2
	702.8241	1.3	1.8	6.5	12.5	1.6	C12 H31 N6 P4 78Se2 82Se2
	702.8231	2.3	3.3	6.5	12.5	1.6	C12 H31 N6 P4 78Se 80Se2 82Se
	702.8222	3.2	4.6	6.5	12.5	1.6	C12 H31 N6 P4 80Se4
	702.8287	-3.3	-4.7	6.5	12.5	1.6	C12 H31 N6 P4 74Se 82Se3

Figure S9: HRMS spectrum of $P_4(\mu\text{-}N^tBu)_3(\mu\text{-}NH)_3Se_4$ (**2**)

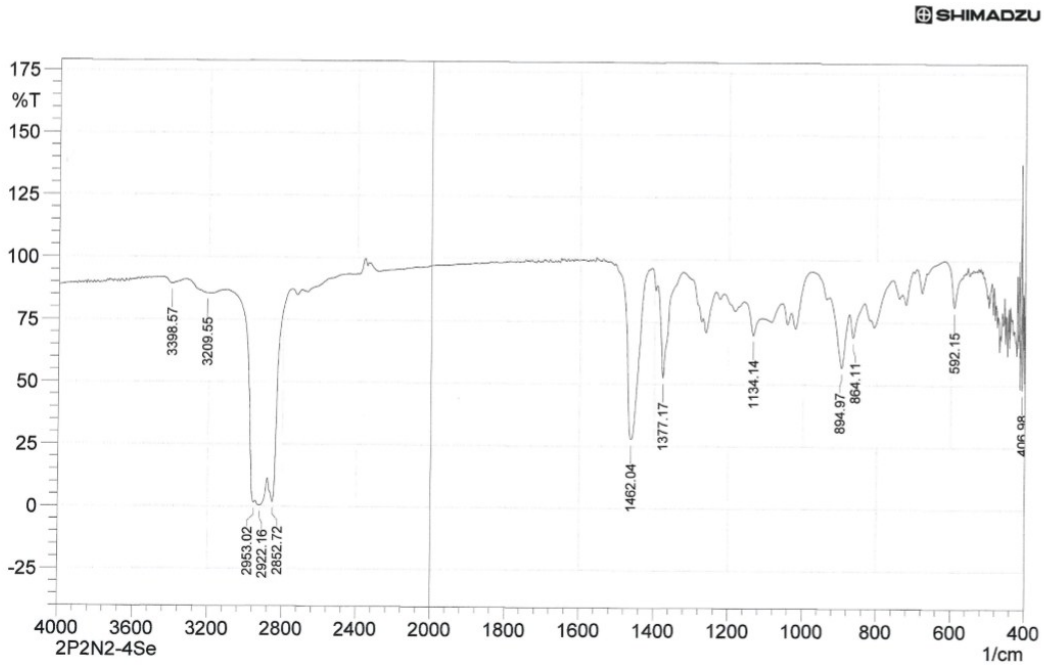


Figure S10: FTIR spectrum of $P_4(\mu\text{-}N^tBu)_3(\mu\text{-}NH)_3Se_4$ (**2**)

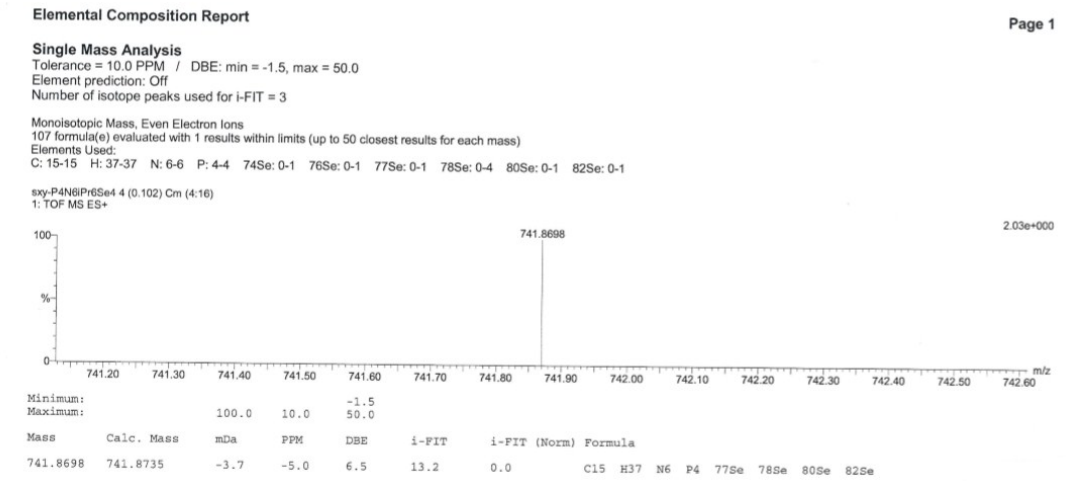


Figure S11: HRMS spectrum of $P_4(\mu\text{-}N^iPr)_5(\mu\text{-}NH)Se_4$ (**4**)

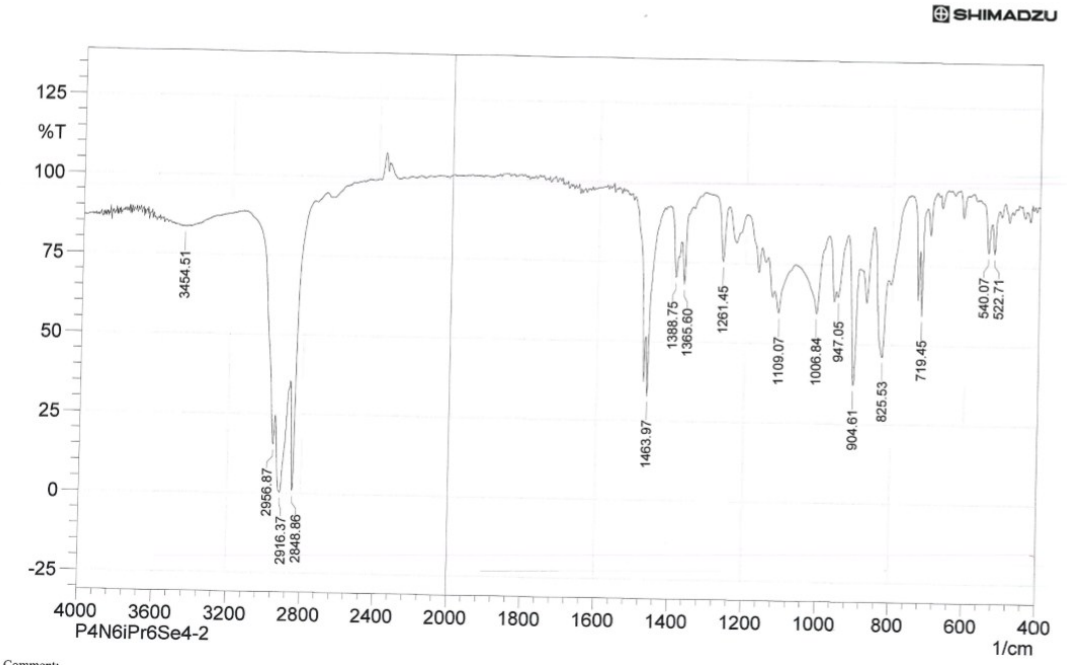


Figure S12: IR spectrum of $P_4(\mu\text{-}N^iPr)_5(\mu\text{-}NH)Se_4$ (**4**)

4 X-ray Analyses

Crystallographic Analyses. Diffraction-quality crystals were obtained by slow evaporation of solvent from solutions in tolune solvent mixtures at room temperature. The crystals were mounted onto quartz fibers, and the X-ray diffraction intensity data were measured at 103 K with a Bruker Kappa diffractometer equipped with a CCD detector, employing Mo K α radiation (λ = 0.71073 Å), with the SMART suite of programs.[3] All data were processed and corrected for Lorentz and polarization effects with SAINT and for absorption effects with SADABS.[4] Structural solution and refinement were carried out with the SHELXTL suite of programs.[5] The structures were solved by direct methods or Patterson maps to locate the heavy atoms, followed by difference maps for the light, non-hydrogen atoms. All non-hydrogen atoms were refined with anisotropic thermal parameters.

The crystals of **4** contained toluene and dimethylamine with full occupancy. The proton of the dimethylamine, H7, participates in a weak H-bonding with N5 of the P_4N_6 moiety (D-H···A, N7-H7···N5, 2.32 Å). In **1** all the *tert*-butyl group is disordered whereas one of the *iso*-propyl groups in **3** is disordered; these are modeled in two alternative sites and refined with appropriate restraints. In **4** the five *iso*-propyl groups are disordered over six positions and the occupancy of the group is fixed at 0.83 and appropriate restraints are applied.

Table S1. X-Ray data of compounds **1**, **2**, **3** and **4**.

	1	2	3	4
Empirical formula	$C_{18}H_{40.50}N_{4.5}P_3$	$C_{21}H_{42}N_6P_4Se_4$	$C_{18}H_{42}N_6P_4$	$C_{15}H_{36}N_6P_4Se_4$
Formula weight	412.96	832.33	466.45	740.22
Crystal system	Monoclinic	Triclinic	Monoclinic	Monoclinic
Space group	C 1 2/m 1	P-1	P 1 21/n 1	$P2_{1/c}$
a/ Å	28.4547(19)	10.5460(4)	8.9073(11)	13.8909(11)
b /Å	16.8252(11)	12.3897(5)	15.7025(18)	15.9194(13)
c/ Å	9.7507(7)	14.0003(6)	9.9032(11)	13.2049(11)
α/°	90	78.264(2)	90	90
β/°	94.991(3)	70.648(2)	113.061(4)	90.007(3)
γ/°	90	75.644(2)	90	90
Volume/ $Å^3$	4650.5(5)	1657.28(12)	1274.4(3)	2920.1(4)
Z	8	2	2	4
ρ (Calc)/$Mg.m^{-3}$	1.180	1.668	1.216	1.684
Absorp. Coeff./ mm^{-1}	0.267	4.644	0.312	5.259
F(000)	1800	826	504	1456
Crystal Size/ mm^3	0.220 x 0.400 x 0.420	0.010 x 0.020 x 0.040	0.060 x 0.120 x 0.180	0.120 x 0.080 x 0.060
Θ range/ °	1.41 to 25.09	1.55 to 26.45	2.61 to 29.55	1.466 to 25.709
Index range	-33<=h<=33 -19<=k<=20 -11<=l<=11	-13<=h<=13 -15<=k<=15 -17<=l<=17	-12<=h<=12 -21<=k<=21 -13<=l<=13	-16<=h<=14 -19<=k<=19 -15<=l<=16
Refl. collected	18856	38958	19035	37170
Indep. Refns. (R_{int})	4282 (0.0806)	6816 (0.0800)	3562 (0.1107)	5560 (0.1620)
Completeness to Θ =	multi-scan	99.7 %	99.9 %	100 %
Absorp. Corr.	0.9440, 0.8960	multi-scan	multi-scan	Semi-empirical from equivalents
Max., min., transmission	0.7073, 1.0000	0.9550, 0.8360	0.9810, 0.9460	0.74, 0.63
Refinement Method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data/ restraint/parameters	4282 / 523 / 428	6816 / 0 / 337	3562 / 108 / 163	5560 / 180 / 301
Goodness-of-fit on F^2	1.099	1.064	1.019	1.045
Final R indices [I>2σ(I)]	R1 = 0.0895, wR2 = 0.2587	R1 = 0.0427, wR2 = 0.1152	R1 = 0.0691, wR2 = 0.1467	R1 = 0.0769, wR2 = 0.2078
R indices (all data)	R1 = 0.1354 wR2 = 0.3082	R1 = 0.0727 wR2 = 0.1477	R1 = 0.1459 wR2 = 0.1835	R1 = 0.1665, wR2 = 0.2539
Largest diff. peak and hole/ e. $Å^{-3}$	0.04, -1.574	1.310, -1.096	0.883, -0.638	1.397, -1.258
	*Data in common: T = 103(2) K, λ = 0.71073 Å			

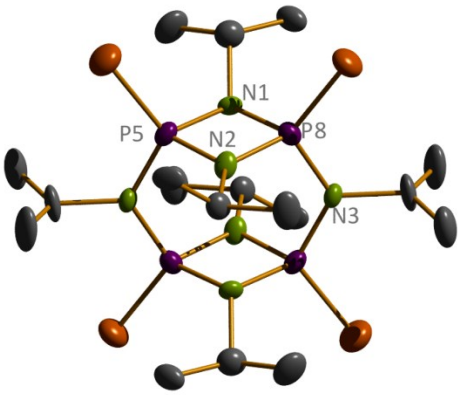
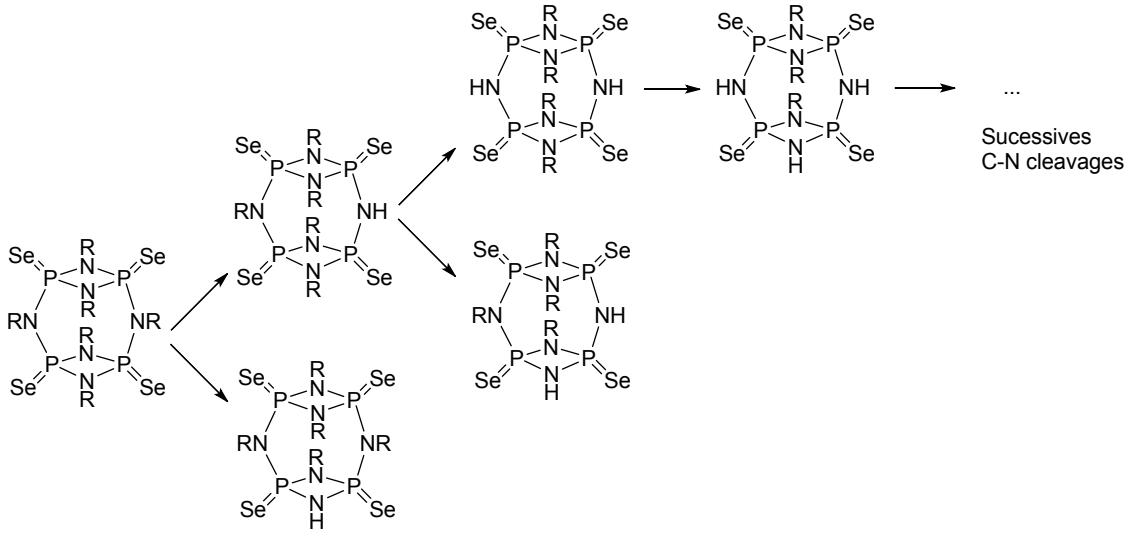


Figure S13. ORTEP diagram for 4. Selected Bond Lengths [Å] and Angles [deg]: N(1)–P(5) 1.695(10), N(1)–P(8) 1.711(10), N(2)–P(5) 1.683(10), N(2)–P(8) 1.678(10), N(3)–P(5)#1 1.723(10), N(3)–P(8) 1.696(10), P(5) –Se(4) 2.075(3), P(8)–Se(2) 2.075(4), N(1)–P(5)-Se(4) 114.5(4), N(2)–P(5)-Se(4) 118.0(4), N(1)–P(8)–Se(2) 117.6(4), N(2)–P(8)–Se(2) 116.7(4), N(3)#1–P(5)–Se(4) 117.5(4). Ellipsoids are drawn at 50% probability. H atoms have been omitted for clarity.

5 Theoretical Studies

Quantum chemical computations were carried out with the Gaussian 09 software package.[6] Full geometry optimizations of stable species were performed in the gas phase by employing the hybrid density functional B3LYP[7] with the Dunning's correlation consistent basis sets cc-pvdz.[8] The B3LYP functional combines the Becke's three-parameter nonlocal hybrid exchange potential with the nonlocal correlation functional of Lee, Yang, and Parr.



n = 2' R = ^{t}Bu
n = 4' R = ^{i}Pr
n = 6' R = ^{n}Pr

n'$_{1C\text{-}N}$ **n'**$_{2C\text{-}N}$ **n'**$_{3C\text{-}N}$

The hypothetical products obtained following different C-N cleavages combinations are denoted as **2**, **4** or **6** where the subscript indicates the number of C-N bond cleaved, i.e. **2**$_{4C\text{-}N}$ for 4 C-N bonds cleavaged.

Scheme S4

Table S2. Electronic and zero-point energies, and thermodynamic magnitudes of the species involved in the cleavage of the C–N bond in the macrocycle $[\{P(\mu\text{-NR})\}_2(\mu\text{-NR})]_2$ at the B3LYP/cc-pvdz theory level.

Species	Number of C-N bonds cleaved	E (hartree)	ZPE	H (hartree)
2'	0	-12247,34117	0,777685	-12246,51226
$\mathbf{2}_{\mathbf{1C\text{-}N}}$	1 (from μ-N)	-12090,16985	0,665365	-12089,45825
$\mathbf{2}_{\mathbf{1C\text{-}N}}$	1 (from P_2N_2)	-12090,14938	0,665691	-12089,43767
$\mathbf{2}_{\mathbf{2C\text{-}N}}$	2 (from μ-N)	-11933,0003	0,55345	-11932,4057
$\mathbf{2}_{\mathbf{2C\text{-}N}}$	2 (from P_2N_2)	-11932,95607	0,553402	-11932,36175
2	3	-11775,76672	0,441759	-11775,28935
$\mathbf{2}_{\mathbf{4C\text{-}N}}$	4	-11618,52608	0,330926	-11618,16544
$\mathbf{2}_{\mathbf{5C\text{-}N}}$	5	-11461,26767	0,219025	-11461,02428
$\mathbf{2}_{\mathbf{6C\text{-}N}}$	6	-11304,01417	0,108037	-11303,88755
4'	0	-12011,588473	0,612305	-12010,932170
4	1 (from μ-N)	-11893,674543	0,528879	-11893,105895
4	1 (from P_2N_2)	-11893,661321	0,528724	-11893,092929
$\mathbf{4}_{\mathbf{2C\text{-}N}}$	2 (from μ-N)	-11775,755371	0,443832	-11775,275503
$\mathbf{4}_{\mathbf{2C\text{-}N}}$	2 (from P_2N_2)	-11775,745297	0,444786	-11775,265058
$\mathbf{4}_{\mathbf{3C\text{-}N}}$	3	-11657,827350	0,359595	-11657,436010
$\mathbf{4}_{\mathbf{4C\text{-}N}}$	4	-11539,897506	0,276453	-11539,593981
$\mathbf{4}_{\mathbf{5C\text{-}N}}$	5	-11421,954036	0,191782	-11421,739209
$\mathbf{4}_{\mathbf{6C\text{-}N}}$	6	-11304,01417	0,108037	-11303,887549
6'	0	-12011,624829	0,615172	-12010,965018
$\mathbf{6}_{\mathbf{1C\text{-}N}}$	1 (from μ-N)	-11893,696414	0,531189	-11893,125139
$\mathbf{6}_{\mathbf{1C\text{-}N}}$	1 (from P_2N_2)	-11893,68612	0,530769	-11893,115308
$\mathbf{6}_{\mathbf{2C\text{-}N}}$	2 (from μ-N)	-11775,771716	0,446245	-11775,289327
$\mathbf{6}_{\mathbf{2C\text{-}N}}$	2 (from P_2N_2)	-11775,758585	0,446105	-11775,276561
$\mathbf{6}_{\mathbf{3C\text{-}N}}$	3	-11657,832828	0,361529	-11657,439559
$\mathbf{6}_{\mathbf{4C\text{-}N}}$	4	-11539,896965	0,277203	-11539,592547
$\mathbf{6}_{\mathbf{5C\text{-}N}}$	5	-11421,955202	0,19265	-11421,739754
$\mathbf{6}_{\mathbf{6C\text{-}N}}$	6	-11304,01417	0,108037	-11303,887549
Isobutylene	---	-157,2313901	0,107021	-157,1181031
Propene	---	-117,911684	0,079114	-117,827536

Table S3. Relative electronic energy (ΔE) including zero-point energy correction and enthalpy (ΔH) of the species involved in the cleavage of C-N bonds in macrocycles [{P(μ-NR)}$_2$(μ-NR)]$_2$ at the B3LYP/cc-pvdz theory level.

Species	Number of C-N bonds cleaved	ΔE[a](kcal/mol)	ΔH[a] (Kcal/mol)
2'	0	0	0
2$_{1C-N}$	1 (from μ-N)	-41,0	-40,2
2$_{1C-N}$	1 (from P_2N_2)	-28,0	-27,3
2$_{2C-N}$	2 (from μ-N)	-82,9	-81,4
2$_{2C-N}$	2 (from P_2N_2)	-55,2	-53,8
2	3	-84,4	-82,5
2$_{4C-N}$	4	-81,0	-78,8
2$_{5C-N}$	5	-67,1	-64,3
2$_{6C-N}$	6	-55,8	-52,7
4'	0	0	0
4	1 (from μ-N)	-1,3	-0,8
4	1 (from P_2N_2)	6,9	7,3
4$_{2C-N}$	2 (from μ-N)	-0,3	1,0
4$_{2C-N}$	2 (from P_2N_2)	6,6	7,5
4$_{3C-N}$	3	6,7	8,5
4$_{4C-N}$	4	15,6	17,6
4$_{5C-N}$	5	32,0	34,7
4$_{6C-N}$	6	46,8	49,8
6'	0	0	0
6$_{1C-N}$	1 (from μ-N)	7,4	7,7
6$_{1C-N}$	1 (from P_2N_2)	13,6	13,9
6$_{2C-N}$	2 (from μ-N)	11,9	12,9
6$_{2C-N}$	2 (from P_2N_2)	20,1	20,9
6$_{3C-N}$	3	25,5	26,9
6$_{4C-N}$	4	37,4	39,1
6$_{5C-N}$	5	52,9	55,0
6$_{6C-N}$	6	67,8	70,4

[a] The relative electronic energies and enthalpies were calculated taking the oxidized macrocycle (**2'**, **4'** or **6'**) as zero where all nitrogen atoms retain their substituents. The successive loss of isobutylene (**2**) and propene (**4** and **6**) from varying positions within the macrocycle has been included to the energy of the new product formed in order to compare their energies with the zero reference compounds.

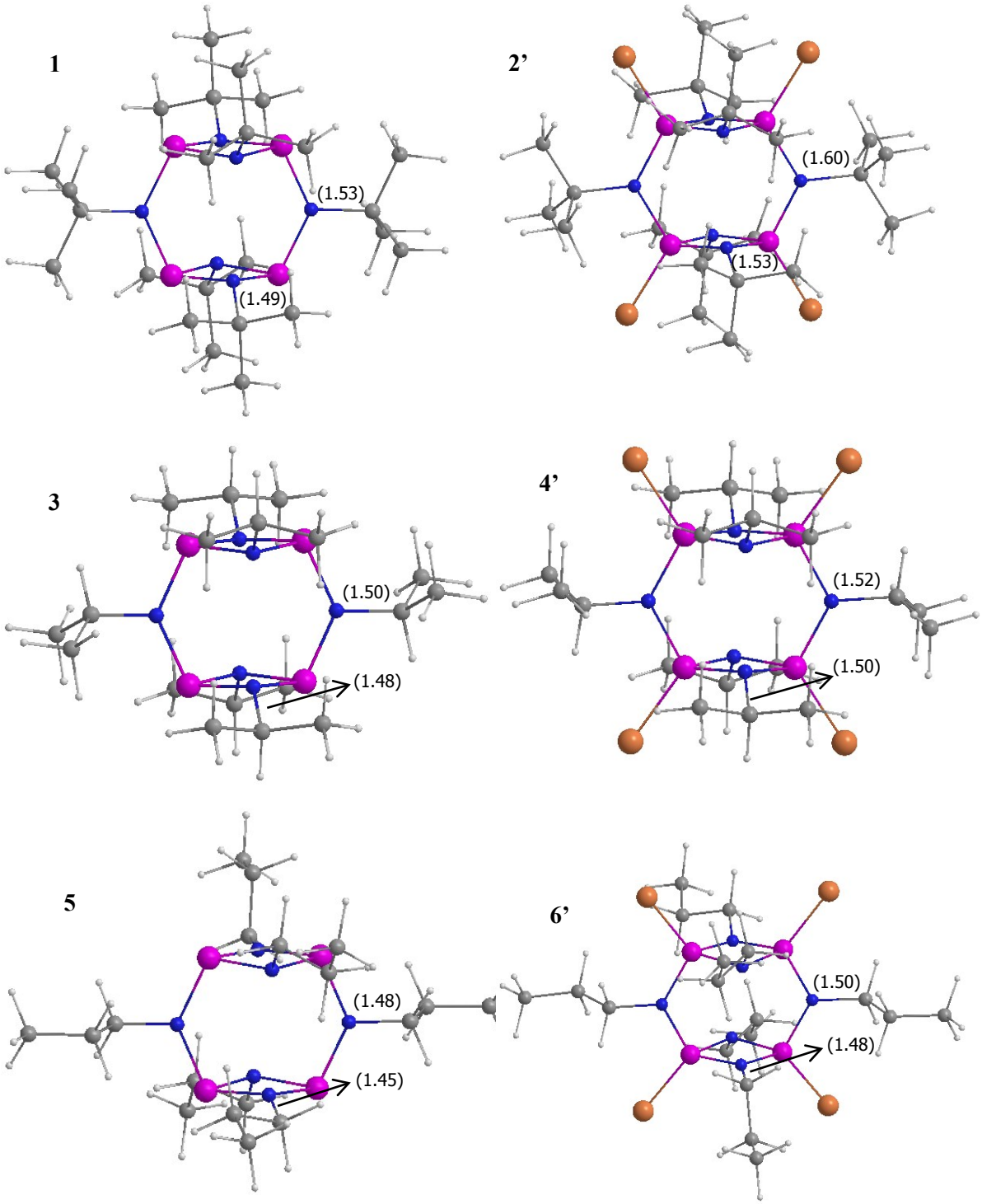
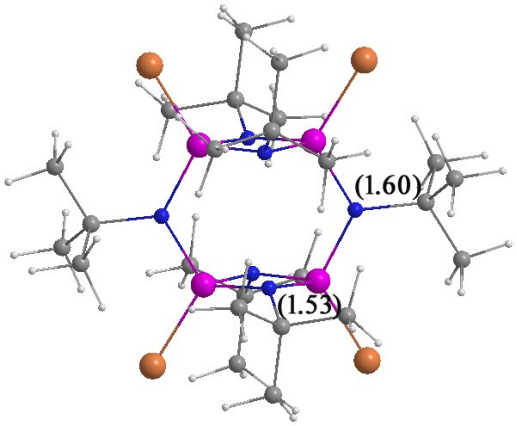


Figure S14. B3LYP/cc-pvdz optimized geometries for the unoxidized macrocycles (**1**, **3** and **5**) and their corresponding fully oxidized counterparts (**2'**, **4'** and **6'**). The C–N bond distances shown in brackets are given in Å.

A complete theoretical study of the reaction mechanism would be very computationally intensive, since it requires the modelling of the selenium atoms in the solid phase and the cyclophosphazane in the liquid phase. These lengthy studies are currently undergoing. Enthalpies of the oxidized products were used instead instead to have a basis by which we could rationalize the experimental results. From the analysis of the optimized geometries we observed that the C–N bond distance between the substituents and the bridging and P_2N_2 ring nitrogen atoms are different, with the former being slightly longer (Figure S14). In order to re-validate the calculated parameters the geometry optimization of **2'** was performed again, using a Popple´s base[9] at B3LYP/6-31+g**. The results were in agreement with the ones obtained using Dunning's correlation basis set re-confirming the validity of the original calculated values.



Scheme S5 B3LYP/6-31+G** optimized geometry for **2'** (bond distances shown in brackets are given in Å)

The difference in bond distance observed between bridging and P_2N_2 positions (1.60 *vs.* 1.53 Å; 1.52 *vs.* 1.50 Å and 1.50 *vs.* 1.48 Å. for **2'**, **4'** to **6'**, respectively), suggests that the loss of the first molecule of isobutylene (**2'**) and propene (**4'** and **6'**) would

occur preferentially at the bridging positions (as observed experimentally). Furthermore, the second substituent loss is expected to occur at the bridging position, since the calculated bridging C–N bond distance is greater than that calculated for the P_2N_2 ring (Table S3). As a result, more thermodynamically stable products are obtained when the second elimination occurs at a bridging position than at the P_2N_2 ring (-81.4, 1.0 and 12.9 kcal/mol *versus* -53.8, 7.5 and 20.9 kcal/mol for **2′**, **4′** and **6′**, respectively).

It can be concluded that the experimental results observed is directly related to the steric congestion present within the macrocycles upon oxidation (see table S4). Going from **1** to **2′** an enhanced ring strain and steric congestion occurs throughout the structure resulting in a decrease in bond angles, especially in the cycle μ-N (angle decreasing by 9º). In the case of ^{i}Pr (from **3** to **4′**) and the hypothetical ^{n}Pr (from **5** to **6′**) the decrease is 8º in both cases. The angles within the P_2N_2 are not affected as much upon oxidation, as observed in the optimized geometries, since their change is ~2º. The dihedral angle formed by phosphorus atoms is not affected at any time, maintaining planarity as shown in the table in all cases.

Table S4. Different angles and dihedral angles for the optimized structures.

	unoxidized macrocycles (**1**, **3**, **5**)			oxidized macrocycles (**2′**, **4′**, **6′**)		
	dihedral	angles	angles	dihedral	angles	angles
	P-P-P-P	PNP (μ-N)	PNP (P_2N_2)	P-P-P-P	PNP (μ-N)	PNP (P_2N_2)
^{t}Bu	0	129	97	0	120	95
^{i}Pr	0	130	97	0	122	94
^{n}Pr	0	131	97	0	123	95

Table S5. B3LYP/cc-pvdz optimized cartesian coordinates of the structures.

Isobutylene

C	-0.000002	1.463015	-0.000001
H	0.932638	2.033895	-0.000041
H	-0.932642	2.033894	0.000031
C	0.000000	0.123321	0.000002
C	1.276348	-0.679458	-0.000037
H	1.327025	-1.340211	0.884260
H	1.326944	-1.340262	-0.884301
H	2.168305	-0.035669	-0.000094
C	-1.276347	-0.679460	0.000038
H	-1.327021	-1.340211	-0.884262
H	-1.326940	-1.340268	0.884299
H	-2.168305	-0.035673	0.000098

Propene

C	1.285524	-0.220683	-0.000029
H	1.306707	-1.315653	-0.000135
H	2.249763	0.294117	0.000018
C	0.132559	0.454288	0.000043
C	-1.235383	-0.163207	-0.000009
H	-1.815799	0.155315	0.884254
H	-1.815816	0.155500	-0.884194
H	-1.185479	-1.263454	-0.000124
H	0.164430	1.551783	0.000151

1

C	-1.427874	-2.121461	3.120874
C	-0.088728	-2.371303	2.405532
C	1.059753	-1.963064	3.340104
H	-1.574205	-1.051318	3.323135
H	-1.449518	-2.665901	4.078444
H	-2.277510	-2.478058	2.517744
H	0.971292	-0.906924	3.630326
H	1.043233	-2.577797	4.254816
H	2.038584	-2.108426	2.860086
N	-2.096940	0.038503	0.000106
N	0.039963	1.533034	1.169606
N	-0.039924	-1.531388	1.171498
N	2.096935	-0.038507	-0.000101
P	-1.369035	-1.575883	0.001018
P	1.369032	1.575879	-0.001011
P	1.288899	-1.631879	0.001007
C	0.029834	-3.878099	2.084460
H	0.990565	-4.101755	1.594351
H	-0.031299	-4.483338	3.004413
H	-0.782927	-4.198536	1.413026
C	0.088717	2.371319	-2.405508
C	-0.029857	3.878110	-2.084418
H	0.031289	4.483363	-3.004361
H	-0.990595	4.101758	-1.594319
H	0.782893	4.198537	-1.412966
C	1.427867	2.121495	-3.120848
H	1.574208	1.051355	-3.323114
H	1.449507	2.665940	-4.078416
H	2.277499	2.478097	-2.517714
C	-1.059763	1.963083	-3.340082
H	-1.043249	2.577826	-4.254786

H	-0.971298	0.906946	-3.630315
H	-2.038593	2.108432	-2.860059
N	0.039917	1.531392	-1.171484
P	-1.288902	1.631876	-0.000991
C	0.088830	2.374842	2.402339
C	-1.059797	1.968256	3.337460
H	-2.038566	2.113105	2.857161
H	-0.971603	0.912535	3.629306
H	-1.043202	2.584363	4.251247
C	-0.029418	3.881174	2.078954
H	0.031817	4.487811	2.997980
H	0.783442	4.200403	1.407065
H	-0.990071	4.104309	1.588452
C	1.427895	2.125887	3.118158
H	1.574078	1.056029	3.322041
H	2.277624	2.481469	2.514564
H	1.449529	2.671738	4.074928
N	-0.039961	-1.533043	-1.169593
C	-0.088814	-2.374855	-2.402324
C	-1.427858	-2.125889	-3.118178
H	-1.449478	-2.671752	-4.074942
H	-2.277606	-2.481450	-2.514599
H	-1.574018	-1.056031	-3.322079
C	1.059840	-1.968284	-3.337419
H	2.038594	-2.113113	-2.857082
H	1.043280	-2.584414	-4.251190
H	0.971651	-0.912571	-3.629294
C	0.029414	-3.881186	-2.078930
H	-0.031802	-4.487826	-2.997956
H	0.990050	-4.104329	-1.588401
H	-0.783467	-4.200405	-1.407062
C	-3.623053	0.127951	-0.000040
C	-4.110260	0.873410	1.259380
H	-3.727822	1.904193	1.290951
H	-5.211612	0.925024	1.270568
H	-3.781166	0.350332	2.170324
C	-4.301097	-1.256204	0.000826
H	-4.048118	-1.851779	-0.887629
H	-4.048352	-1.850571	0.890155
H	-5.391444	-1.096008	0.000569
C	-4.110203	0.871763	-1.260453
H	-3.727880	1.902549	-1.293342
H	-3.781001	0.347553	-2.170707
H	-5.211560	0.923260	-1.271802
C	3.623048	-0.127954	-0.000001
C	4.110244	-0.871809	1.260369
H	3.781064	-0.347638	2.170653
H	3.727930	-1.902600	1.293229
H	5.211601	-0.923298	1.271683
C	4.110211	-0.873366	-1.259466
H	5.211563	-0.924961	-1.270704
H	3.727788	-1.904154	-1.291052
H	3.781068	-0.350264	-2.170379
C	4.301087	1.256203	-0.000847
H	4.048274	1.850612	-0.890129
H	4.048172	1.851733	0.887655
H	5.391434	1.096010	-0.000679

2' C-N cleavages = 0

N	0.074518	2.187743	0.000064
N	-1.526103	0.018697	-1.182222

N	1.526105	-0.018868	-1.182240
N	-0.074461	-2.187723	0.000227
P	1.614936	1.271827	-0.000149
P	-1.614874	-1.271824	0.000018
P	1.533244	-1.314912	0.000083
C	-2.208263	-0.013485	2.557000
C	-3.732048	0.238218	2.525586
H	-4.134928	-0.042163	3.513220
H	-3.968751	1.292326	2.345962
H	-4.233721	-0.370263	1.765274
C	-1.975027	-1.410233	3.171108
H	-0.963929	-1.784333	2.976012
H	-2.113627	-1.347398	4.262041
H	-2.693291	-2.141084	2.778987
C	-1.583876	1.065639	3.449672
H	-2.161009	1.124224	4.385788
H	-0.545433	0.843399	3.708488
H	-1.628327	2.057050	2.976906
N	-1.526170	0.018845	1.182118
P	-1.533210	1.314924	-0.000161
C	-2.207846	-0.013836	-2.557285
C	-1.583324	1.065277	-3.449867
H	-1.628127	2.056735	-2.977225
H	-0.544751	0.843182	-3.708238
H	-2.160116	1.123658	-4.386206
C	-3.731683	0.237646	-2.526436
H	-4.134152	-0.043005	-3.514163
H	-4.233537	-0.370768	-1.766194
H	-3.968619	1.291747	-2.347125
C	-1.974290	-1.410632	-3.171173
H	-0.963309	-1.784734	-2.975509
H	-2.692770	-2.141434	-2.779363
H	-2.112304	-1.347877	-4.262185
N	1.526208	-0.018658	1.182111
C	2.207852	0.013922	2.557192
C	1.974180	1.410701	3.171039
H	2.112487	1.348057	4.262019
H	2.692448	2.141607	2.779017
H	0.963076	1.784578	2.975587
C	1.583330	-1.065207	3.449749
H	1.628363	-2.056691	2.977193
H	2.159954	-1.123430	4.386202
H	0.544671	-0.843237	3.707907
C	3.731699	-0.237475	2.526370
H	4.134120	0.042950	3.514180
H	3.968686	-1.291523	2.346795
H	4.233549	0.371152	1.766292
Se	3.278871	-2.535548	0.000198
Se	3.478644	2.307105	-0.000387
Se	-3.478560	-2.307145	-0.000095
Se	-3.278836	2.535551	-0.000524
C	2.208069	0.013366	-2.557228
C	-0.002960	-3.786320	0.000567
C	0.003037	3.786356	0.000468
C	-1.346750	-4.541621	0.000886
H	-1.953546	-4.357797	0.891680
H	-1.953644	-4.358370	-0.889951
H	-1.067122	-5.607218	0.001214
C	0.671572	-4.258786	-1.304836
H	0.771334	-5.355384	-1.272374
H	0.022130	-4.010624	-2.158853
H	1.667996	-3.847562	-1.476594

C	0.671802	-4.258247	1.306051
H	1.668242	-3.846937	1.477497
H	0.022486	-4.009788	2.160076
H	0.771586	-5.354852	1.273980
C	-0.671888	4.258262	1.305880
H	-1.668211	3.846714	1.477396
H	-0.022498	4.010106	2.159937
H	-0.771984	5.354834	1.273656
C	1.346787	4.541738	0.001137
H	1.953299	4.358073	0.892157
H	1.953979	4.358422	-0.889480
H	1.067069	5.607311	0.001246
C	-0.671219	4.258901	-1.305042
H	-1.667702	3.847861	-1.476908
H	-0.770765	5.355523	-1.272661
H	-0.021711	4.010547	-2.158952
C	1.974700	1.410045	-3.171463
H	2.112717	1.346993	-4.262459
H	0.963764	1.784337	-2.975915
H	2.693260	2.140858	-2.779829
C	1.583578	-1.065877	-3.449682
H	0.545086	-0.843717	-3.708338
H	2.160557	-1.124559	-4.385886
H	1.628156	-2.057230	-2.976797
C	3.731876	-0.238272	-2.526159
H	3.968681	-1.292393	-2.346780
H	4.134508	0.042292	-3.513844
H	4.233700	0.370114	-1.765877

2 C-N cleavages = 1 (from P_2N_2)

N	0.004561	1.909870	0.039839
N	1.601579	-0.275849	1.159398
N	-1.535591	-0.377103	1.171892
N	-0.039592	-2.207299	-0.169178
P	-1.597261	1.066656	0.181322
P	1.547686	-1.557862	-0.032799
P	-1.609349	-1.499414	-0.149896
N	1.580748	-0.271983	-1.197135
P	1.608373	1.025490	-0.025834
N	-1.679258	-0.078286	-1.158812
Se	-2.989671	-3.091143	-0.347644
Se	-3.333247	2.215099	0.610136
Se	2.874493	-3.204779	-0.001243
Se	3.392515	2.204325	-0.066048
H	-0.054825	-3.223818	-0.243984
C	-2.106113	-0.642875	2.561093
C	0.110446	3.510103	-0.096775
C	2.395589	-0.287157	2.474968
C	2.152256	-0.371000	-2.601175
C	-2.473026	0.106975	-2.447324
C	-3.988922	-0.073938	-2.230383
H	-4.366340	0.605458	-1.455405
H	-4.511502	0.153690	-3.173930
H	-4.232458	-1.104825	-1.943305
C	-1.990995	-0.917046	-3.484447
H	-2.043206	-1.945761	-3.098803
H	-2.646391	-0.862200	-4.367805
H	-0.966167	-0.707470	-3.813137
C	1.631971	-1.672122	-3.240226
H	0.543718	-1.761642	-3.154074
H	1.898791	-1.675059	-4.308651
H	2.089944	-2.557505	-2.778564

C	3.692351	-0.413916	-2.584433
H	4.057881	-1.250909	-1.973010
H	4.055751	-0.559945	-3.614942
H	4.117321	0.518448	-2.192874
C	2.178410	1.056652	3.192788
H	2.522093	0.958188	4.234523
H	2.754119	1.864095	2.723924
H	1.119982	1.347289	3.209450
C	3.907205	-0.503248	2.256801
H	4.417077	-0.391163	3.227813
H	4.119032	-1.509762	1.874618
H	4.326397	0.235150	1.563536
C	-3.648818	-0.658945	2.583415
H	-4.051747	-1.331334	1.813576
H	-3.975045	-1.036964	3.566463
H	-4.074410	0.339156	2.436558
C	-1.621465	-2.036105	3.009238
H	-0.555262	-2.182831	2.814219
H	-1.796257	-2.144432	4.091279
H	-2.177406	-2.834006	2.498262
C	-1.594126	0.436896	3.521326
H	-0.504912	0.393824	3.632098
H	-1.880939	1.443362	3.183760
H	-2.045365	0.276756	4.513058
C	1.873069	-1.424012	3.365427
H	0.869420	-1.216063	3.750910
H	1.866288	-2.389636	2.839035
H	2.549035	-1.526537	4.228592
C	1.681183	0.834724	-3.420826
H	0.586341	0.881991	-3.471784
H	2.059764	1.778739	-3.007073
H	2.069477	0.744774	-4.447231
C	-2.210339	1.525899	-2.977251
H	-1.136023	1.740559	-3.052357
H	-2.649037	1.617502	-3.983089
H	-2.680616	2.286266	-2.338799
C	0.781932	4.057073	1.176872
H	0.863947	5.153064	1.095852
H	0.144658	3.832962	2.046605
H	1.785234	3.663819	1.355537
C	-1.209139	4.302598	-0.203883
H	-1.852353	3.983615	-1.030239
H	-1.790330	4.314090	0.719689
H	-0.893893	5.336750	-0.414587
C	0.817032	3.863780	-1.424907
H	1.788092	3.392668	-1.573720
H	0.156834	3.613963	-2.269354
H	0.984345	4.952110	-1.445170

2 C-N cleavages = 1 (from μ-N)

N	0.135887	-2.166875	0.122923
N	1.195713	0.011486	-1.333533
N	-1.404432	-0.011364	-1.170280
N	0.112307	2.175299	0.096787
P	-1.443688	-1.315698	-0.032181
P	1.610530	1.318520	-0.281250
P	-1.462705	1.280689	-0.026625
N	1.887694	0.029034	0.900527
P	1.625135	-1.276388	-0.270412
N	-1.429756	-0.021501	1.152090
Se	-3.208544	2.480836	-0.231220

Se	-3.178164	-2.517697	-0.262984	C	-1.017267	-1.268657	-3.289605
Se	3.262799	2.355125	-1.128833	H	0.067436	-1.322864	-3.135928
Se	3.264484	-2.334130	-1.131500	H	-1.480125	-2.182703	-2.890291
C	-1.643440	-0.008484	-2.667562	H	-1.206632	-1.253005	-4.374187
C	0.249519	-3.739161	0.349709	C	2.313519	-1.000587	3.116052
C	2.781846	0.061840	2.114944	H	1.286723	-0.808833	3.455923
C	-2.021811	-0.054092	2.545066	H	2.360718	-2.008923	2.686008
C	-3.556330	0.086537	2.539662	H	2.975250	-0.988692	3.996425
H	-4.023698	-0.698397	1.929241	C	-1.654796	-1.395537	3.195820
H	-3.926850	-0.010619	3.573503	H	-0.578149	-1.599817	3.126083
H	-3.872407	1.061577	2.148161	H	-1.935888	-1.365411	4.259906
C	-1.403499	1.084745	3.363728	H	-2.207253	-2.222508	2.730752
N	-1.676716	2.066293	2.958429	C	0.287939	-4.426545	-1.022621
N	-1.784846	1.037738	4.395818	H	0.373105	-5.516742	-0.883316
N	-0.307925	1.006057	3.394875	H	-0.647140	-4.231803	-1.568606
C	2.670499	1.446581	2.768952	H	1.138523	-4.090850	-1.628578
H	3.210632	1.434187	3.728096	C	-0.901405	-4.356557	1.173176
H	3.134122	2.219789	2.141082	H	-1.078010	-3.815032	2.110312
H	1.625200	1.721753	2.968554	H	-1.840954	-4.443746	0.628176
C	4.255081	-0.192034	1.741309	H	-0.570079	-5.371218	1.444129
H	4.882532	-0.079676	2.640776	C	1.487024	-4.067124	1.216653
H	4.403125	-1.204313	1.341988	H	1.599919	-5.162034	1.221430
H	4.599388	0.526244	0.983777	H	2.432987	-3.655568	0.860828
C	-3.155247	-0.006301	-2.975360	H	1.313003	-3.753830	2.256537
H	-3.297028	-0.015535	-4.068526	C	0.102877	3.746346	0.342189
H	-3.647694	-0.890971	-2.552396	C	-0.803136	4.104910	1.539152
H	-3.642022	0.889346	-2.568867	H	-1.819760	3.712813	1.479494
C	-1.015955	1.250718	-3.290075	H	-0.334142	3.776351	2.478598
H	-1.221732	1.243149	-4.371769	H	-0.882502	5.202416	1.576812
H	-1.464429	2.166834	-2.879775	C	1.471497	4.325101	0.761249
H	0.071054	1.295484	-3.152600	H	1.932104	3.763426	1.582538

H	2.184099	4.405757	-0.060241
H	1.269031	5.339483	1.138364
C	-0.310341	4.446004	-0.961875
H	-1.330569	4.190048	-1.269974
H	-0.261939	5.537767	-0.817525
H	0.392607	4.181247	-1.766095
H	1.766953	0.009147	-2.179629

2 C-N cleavages = 2 (from P_2N_2)

N	-0.000231	-1.920858	0.000479
N	1.674300	0.044320	-1.174058
N	-1.674631	-0.044504	-1.174040
N	-0.000181	1.920892	-0.000032
P	-1.611407	-1.285952	0.049485
P	1.611007	1.285999	0.049303
P	-1.611325	1.286002	-0.049604
N	1.674238	-0.044341	1.174069
P	1.610960	-1.286011	-0.049187
N	-1.674674	0.044558	1.173936
Se	-2.931721	2.931833	-0.154294
Se	-2.931811	-2.931784	0.153833
Se	2.931207	2.932000	0.153755
Se	2.931129	-2.932049	-0.153449
H	-0.000192	2.941057	-0.000096
H	-0.000257	-2.941021	-0.000528
C	-2.375130	-0.118948	-2.519036
C	2.376472	0.118455	-2.518332
C	1.879677	-1.036628	-3.398635
H	2.448921	-1.038185	-4.341277
H	2.028008	-2.014327	-2.917939
H	0.816989	-0.916963	-3.646262
C	2.020401	1.457583	-3.185637
H	2.492258	2.306121	-2.672657
H	2.383935	1.444556	-4.225126
H	0.935339	1.622804	-3.202301
C	3.903898	0.028114	-2.340744
H	4.200788	-0.938508	-1.910842
H	4.393179	0.133418	-3.322793
H	4.271492	0.834679	-1.689749
C	-3.902784	-0.028832	-2.343049
H	-4.200162	0.937706	-1.913284
H	-4.391111	-0.134051	-3.325579
H	-4.270949	-0.835499	-1.692497
C	-2.018047	-1.458141	-3.185610
H	-2.489585	-2.306697	-2.672366
H	-2.381253	-1.445836	-4.225222
H	-0.932880	-1.622691	-3.201803
C	-1.877591	1.036052	-3.398991
H	-2.445240	1.036897	-4.342594
H	-2.027287	2.013848	-2.918910
H	-0.814420	0.916872	-3.644741
C	-2.375639	0.118989	2.518757
C	-3.903225	0.028598	2.342344
H	-4.200344	-0.937990	1.912530
H	-4.391795	0.133774	3.324759
H	-4.271317	0.835220	1.691694
C	-1.878126	-1.035922	3.398808
H	-0.814974	-0.916798	3.644608
H	-2.445881	-1.036833	4.342349
H	-2.027697	-2.013687	2.918676
C	-2.019049	1.458309	3.185356
H	-2.491020	2.306689	2.672216

H	-2.382121	1.445802	4.225014
H	-0.933959	1.623377	3.201452
C	2.019542	-1.457828	3.185671
H	2.382006	-1.444512	4.225534
H	0.934619	-1.624102	3.201201
H	2.492572	-2.306011	2.673173
C	2.375513	-0.118473	2.518682
C	1.877971	1.036390	3.398839
H	2.446549	1.037841	4.341881
H	2.026485	2.014198	2.918415
H	0.815130	0.916501	3.645667
C	3.903049	-0.027778	2.341991
H	4.391817	-0.133207	3.324276
H	4.271161	-0.834127	1.691020
H	4.199966	0.939000	1.912458

2 C-N cleavages = 2 (from μ-N)

N	-0.214194	1.859688	0.017709
N	-1.299524	-0.375727	-1.401960
N	1.420387	-0.292899	-1.146143
N	-0.065353	-2.265566	0.152967
P	1.415559	1.074077	-0.080483
P	-1.610114	-1.636528	-0.251605
P	1.488342	-1.508445	0.072593
N	-1.938710	-0.327832	0.850462
P	-1.704363	0.947314	-0.352700
N	1.471714	-0.159754	1.175410
Se	2.933548	-3.048659	0.094409
Se	3.093240	2.335917	-0.390385
Se	-2.945977	-3.180593	-0.750731
Se	-3.383251	1.958934	-1.190978
H	-0.016568	-3.283650	0.134495
C	1.713863	-0.405439	-2.626067
C	-0.367661	3.432820	0.241890
C	-2.763298	-0.402475	2.108500
C	2.121907	-0.111555	2.541879
C	3.657262	-0.202490	2.449934
H	4.064268	0.616467	1.840684
H	4.086485	-0.126772	3.462472
H	3.977345	-1.156913	2.011370
C	1.575829	-1.284989	3.370491
H	1.774574	-2.254186	2.890074
H	2.073259	-1.293806	4.352998
H	0.494548	-1.183824	3.536944
C	-2.407368	-1.709759	2.837946
H	-2.947122	-1.743648	3.796953
H	-2.706618	-2.594190	2.257047
H	-1.330288	-1.774513	3.042322
C	-4.265390	-0.391164	1.768857
H	-4.855325	-0.478481	2.695845
H	-4.551177	0.540887	1.260980
H	-4.525714	-1.233592	1.111814
C	3.238059	-0.455198	-2.852267
H	3.444214	-0.570868	-3.928916
H	3.723235	0.464633	-2.500512
H	3.684509	-1.308686	-2.322188
C	1.089677	-1.702207	-3.172168
H	1.342335	-1.788985	-4.240367
H	1.496962	-2.590415	-2.666455
H	-0.002921	-1.709546	-3.078304
C	1.117618	0.806681	-3.358571

H	0.028285	0.863405	-3.234929
H	1.566243	1.748616	-3.011623
H	1.335836	0.711860	-4.433764
C	-2.425422	0.789160	3.009506
H	-1.351457	0.825657	3.240840
H	-2.722603	1.738748	2.546180
H	-2.979918	0.698046	3.956443
C	1.740579	1.207277	3.226064
H	0.652733	1.365649	3.225294
H	2.084144	1.181411	4.271787
H	2.229257	2.061427	2.738287
C	-0.428436	4.110527	-1.133709
H	-0.527723	5.200359	-1.000600
H	0.503421	3.924024	-1.688032
H	-1.280730	3.759360	-1.728908
C	0.772217	4.076573	1.061250
H	0.988340	3.516852	1.979280
H	1.697072	4.216395	0.502568
H	0.406844	5.069253	1.366710
C	-1.606552	3.738065	1.114588
H	-1.736300	4.831117	1.120754
H	-2.547564	3.313472	0.761837
H	-1.424201	3.424128	2.152329
H	-1.903642	-0.396625	-2.225334

2 C-N cleavages = 3

N	0.128128	1.951353	-0.063100
N	-1.548736	0.000046	-1.112634
N	1.420990	0.000046	-1.550861
N	0.128147	-1.951340	-0.063228
P	1.683848	1.296873	-0.451781
P	-1.464282	-1.290978	0.053886
P	1.683873	-1.296822	-0.451833
C	-1.735240	-0.000162	2.674874
C	-3.260274	0.000168	2.879785
H	-3.491987	0.000037	3.957352
H	-3.716518	0.893190	2.428440
H	-3.716952	-0.892473	2.428127
C	-1.114132	-1.255802	3.305198
H	-0.030510	-1.289523	3.127159
H	-1.289591	-1.241743	4.392061
H	-1.563990	-2.175944	2.904232
C	-1.113538	1.255013	3.305539
H	-1.288993	1.240736	4.392401
H	-0.029900	1.288273	3.127504
H	-1.562968	2.175475	2.904833
N	-1.409021	-0.000061	1.205414
P	-1.464287	1.290961	0.054009
C	-2.118606	0.000141	-2.508967
C	-1.621614	1.257776	-3.243671
H	-1.953236	2.178852	-2.742768
H	-0.523928	1.289545	-3.335037
H	-2.035947	1.263339	-4.263590
C	-3.657290	0.000319	-2.457614
H	-4.066552	0.000431	-3.480843
H	-4.030689	-0.892313	-1.935402
H	-4.030482	0.892976	-1.935293
C	-1.621896	-1.257553	-3.243766
H	-0.524217	-1.289570	-3.335136
H	-1.953731	-2.178591	-2.742939
H	-2.036219	-1.262946	-4.263691
N	2.107459	0.000005	0.651028

C	3.164197	-0.000013	1.733851
C	2.968917	1.251431	2.604153
H	3.738481	1.263176	3.391755
H	3.074870	2.177587	2.021148
H	1.984720	1.248328	3.094561
C	2.969162	-1.251738	2.603788
H	3.075207	-2.177702	2.020491
H	3.738788	-1.263602	3.391327
H	1.985000	-1.248924	3.094267
C	4.576036	0.000187	1.119296
H	5.329781	0.000090	1.923278
H	4.735652	-0.892766	0.498197
H	4.735540	0.893380	0.498518
H	0.136606	2.971067	-0.040485
H	0.136631	-2.971056	-0.040679
H	0.694193	0.000036	-2.261388
Se	2.963203	-2.890928	-0.937262
Se	2.963135	2.891008	-0.937249
Se	-2.853002	-2.872797	0.152037
Se	-2.853026	2.872751	0.152363

2 C-N cleavages = 4

N	0.000192	-1.991194	-0.001683
N	1.814874	-0.000204	-0.717268
N	-1.177171	0.000023	-1.519722
N	0.000497	1.991051	-0.001605
P	-1.524789	-1.292792	-0.398933
P	1.524707	1.292668	0.398204
P	-1.524580	1.292852	-0.398861
N	1.177082	-0.000081	1.519483
P	1.524423	-1.292887	0.398205
N	-1.815021	0.000034	0.716660
Se	-2.913227	2.785838	-0.889053
Se	-2.913965	-2.785212	-0.889279
Se	2.913424	2.785095	0.889902
Se	2.912933	-2.785531	0.889928
H	-0.000583	3.010122	0.002732
H	-0.000901	-3.010264	0.003139
H	1.717234	-0.000293	2.386186
H	-1.714947	0.000027	-2.387839
C	-2.412137	0.000063	2.092302
C	-3.946645	0.000555	1.971609
H	-4.405330	0.000467	2.973729
H	-4.295820	0.892562	1.430253
H	-4.296375	-0.890999	1.429860
C	-1.934807	1.257029	2.836550
H	-2.371103	1.265483	3.847479
H	-0.839971	1.272662	2.928939
H	-2.262743	2.176865	2.327665
C	-1.935563	-1.257353	2.836284
H	-0.840718	-1.273765	2.928363
H	-2.371541	-1.265601	3.847353
H	-2.264324	-2.176868	2.327352
C	1.936420	-1.257473	-2.836875
H	2.264504	-2.177019	-2.327559
H	0.841649	-1.273647	-2.929721
H	2.373256	-1.265856	-3.847562
C	2.412752	-0.000102	-2.092623
C	3.947204	0.000193	-1.970902
H	4.296116	0.891991	-1.429023
H	4.296510	-0.891575	-1.429241
H	4.406626	0.000430	-2.972678

C	1.936024	1.256951	-2.837108
H	0.841217	1.272904	-2.929824
H	2.264043	2.176746	-2.328269
H	2.372501	1.264952	-3.847973

2 C-N cleavages = 5

N	0.285034	-1.994545	-0.219144
N	-1.519720	-0.000038	0.658101
N	1.688697	-0.000019	1.051377
N	0.284959	1.994532	-0.218875
P	1.846611	-1.304372	-0.057912
P	-1.278089	1.296385	-0.478783
P	1.846575	1.304379	-0.057910
N	-1.090293	0.000039	-1.604279
P	-1.278026	-1.296381	-0.478802
N	1.937050	0.000035	-1.233433
Se	3.333211	2.764851	0.074232
Se	3.333293	-2.764787	0.074294
Se	-2.662044	2.836758	-0.804135
Se	-2.662029	-2.836694	-0.804281
H	0.284127	3.012534	-0.277118
C	-2.190635	-0.000120	2.000757
C	-1.731406	1.254795	2.761718
H	-2.185580	1.259899	3.764637
H	-0.636946	1.273165	2.881494
H	0.284136	-3.012559	-0.277135
H	-0.369630	0.000061	-2.325288
H	1.538469	-0.000052	2.055538
H	2.748732	0.000057	-1.853986
C	-3.720301	-0.000158	1.839469
H	-4.054844	0.891944	1.290146
H	-4.054788	-0.892131	1.289901
H	-4.204232	-0.000302	2.829662
C	-1.731319	-1.255060	2.761604
H	-2.041913	-2.177162	2.247955
H	-0.636858	-1.273357	2.881371
H	-2.185487	-1.260273	3.764527
H	-2.042035	2.176916	2.248130

2 C-N cleavages = 6

N	-0.000093	-1.999187	-0.000003
N	-1.588337	0.000057	-1.152930
N	0.000077	1.999187	0.000000
P	-1.572594	-1.301476	0.016476
P	1.572592	1.301505	-0.016480
P	-1.572452	1.301597	0.016484
N	1.588362	-0.000057	1.152873
P	1.572449	-1.301625	-0.016487
Se	-3.049168	2.777715	0.008826
Se	-3.049361	-2.777539	0.008828
Se	3.049357	2.777574	-0.008825
Se	3.049164	-2.777749	-0.008823
H	0.000099	3.018696	0.000029
H	-0.000134	-3.018696	-0.000031
H	2.312330	-0.000109	1.872854
H	-2.312288	0.000109	-1.872929
N	-1.519209	0.000049	1.143247
H	-1.141920	0.000017	2.087679
N	1.519243	-0.000049	-1.143200
H	1.141948	-0.000017	-2.087627

3

C	-0.411962	-2.379084	-2.351257
C	0.898241	-3.171785	-2.338222
H	1.140165	-3.505393	-1.317012
H	0.811876	-4.058616	-2.986748
H	1.739987	-2.567089	-2.711419
N	-2.029418	0.001393	0.369079
N	0.285638	-1.169759	1.506414
N	-0.286934	-1.172142	-1.504852
N	2.029364	-0.001405	-0.369334
P	-1.608741	-0.000336	-1.349913
P	1.608679	0.000323	1.349630
P	1.005239	-0.002090	-1.808176
C	0.411992	2.378836	2.351415
C	1.577701	3.252257	1.883400
H	1.410680	3.609169	0.855113
H	1.682677	4.128169	2.544212
H	2.530624	2.702390	1.906379
N	0.286879	1.172185	1.504571
P	-1.005291	0.002080	1.807892
C	0.409283	-2.375803	2.354276
C	1.574075	-3.250898	1.887126
H	1.406901	-3.608197	0.859003
H	2.527636	-2.702131	1.910028
H	1.677860	-4.126531	2.548495
N	-0.285694	1.169694	-1.506686
C	-0.409232	2.376033	-2.354107
C	0.901859	3.167264	-2.341408
H	1.742980	2.561315	-2.713985
H	0.816661	4.053715	-2.990608
H	1.143964	3.501302	-1.320383
C	-3.491790	0.002237	0.698809
C	-4.213271	-1.265912	0.224791
H	-4.253719	-1.316876	-0.875518
H	-3.704495	-2.169229	0.594025
H	-5.251544	-1.277104	0.596898
C	-4.212064	1.270620	0.223593
H	-3.702636	2.173806	0.592254
H	-4.252162	1.320742	-0.876768
H	-5.250430	1.282994	0.595403
C	3.491740	-0.002259	-0.699042
C	4.212038	-1.270552	-0.223623
H	4.252142	-1.320492	0.876746
H	3.702623	-2.173808	-0.592131
H	5.250403	-1.282971	-0.595437
C	4.213191	1.265977	-0.225207
H	3.704401	2.169230	-0.594581
H	4.253629	1.317106	0.875094
H	5.251467	1.277134	-0.597306
H	-3.527197	0.002777	1.802528
H	3.527156	-0.002962	-1.802760
C	-1.574013	3.251013	-1.886716
H	-2.527604	2.702313	-1.909939
H	-1.406919	3.607868	-0.858428
H	-1.677679	4.126921	-2.547739
C	-1.577587	-3.252436	-1.882907
H	-2.530557	-2.702658	-1.906087
H	-1.682492	-4.128604	-2.543388
H	-1.410526	-3.608930	-0.854484
H	-0.613279	2.089308	-3.408649
H	-0.615932	-2.093033	-3.405999

C	-0.898134	3.171666	2.338630
H	-1.739975	2.566871	2.711450
H	-0.811744	4.058175	2.987596
H	-1.139929	3.505813	1.317565
C	-0.901761	-3.167117	2.341955
H	-0.816500	-4.053251	2.991579
H	-1.742918	-2.561043	2.714244
H	-1.143854	-3.501680	1.321099
H	0.613380	-2.088689	3.408702
H	0.615909	2.092402	3.406064

4' C-N cleavages = 0

N	-0.039588	-2.133501	-0.008940
N	1.418103	-0.026739	-1.184076
N	-1.520973	0.038088	-1.180985
N	-0.038355	2.133570	0.008738
P	-1.589758	-1.281113	-0.038597
P	1.502790	1.285101	-0.025178
P	-1.588898	1.282110	0.038728
C	2.220131	0.029584	2.452332
C	2.068860	1.351438	3.208413
H	1.021010	1.539355	3.483263
H	2.659051	1.292482	4.136769
H	2.442753	2.206200	2.631613
C	1.819414	-1.139219	3.353092
H	2.511235	-1.180333	4.209471
H	0.801169	-1.005380	3.745171
H	1.881217	-2.105946	2.836674
N	1.418387	0.026002	1.183968
P	1.501901	-1.285961	0.024998
C	2.219503	-0.030997	-2.452644
C	2.066953	-1.352798	-3.208548
H	2.439850	-2.207868	-2.631550
H	1.018942	-1.539619	-3.483536
H	2.657356	-1.294624	-4.136814
C	1.819549	1.138099	-3.353350
H	0.800894	1.005342	-3.744709
H	1.882783	2.104830	-2.837112
H	2.510847	1.178273	-4.210195
N	-1.520602	-0.037192	1.181048
C	-2.308349	-0.057725	2.456427
C	-2.138408	-1.387763	3.194960
H	-2.729300	-1.351005	4.123935
H	-2.500360	-2.239940	2.605276
H	-1.087672	-1.563306	3.466564
C	-1.906975	1.107049	3.362674
H	-1.998002	2.078056	2.856804
H	-2.580315	1.127313	4.234379
H	-0.877893	0.986079	3.729462
Se	-3.308609	2.516704	0.146635
Se	-3.310152	-2.514780	-0.145943
Se	3.256193	2.467187	-0.117812
Se	3.254705	-2.468986	0.117307
H	-3.373603	0.061428	2.189633
H	3.281524	-0.095323	2.173933
H	3.281066	0.093016	-2.174476
C	-2.309299	0.059181	-2.456002
H	-3.374554	-0.058889	-2.188717
C	-2.138475	1.388898	-3.194907
H	-2.730556	1.352775	-4.123152
H	-2.498655	2.241643	-2.604965

H	-1.087854	1.563062	-3.467835
C	-1.909463	-1.106122	-3.362250
H	-2.001478	-2.076988	-2.856289
H	-2.583025	-1.125673	-4.233805
H	-0.880332	-0.986353	-3.729309
C	-0.119481	3.655193	0.007914
H	-1.202269	3.830410	0.047098
C	-0.121617	-3.655112	-0.008074
H	-1.204512	-3.829615	-0.047090
C	0.454653	-4.301400	-1.270551
H	0.033635	-3.835869	-2.174970
H	1.549856	-4.243132	-1.316715
H	0.169501	-5.366456	-1.279097
C	0.364167	-4.292721	1.296366
H	1.452855	-4.225903	1.421044
H	-0.125504	-3.826405	2.165098
H	0.086621	-5.359764	1.289313
C	0.457327	4.301092	1.270337
H	0.035786	3.836016	2.174749
H	1.552470	4.241836	1.316594
H	0.173193	5.366422	1.278779
C	0.366421	4.292473	-1.296651
H	1.455046	4.225077	-1.421549
H	-0.123667	3.826294	-2.165220
H	0.089450	5.359666	-1.289650

4 C-N cleavages = 1 (from P_2N_2)

N	0.054680	1.859998	-0.079013
N	1.580763	-0.234709	1.154183
N	-1.564978	-0.165672	1.206766
N	-0.083188	-2.238004	0.143950
P	-1.542046	1.098267	0.017501
P	1.506977	-1.591763	0.060110
P	-1.635269	-1.490170	0.098782
N	1.516148	-0.362013	-1.157154
P	1.610153	0.990219	-0.082270
N	-1.625387	-0.242129	-1.097784
Se	-3.097208	-3.005815	0.134754
Se	-3.175179	2.441833	0.019640
Se	2.849704	-3.213905	0.065744
Se	3.310304	2.255775	-0.219522
H	-0.110910	-3.256674	0.125432
C	-1.479715	-0.165309	2.687324
C	0.174115	3.374491	-0.257853
C	2.188649	-0.203485	2.521243
C	1.919664	-0.489790	-2.583497
C	-2.228154	-0.249508	-2.463381
C	-3.762862	-0.253250	-2.473265
H	-4.169779	0.594157	-1.907362
H	-4.115236	-0.177259	-3.515223
H	-4.155282	-1.185440	-2.042068
C	-1.677535	-1.420008	-3.284080
H	-2.012672	-2.382810	-2.868181
H	-2.057067	-1.352810	-4.315737
H	-0.580980	-1.418796	-3.320253
C	3.434429	-0.650509	-2.766908
H	3.654348	-0.836456	-3.831185
H	3.965150	0.260713	-2.454933
H	3.819484	-1.497232	-2.182400
C	1.383823	0.684984	-3.405188
H	1.583518	0.505800	-4.473098
H	0.302081	0.818741	-3.273032

H	1.891299	1.620639	-3.123441
C	1.882490	1.122280	3.226564
H	2.231613	1.061119	4.269066
H	2.415468	1.954691	2.743416
H	0.810793	1.356317	3.239326
C	3.698404	-0.478014	2.530463
H	4.052817	-0.502103	3.574120
H	3.938287	-1.442744	2.065377
H	4.243370	0.314834	1.997249
C	-1.916972	1.183091	3.264152
H	-1.764153	1.167994	4.354779
H	-1.336436	2.023483	2.856453
H	-2.979411	1.377381	3.057933
C	-2.312919	-1.297453	3.295529
H	-1.974572	-2.289585	2.965109
H	-2.214482	-1.255347	4.392119
H	-3.376639	-1.196484	3.032707
C	-0.250242	4.176005	0.976035
H	-1.331678	4.150975	1.159331
H	0.276235	3.809453	1.871357
H	0.047535	5.227226	0.827017
C	-0.388101	3.889648	-1.586882
H	0.025399	3.313962	-2.429679
H	-1.483444	3.857011	-1.638177
H	-0.069810	4.937613	-1.715322
H	-0.427398	-0.338948	2.959162
H	1.682145	-1.017591	3.068741
H	1.259233	3.511529	-0.330413
H	-1.880826	0.693691	-2.919072
H	1.428933	-1.414884	-2.930111

4 C-N cleavages = 1 (from μ-N)

N	1.078003	-1.808281	-0.051003
N	-1.222482	-0.592744	1.125769
N	1.542355	0.867093	0.872197
N	-0.868405	1.993721	-0.069976
P	2.057380	-0.372338	-0.235646
P	-1.869850	0.555740	-0.027636
P	0.871223	1.927128	-0.324622
N	-1.235197	-0.562211	-1.178775
P	-0.698581	-1.753849	-0.061126
N	1.267820	0.644306	-1.424030
Se	1.771201	3.775930	-0.812248
Se	4.125152	-0.639988	-0.559350
Se	-3.946621	0.943192	-0.031817
Se	-1.601203	-3.669357	-0.136704
C	1.647100	1.039634	2.338367
C	1.708700	-3.196268	0.029552
C	-1.666523	-0.832308	2.531403
C	-1.384542	-0.569913	-2.657449
C	-2.811691	-0.931406	-3.087706
H	-2.879040	-0.911939	-4.187870
H	-3.072545	-1.942544	-2.738489
H	-3.550145	-0.227226	-2.682933
C	-0.370242	-1.506616	-3.319265
H	-0.469199	-1.419383	-4.412341
H	0.662680	-1.257229	-3.048088
H	-0.568604	-2.555760	-3.050209
C	-0.650052	-1.707713	3.272855

H	-0.945469	-1.786352	4.330744
H	-0.637813	-2.727509	2.857169
H	0.367593	-1.300257	3.231439
C	-3.073936	-1.430025	2.666967
H	-3.337030	-1.482277	3.736536
H	-3.826939	-0.819063	2.154618
H	-3.108931	-2.447834	2.252106
C	2.721720	0.121243	2.923606
H	2.715893	0.215428	4.020769
H	2.545088	-0.935299	2.678681
H	3.720427	0.392937	2.551716
C	1.937849	2.497091	2.710493
H	1.160966	3.186573	2.349205
H	1.975083	2.582882	3.808264
H	2.901692	2.829391	2.296767
C	2.618805	-3.389240	1.245422
H	3.545055	-2.802672	1.189396
H	2.086686	-3.137105	2.175766
H	2.895799	-4.454555	1.303910
C	2.321457	-3.663808	-1.292955
H	1.583375	-3.595609	-2.106158
H	3.216060	-3.092737	-1.572760
H	2.607196	-4.723970	-1.192470
H	0.671467	0.763844	2.773406
H	-1.665953	0.170344	2.994456
H	0.835602	-3.837971	0.201899
H	-1.154828	0.461971	-2.975634
C	-1.432433	3.390775	0.176095
H	-0.524668	4.006206	0.216623
C	-2.109254	3.545056	1.542075
H	-3.074374	3.026852	1.605684
H	-1.454396	3.173006	2.347127
H	-2.283186	4.618149	1.725370
C	-2.241424	3.927074	-1.006601
H	-2.469196	4.990782	-0.826138
H	-1.645237	3.866496	-1.930106
H	-3.187608	3.391384	-1.152528
H	1.884098	0.943771	-2.182866

4 C-N cleavages = 2 (from P_2N_2)

N	-0.000044	-1.977042	-0.000003
N	1.576084	-0.020294	-1.176556
N	-1.576238	0.020441	-1.176538
N	-0.000027	1.977118	0.000257
P	-1.585772	-1.285210	-0.020003
P	1.585683	1.285267	-0.019829
P	-1.585704	1.285248	0.020019
N	1.576234	0.020340	1.176596
P	1.585673	-1.285230	0.019913
N	-1.576180	-0.020412	1.176583
Se	-3.050735	2.790873	0.134673
Se	-3.050605	-2.791005	-0.134811
Se	3.050563	2.791030	-0.134547
Se	3.050465	-2.791084	0.134559
H	-0.000025	2.996546	-0.000032
H	-0.000020	-2.996469	-0.000095
C	-2.314722	-0.018109	-2.478499
C	2.315025	0.018420	-2.478292
C	2.235254	-1.324795	-3.207230
H	2.752051	-1.230854	-4.175394
H	2.718705	-2.132499	-2.643260
H	1.191205	-1.610935	-3.404542

C	1.778007	1.145265	-3.363384
H	1.792634	2.117936	-2.851754
H	2.415534	1.232398	-4.257529
H	0.751593	0.930259	-3.693824
C	-1.777493	-1.144881	-3.363559
H	-1.792276	-2.117590	-2.852007
H	-2.414799	-1.231907	-4.257870
H	-0.750986	-0.929892	-3.693739
C	-2.234775	1.325170	-3.207290
H	-2.751542	1.231361	-4.175482
H	-2.718180	2.132857	-2.643258
H	-1.190702	1.611249	-3.404573
C	-2.314955	0.018138	2.478383
C	-2.234931	-1.325071	3.207303
H	-2.751924	-1.231282	4.175376
H	-2.718099	-2.132891	2.643249
H	-1.190854	-1.610961	3.404802
C	-1.778042	1.145074	3.363422
H	-1.793098	2.117770	2.851850
H	-2.415358	1.231948	4.257742
H	-0.751467	0.930375	3.693569
C	2.235212	1.324841	3.207359
H	2.752198	1.230927	4.175425
H	2.718471	2.132619	2.643333
H	1.191171	1.610854	3.404911
C	2.315021	-0.018357	2.478399
C	1.777983	-1.145223	3.363451
H	2.415409	-1.232259	4.257677
H	0.751512	-0.930290	3.693769
H	1.792743	-2.117906	2.851851
H	-3.374978	0.231435	2.251580
H	-3.374754	-0.231586	-2.251913
H	3.374981	0.231890	-2.251357
H	3.374997	-0.231808	2.251536

4 C-N cleavages = 2 (from μ-N)

N	0.250284	-1.820542	-0.090518
N	-1.396378	0.169349	1.139837
N	1.779270	0.428311	0.863649
N	0.002908	2.306003	-0.049655
P	1.737472	-0.903537	-0.257388
P	-1.515608	1.493142	0.015043
P	1.580451	1.681555	-0.312217
N	-1.448587	0.236010	-1.163641
P	-1.375431	-1.089829	-0.070894
N	1.453783	0.359601	-1.435511
Se	2.940227	3.226577	-0.713393
Se	3.519525	-1.989939	-0.570564
Se	-3.019831	2.961522	0.101797
Se	-2.947862	-2.508200	-0.143751
H	-0.072427	3.319270	-0.130477
C	1.868912	0.518011	2.338706
C	0.282047	-3.348176	-0.041601
C	-1.926987	0.122689	2.535243
C	-1.626922	0.334907	-2.633940
C	-3.099790	0.547769	-3.004481
H	-3.191016	0.693291	-4.093365
H	-3.700156	-0.329800	-2.718015
H	-3.517109	1.431314	-2.501715
C	-1.045936	-0.884123	-3.353064
H	-1.150316	-0.740805	-4.439713

H	0.018289	-1.023525	-3.124883
H	-1.595603	-1.799566	-3.083366
C	-1.371231	-1.093031	3.284448
H	-1.696107	-1.047653	4.335625
H	-1.762062	-2.029836	2.857900
H	-0.273920	-1.131074	3.267900
C	-3.458689	0.156422	2.617791
H	-3.762694	0.207458	3.676295
H	-3.870913	1.031751	2.098986
H	-3.893707	-0.750968	2.174124
C	2.554508	-0.719310	2.920891
H	2.551154	-0.648603	4.019962
H	2.037576	-1.649646	2.645167
H	3.596147	-0.795697	2.575605
C	2.603994	1.792531	2.764137
H	2.095585	2.702983	2.414252
H	2.640884	1.831601	3.864317
H	3.633326	1.806347	2.375155
C	1.025410	-3.910348	1.173213
H	2.110467	-3.750017	1.130412
H	0.632104	-3.475830	2.105567
H	0.845407	-4.997078	1.215435
C	0.667217	-3.994803	-1.374933
H	0.028201	-3.615458	-2.186712
H	1.718836	-3.831304	-1.642598
H	0.496449	-5.081484	-1.299196
H	0.839997	0.570260	2.730963
H	-1.528901	1.036557	3.010017
H	-0.774660	-3.596019	0.115603
H	-1.043064	1.221957	-2.936964
H	2.130817	0.376637	-2.201059

4 C-N cleavages = 3

N	0.077388	1.990565	-0.103643
N	1.931649	-0.000021	0.752827
N	-1.362214	-0.000003	1.178414
N	0.077346	-1.990570	-0.103677
P	-1.492731	1.288681	0.025265
P	1.637208	-1.297189	-0.392519
P	-1.492761	-1.288657	0.025234
N	1.423216	-0.000009	-1.499734
P	1.637234	1.297161	-0.392513
C	2.970820	-0.000047	1.828389
C	2.850129	1.254891	2.696829
H	2.930935	2.179494	2.109369
H	1.896693	1.261887	3.248023
H	3.667755	1.256297	3.434889
C	2.849976	-1.254915	2.696909
H	1.896534	-1.261760	3.248095
H	2.930674	-2.179565	2.109506
H	3.667597	-1.256376	3.434974
N	-1.526009	0.000025	-1.146054
C	-2.182715	0.000049	-2.482767
C	-1.802460	1.260982	-3.264859
H	-2.328849	1.256279	-4.232010
H	-2.088899	2.178929	-2.732730
H	-0.719960	1.299502	-3.474227
C	-1.802447	-1.260843	-3.264918
H	-2.088868	-2.178818	-2.732828
H	-2.328840	-1.256107	-4.232067
H	-0.719948	-1.299338	-3.474294
Se	-2.990738	-2.757382	0.130882
Se	-2.990675	2.757436	0.130970

Se	3.028050	-2.818506	-0.777377
Se	3.028092	2.818457	-0.777396
H	-3.276466	0.000040	-2.327643
H	3.963344	-0.000122	1.343294
C	-1.815082	-0.000005	2.597113
H	-2.920224	0.000072	2.602189
C	-1.322173	-1.261103	3.309734
H	-1.668145	-1.243484	4.355072
H	-1.713548	-2.176395	2.843487
H	-0.222599	-1.305443	3.308090
C	-1.321993	1.260993	3.309786
H	-1.713269	2.176359	2.843603
H	-1.667928	1.243361	4.355136
H	-0.222413	1.305191	3.308101
H	0.087010	3.009936	-0.087835
H	0.086950	-3.009942	-0.087890
H	0.783449	-0.000001	-2.289217

4 C-N cleavages = 4

N	-0.007075	-1.975012	0.061036
N	1.690721	0.024687	-0.866903
N	-1.323572	-0.050341	-1.434308
N	-0.070309	2.019612	-0.101045
P	-1.564449	-1.302308	-0.238477
P	1.484075	1.349517	0.223258
P	-1.607603	1.279833	-0.339680
N	1.271230	0.088355	1.411563
P	1.533700	-1.237759	0.300838
N	-1.751156	0.030187	0.848099
Se	-3.089872	2.705905	-0.733117
Se	-2.997932	-2.800972	-0.532821
Se	2.884806	2.878852	0.524343
Se	2.995689	-2.687445	0.690094
H	-0.086367	3.038476	-0.117634
H	0.009699	-2.993409	0.095414
H	1.887982	0.125961	2.224735
H	-1.922901	-0.092495	-2.259882
C	-2.260334	0.077758	2.240516
C	-1.819539	1.370977	2.930609
H	-2.253777	1.405638	3.941952
H	-0.723743	1.416418	3.019240
H	-2.170802	2.262575	2.389468
C	-1.803940	-1.156908	3.021568
H	-0.707572	-1.182661	3.111164
H	-2.236919	-1.123485	4.033517
H	-2.144374	-2.089424	2.546550
C	1.561225	-1.263713	-2.988407
H	2.110831	-2.127866	-2.581498
H	0.484107	-1.437473	-2.866875
H	1.783919	-1.205704	-4.065048
C	2.002656	0.037786	-2.315082
C	3.490885	0.321367	-2.548387
H	3.796311	1.263762	-2.071294
H	4.107582	-0.491193	-2.132218
H	3.695520	0.396484	-3.628752
H	-3.364010	0.069563	2.184991
H	1.402620	0.864001	-2.735857

4 C-N cleavages = 5

N	0.151898	-1.960126	-0.199291
N	-1.563587	0.082499	0.747061
N	1.662485	-0.053281	1.083369

N	0.314778	2.019134	-0.119236
P	1.743492	-1.338496	-0.055812
P	-1.280622	1.391294	-0.355023
P	1.850977	1.266829	-0.002570
N	-1.172230	0.115246	-1.515624
P	-1.389876	-1.200317	-0.410200
N	1.862158	-0.013748	-1.206006
Se	3.396550	2.664017	0.133630
Se	3.170774	-2.861242	0.015465
Se	-2.614606	2.995671	-0.527268
Se	-2.834707	-2.687164	-0.709529
H	0.347420	3.038240	-0.124740
C	-2.232015	0.131568	2.071287
H	0.109620	-2.976460	-0.270004
H	-0.469776	0.100594	-2.254325
H	1.547886	-0.070117	2.092113
H	2.658432	-0.033411	-1.845828
C	-3.759246	0.062658	1.968735
H	-4.140278	0.851544	1.304348
H	-4.084569	-0.912530	1.576794
H	-4.206056	0.204549	2.966298
C	-1.659833	-0.950916	2.990801
H	-1.889427	-1.958444	2.607994
H	-0.567615	-0.859150	3.092109
H	-2.105989	-0.864232	3.993594
H	-1.953522	1.118277	2.480740

5

N	-1.042710	1.660510	0.642602
N	-0.945810	-1.115057	1.328934
N	-1.023927	-0.028570	-1.572876
N	1.042449	-1.660608	-0.642560
P	-0.745282	1.625447	-1.099964
P	0.745185	-1.625505	1.100065
P	0.607648	-0.529136	-1.926584
C	2.268742	0.752664	1.722640
C	3.027394	0.438985	3.019471
H	2.371237	0.667610	3.877982
H	3.224461	-0.647175	3.063471
N	1.023780	0.028465	1.573110
P	-0.607840	0.529075	1.926657
C	-1.886992	-1.969611	2.068010
C	-2.253128	-3.246752	1.308596
H	-2.682599	-2.973420	0.330625
H	-1.330420	-3.816930	1.096357
N	0.945702	1.115080	-1.328932
C	1.886383	1.969667	-2.068635
C	2.254211	3.246089	-1.308817
H	1.332050	3.816460	-1.094726
H	2.685046	2.971833	-0.331701
C	-2.268903	-0.752725	-1.722442
C	1.814331	-2.838726	-1.104548
C	-1.814153	2.838892	1.104676
C	3.333289	-2.640876	-1.077847
H	3.587691	-1.768451	-1.707003
H	3.639290	-2.380175	-0.048176
C	-3.333167	2.641480	1.078108
H	-3.587741	1.769100	1.707254
H	-3.639336	2.380897	0.048456
C	-3.027569	-0.439080	-3.019276
H	-3.224563	0.647095	-3.063322
H	-2.371460	-0.667798	-3.877793

H	1.545386	-3.705933	-0.475778
H	1.501315	2.249916	-3.072168
H	-1.544998	3.706022	0.475890
H	-2.041719	-1.832702	-1.674189
H	-2.803513	-1.378015	2.243449
H	2.041551	1.832643	1.674425
C	-4.341695	-1.213709	-3.136984
H	-4.870609	-0.971435	-4.072469
H	-4.168998	-2.303906	-3.126033
H	-5.022657	-0.980356	-2.300247
C	-4.098247	3.876876	1.556909
H	-5.186962	3.711210	1.530857
H	-3.826612	4.141062	2.593397
H	-3.880028	4.754437	0.924385
C	-3.230931	-4.128219	2.089175
H	-3.482284	-5.042002	1.527698
H	-2.807492	-4.439245	3.059328
H	-4.174692	-3.594976	2.296356
C	4.098752	-3.876081	-1.556540
H	5.187419	-3.710110	-1.530413
H	3.880726	-4.753676	-0.923997
H	3.827266	-4.140378	-2.593038
C	4.341461	1.213698	3.137263
H	4.168678	2.303880	3.126484
H	4.870407	0.971319	4.072701
H	5.022427	0.980524	2.300477
C	3.231179	4.127755	-2.090215
H	2.806284	4.439902	-3.059370
H	3.483970	5.040878	-1.528311
H	4.174300	3.594188	-2.299469
H	1.495425	-3.087972	-2.131871
H	-1.495072	3.088020	2.131973
H	-2.911933	-0.544991	-0.846861
H	-1.503123	-2.248950	3.072252
H	2.802334	1.377699	-2.245748
H	2.911758	0.544982	0.847041

6′ C-N cleavages = 0

N	1.808180	-0.881062	-0.471879
N	-0.610592	-1.535400	0.961410
N	0.806042	1.002675	1.302553
N	-1.857981	1.007899	0.477877
P	1.843095	0.817776	-0.061642
P	-1.892785	-0.702708	0.109158
P	-0.392940	1.961067	0.517048
C	-1.075595	-0.632557	-2.668841
C	-1.910939	-1.674128	-3.421129
H	-1.428066	-2.659187	-3.311730
H	-2.899431	-1.755214	-2.940299
N	-0.874736	-0.938158	-1.254761
P	0.349055	-1.854770	-0.469163
C	-0.865913	-2.557847	1.996873
C	-1.334881	-1.958457	3.323310
H	-0.576809	-1.250548	3.696518
H	-2.258155	-1.378929	3.152658
N	0.556406	1.647415	-0.924625
C	0.827410	2.714631	-1.914310
C	1.317383	2.185576	-3.262582
H	2.217713	1.566680	-3.106773
H	0.549657	1.531142	-3.705325
Se	-0.676691	3.955893	1.126435

Se	3.759284	1.694072	-0.083753
Se	-3.822893	-1.547700	0.183322
Se	0.685726	-3.865373	-1.002431
C	1.121101	1.031680	2.736713
C	-3.158021	1.708994	0.719044
C	3.088703	-1.530915	-0.901542
C	-3.791878	2.289666	-0.544599
H	-3.088458	3.004844	-1.004825
H	-3.958871	1.475392	-1.270575
C	3.878792	-2.179929	0.234545
H	3.235369	-2.912658	0.749191
H	4.155948	-1.407352	0.970394
C	2.076179	-0.078327	3.176097
H	1.660702	-1.056943	2.886642
H	3.032454	0.034399	2.640015
H	-3.835129	0.980743	1.185030
H	1.562489	3.431388	-1.506960
H	3.695816	-0.754943	-1.387836
H	1.544966	2.017169	3.000792
H	0.079118	-3.106097	2.138529
H	-0.078039	-0.535965	-3.127594
C	2.329280	-0.032560	4.684884
H	3.030041	-0.824516	4.991150
H	2.764542	0.933932	4.988904
H	1.396247	-0.171805	5.256983
C	5.137120	-2.874175	-0.292154
H	5.708279	-3.334907	0.528973
H	4.882517	-3.671687	-1.010415
H	5.805849	-2.161538	-0.804100
C	-1.599676	-3.045496	4.367893
H	-1.940510	-2.606398	5.318415
H	-2.378203	-3.747409	4.025936
H	-0.689901	-3.633236	4.577947
C	-5.115966	2.992189	-0.235977
H	-5.567278	3.406886	-1.150871
H	-5.845108	2.294902	0.209749
H	-4.971093	3.825474	0.472087
C	-2.065811	-1.315355	-4.899929
H	-1.087505	-1.257929	-5.407821
H	-2.669363	-2.069298	-5.428637
H	-2.565530	-0.339822	-5.030687
C	1.646196	3.330812	-4.223905
H	2.441405	3.977835	-3.818305
H	1.992030	2.944608	-5.195333
H	0.763236	3.965118	-4.411712
H	-2.965897	2.505787	1.450081
H	2.833567	-2.281731	-1.661435
H	0.163994	0.937081	3.276233
H	-1.608550	-3.290538	1.634326
H	-0.115949	3.268145	-2.046118
H	-1.541083	0.365957	-2.736070

6 C-N cleavages = 1 (from P_2N_2)

N	-0.142553	1.716060	-0.594363
N	1.530303	0.306670	1.280854
N	-1.604827	-0.162353	1.003225
N	0.340262	-2.163779	0.618578
P	-1.590399	0.725311	-0.507263
P	1.800218	-1.251910	0.550345
P	-1.288081	-1.720047	0.271204
C	2.077234	-0.758481	-2.293218
C	3.578395	-0.714142	-2.600293

H	3.949578	0.307686	-2.421734
H	4.105212	-1.371259	-1.889405
N	1.724692	-0.366793	-0.926459
P	1.495299	1.190989	-0.226603
N	-1.230677	-0.817312	-1.195171
Se	-2.556445	-3.358122	0.604314
Se	-3.348528	1.730903	-1.093334
Se	3.422827	-2.450380	1.127156
Se	2.944813	2.693976	-0.518852
C	-2.669474	0.004764	2.019794
C	-0.327943	3.166934	-0.930577
C	-0.547197	4.073908	0.279148
H	0.307442	3.972101	0.969374
H	-1.449829	3.745563	0.821134
C	-2.518156	1.271087	2.859733
H	-1.534733	1.265737	3.354199
H	-2.541221	2.152849	2.197693
H	-1.184188	3.231339	-1.614644
H	-3.660854	-0.004185	1.532552
H	1.526291	-0.095949	-2.981555
C	-3.634796	1.384534	3.900607
H	-3.523946	2.300584	4.501427
H	-4.627821	1.416983	3.422113
H	-3.627267	0.526538	4.594178
C	-0.701108	5.536688	-0.144115
H	-0.860653	6.187033	0.730130
H	0.198935	5.898117	-0.669407
H	-1.562045	5.669977	-0.820763
C	3.870718	-1.144067	-4.039042
H	3.371936	-0.483446	-4.769245
H	4.951077	-1.112117	-4.248409
H	3.525731	-2.174440	-4.232963
H	0.564609	3.484389	-1.485343
H	1.686355	-1.775806	-2.460561
H	-2.622360	-0.885884	2.666018
H	0.441068	-3.089059	1.034294
C	2.221644	0.780364	2.499531
H	2.669264	1.758564	2.259900
H	3.061435	0.091839	2.699191
C	1.326124	0.891907	3.732742
H	1.938185	1.343817	4.534053
H	0.513087	1.608139	3.525332
C	0.751889	-0.441544	4.212722
H	0.120988	-0.903977	3.436969
H	1.554566	-1.156187	4.459964
H	0.131409	-0.308169	5.113426
C	-1.251970	-1.261647	-2.592046
H	-0.556292	-2.112017	-2.685208
H	-0.831629	-0.446628	-3.204674
C	-2.638651	-1.655403	-3.113044
H	-3.318128	-0.795524	-3.000329
H	-3.040107	-2.462407	-2.478908
C	-2.582345	-2.105250	-4.573978
H	-3.581877	-2.388716	-4.938130
H	-2.205272	-1.302875	-5.231546
H	-1.921771	-2.979897	-4.704459

6 C-N cleavages = 1 (from μ-N)

N	-1.998618	0.403361	-0.626675
N	0.014055	1.857581	0.763876
N	-0.371556	-1.249712	1.074747

N	2.100469	-0.003421	0.252404	C	-0.148137	2.765297	1.916361
P	-1.383365	-1.217762	-0.358503	H	-0.995805	3.430629	1.682577
P	1.498945	1.593367	-0.107162	H	0.748002	3.410022	1.957374
P	1.130466	-1.464999	0.187574	C	-0.368278	2.078395	3.263008
N	0.454423	1.420747	-1.492797	H	-0.595909	2.873312	3.995926
P	-1.010367	1.839955	-0.646871	H	-1.269783	1.446696	3.202686
N	0.114202	-1.342194	-1.189635	C	0.827904	1.259067	3.748173
Se	2.239483	-3.215722	0.562514	H	1.072689	0.455771	3.035691
Se	-2.843368	-2.719596	-0.589417	H	1.723590	1.892864	3.861823
Se	2.944938	3.119702	-0.101378	H	0.623757	0.791292	4.724625
Se	-2.015873	3.603820	-1.193609	C	0.416162	-1.399632	-2.619279
C	-0.681970	-2.103864	2.246438	H	1.385867	-0.898279	-2.777598
C	-3.476926	0.584902	-0.778600	H	-0.332972	-0.780996	-3.141566
C	-4.213442	0.861900	0.531432	C	0.438316	-2.821385	-3.188817
H	-3.791964	1.766622	1.002400	H	-0.538737	-3.295518	-2.999042
H	-4.043741	0.023112	1.227445	H	1.186654	-3.414781	-2.637847
C	-1.832687	-1.575316	3.100725	C	0.752436	-2.827020	-4.685804
H	-1.597332	-0.557310	3.447553	H	0.764906	-3.853718	-5.083233
H	-2.742855	-1.505475	2.481989	H	0.000815	-2.257974	-5.259771
H	-3.863521	-0.329953	-1.246807	H	1.739069	-2.378452	-4.894838
H	-0.906818	-3.133643	1.917168	H	0.682101	1.980828	-2.314347
C	-2.100828	-2.490868	4.298164	C	3.543438	-0.127174	0.642666
H	-2.933478	-2.109114	4.909331	H	3.617394	-0.963144	1.350900
H	-2.365724	-3.510262	3.971736	H	3.815297	0.790870	1.181349
H	-1.215200	-2.569903	4.951420	C	4.486590	-0.347253	-0.539492
C	-5.714071	1.050453	0.297427	H	4.189969	-1.268620	-1.067860
H	-6.241426	1.248876	1.243533	H	4.378481	0.492116	-1.246606
H	-5.909167	1.899997	-0.378513	C	5.941847	-0.456107	-0.078774
H	-6.165164	0.151091	-0.154560	H	6.269457	0.462131	0.437482
H	-3.629811	1.412089	-1.484961	H	6.080787	-1.301109	0.616566
H	0.240098	-2.155168	2.846182	H	6.616188	-0.615182	-0.934692

6 C-N cleavages = 2 (from P_2N_2)

N	0.067866	0.014874	1.979558
N	-1.561002	1.358350	0.083954
N	1.675894	1.001096	-0.102049
N	-0.184952	-0.001880	-1.972560
P	1.593762	-0.165565	1.193733
P	-1.712788	0.173046	-1.186308
P	1.431629	-0.161012	-1.383614
C	-2.035580	-2.380549	0.155799
C	-3.534632	-2.678818	0.266941
H	-3.923759	-2.200302	1.180622
H	-4.052388	-2.206004	-0.583762
N	-1.714919	-0.952239	0.119129
P	-1.545148	0.201368	1.389133
N	1.358748	-1.295481	-0.088001
Se	2.761837	-0.302136	-2.999054
Se	3.123191	-0.345929	2.619107
Se	-3.241827	0.301089	-2.616996
Se	-2.869546	0.382629	3.006476
C	2.696575	2.070474	-0.163429
C	2.390402	3.241421	0.769085
H	1.411267	3.668484	0.502796
H	2.308909	2.869704	1.804945
H	3.693009	1.655205	0.071551
H	-1.491546	-2.825565	1.005822
C	3.477156	4.316693	0.694892
H	3.249215	5.156454	1.369606
H	4.461448	3.913034	0.985455
H	3.572192	4.724223	-0.325996
C	-3.813751	-4.182415	0.291960
H	-3.321805	-4.672505	1.149832
H	-4.893496	-4.381707	0.371844
H	-3.452305	-4.676925	-0.626174
H	-1.620830	-2.840649	-0.756653
H	2.730982	2.411894	-1.210024
H	-0.235479	0.100255	-2.985875
C	-2.297998	2.641245	0.119314
H	-2.783451	2.708166	1.106453
H	-3.107156	2.585968	-0.629870
C	-1.431373	3.875241	-0.129883
H	-2.083134	4.757221	0.004709
H	-0.660172	3.940244	0.656242
C	-0.785170	3.917115	-1.515053
H	-0.111671	3.058024	-1.664634
H	-1.546625	3.886776	-2.312120
H	-0.191645	4.835346	-1.651047
C	1.371531	-2.760172	-0.089982
H	0.736999	-3.101195	-0.925091
H	0.879388	-3.100323	0.836514
C	2.772504	-3.371576	-0.200151
H	3.385206	-3.002200	0.638536
H	3.247567	-3.006965	-1.125605
C	2.724929	-4.900457	-0.193288
H	3.736872	-5.326991	-0.270649
H	2.271688	-5.287824	0.735498
H	2.134749	-5.291655	-1.039964
H	0.140839	0.117806	2.991336

6 C-N cleavages = 2 (from μ-N)

N	-0.514945	1.671070	-0.485530

N	1.233138	0.199074	1.301810
N	-1.719108	-0.734008	0.431056
N	0.580079	-2.248651	0.036789
P	-1.713778	0.451273	-0.848947
P	1.843322	-1.107282	0.318115
P	-1.026757	-2.017154	-0.522486
C	2.026151	-0.062899	-2.378444
C	3.466404	0.318742	-2.733401
H	3.652619	1.352026	-2.396556
H	4.155561	-0.326102	-2.162923
N	1.729016	0.044694	-0.951051
P	1.152747	1.359781	-0.008250
N	-0.892299	-0.793575	-1.752220
Se	-2.013778	-3.835070	-0.835791
Se	-3.545831	1.169923	-1.591091
Se	3.607526	-2.116616	0.835562
Se	2.301329	3.116484	0.177285
C	-2.791456	-0.941704	1.422354
C	-0.953067	3.102866	-0.569158
C	-1.489186	3.677413	0.741072
H	-0.720657	3.571261	1.525470
H	-2.368149	3.094116	1.062846
C	-2.971330	0.227178	2.388785
H	-2.011602	0.443624	2.882532
H	-3.251005	1.128323	1.817991
H	-1.721039	3.157780	-1.352436
H	-3.744731	-1.145446	0.901972
H	1.307449	0.574308	-2.920638
C	-4.051862	-0.069849	3.431313
H	-4.187269	0.783731	4.113447
H	-5.025219	-0.273295	2.954518
H	-3.790249	-0.949339	4.043749
C	-1.873277	5.150788	0.585224
H	-2.264537	5.560361	1.529577
H	-1.003275	5.761490	0.291077
H	-2.652412	5.283333	-0.184335
C	3.734545	0.188220	-4.233638
H	3.072411	0.846394	-4.822355
H	4.773241	0.461496	-4.475484
H	3.572611	-0.845540	-4.584763
H	-0.087138	3.684399	-0.911437
H	1.808242	-1.098735	-2.688673
H	-2.527832	-1.855210	1.979639
H	0.831316	-3.216527	0.232146
C	1.747960	0.516200	2.652139
H	2.022690	1.583521	2.654673
H	2.684486	-0.050287	2.797753
C	0.770690	0.215652	3.788737
H	1.248457	0.563505	4.722276
H	-0.135764	0.832022	3.662313
C	0.396629	-1.261211	3.920589
H	-0.092642	-1.630203	3.004849
H	1.289512	-1.884830	4.093858
H	-0.296226	-1.424533	4.761575
H	-1.230627	-1.000029	-2.691356

6 C-N cleavages = 3

N	0.036496	1.969733	-0.382047
N	2.068250	0.204388	0.578110
N	-1.235113	-0.017745	1.152825
N	0.370736	-1.970540	-0.110184
P	-1.464910	1.169567	-0.103569

P	1.866854	-1.182221	-0.459148
P	-1.246065	-1.399005	0.087063
N	1.523408	0.019602	-1.642129
P	1.649222	1.399251	-0.620806
N	-1.462014	-0.208015	-1.139873
Se	-2.543028	-3.012591	0.412227
Se	-3.033361	2.558089	-0.022763
Se	3.396303	-2.596138	-0.661224
Se	2.924952	3.015586	-0.996585
C	-1.934195	0.022834	2.454972
C	-1.330205	1.041149	3.421187
H	-0.266866	0.802104	3.579393
H	-1.369868	2.044231	2.962464
H	-3.005845	0.240882	2.299751
C	-2.075635	1.059034	4.757733
H	-1.635933	1.797754	5.445671
H	-3.138154	1.321091	4.621544
H	-2.036146	0.074580	5.254208
H	-1.871147	-0.992539	2.877234
H	0.474599	-2.968322	0.073145
C	3.122335	0.360412	1.599881
H	3.617790	1.326496	1.409149
H	3.877742	-0.425091	1.423152
C	2.615023	0.295291	3.040695
H	3.471535	0.534081	3.696321
H	1.872966	1.096769	3.198748
C	2.025967	-1.060052	3.434230
H	1.154048	-1.311952	2.809203
H	2.767205	-1.867729	3.314466
H	1.694741	-1.061172	4.485052
C	-1.653137	-0.330606	-2.583789
H	-1.055848	-1.191588	-2.935251
H	-1.225823	0.570384	-3.060238
C	-3.118194	-0.501204	-2.999746
H	-3.690817	0.364449	-2.627544
H	-3.524672	-1.391163	-2.491179
C	-3.271004	-0.632814	-4.515544
H	-4.328590	-0.754049	-4.795712
H	-2.889207	0.259750	-5.040528
H	-2.722499	-1.508242	-4.903775
H	-0.025092	2.986845	-0.340937
H	1.055843	-0.075833	-2.538354

6 C-N cleavages = 4

N	0.000682	2.037228	-0.167235
N	-1.919136	0.074021	-0.711387
N	1.114923	-0.133068	-1.524866
N	-0.188056	-1.943695	0.160605
P	1.487225	1.234629	-0.509454
P	-1.674251	-1.138057	0.498018
P	1.365091	-1.344805	-0.295273
N	-1.215658	0.219220	1.499050
P	-1.546618	1.434871	0.291574
N	1.679961	0.023562	0.702351
Se	2.701932	-2.930341	-0.581403
Se	2.964302	2.618914	-1.043181
Se	-3.178589	-2.489184	1.031519
Se	-2.911474	2.992925	0.586371
H	-0.246094	-2.960810	0.191798
C	-2.748393	0.050272	-1.925621
H	-3.266354	1.022990	-1.962647
H	-3.531400	-0.714271	-1.776825

C	-1.995132	-0.200347	-3.235503
H	-2.680723	0.069196	-4.058788
H	-1.141968	0.495709	-3.296755
C	-1.521725	-1.642592	-3.422523
H	-0.833024	-1.950334	-2.620797
H	-2.372837	-2.344331	-3.419141
H	-0.993014	-1.765961	-4.381324
C	1.944875	0.126372	2.136606
H	1.439152	-0.721361	2.629361
H	1.444539	1.036653	2.508454
C	3.437598	0.143616	2.476882
H	3.910731	0.989332	1.950050
H	3.901721	-0.773696	2.077260
C	3.680355	0.250971	3.983167
H	4.757532	0.262294	4.210271
H	3.243657	1.175311	4.398876
H	3.235383	-0.600490	4.526271
H	0.030186	3.046177	-0.308384
H	-1.667818	0.316887	2.408303
H	1.614342	-0.232154	-2.409030

6 C-N cleavages = 5

N	-0.249762	2.042529	-0.147852
N	1.621007	0.082226	0.716626
N	-1.599776	-0.068414	0.990590
N	-0.078367	-1.939962	-0.336041
P	-1.784818	1.281098	-0.058570
P	1.461123	-1.166123	-0.484520
P	-1.673595	-1.321669	-0.184236
N	1.228121	0.170260	-1.555111
P	1.346536	1.417675	-0.366713
N	-1.801398	0.032969	-1.295705
Se	-3.093395	-2.852625	-0.164178
Se	-3.330362	2.674969	0.106842
Se	2.962599	-2.601233	-0.719742
Se	2.717734	2.993136	-0.465509
H	-0.031768	-2.956856	-0.395011
C	2.499211	0.085530	1.897986
H	3.059780	1.034685	1.880092
H	3.237830	-0.725104	1.771069
C	1.751150	-0.068543	3.225144
H	2.470810	0.139324	4.036533
H	0.978835	0.718956	3.294751
C	1.130225	-1.450911	3.437752
H	0.414368	-1.705644	2.638525
H	1.903205	-2.237199	3.438646
H	0.595061	-1.506845	4.399031
H	-0.285757	3.060899	-0.113049
H	0.538232	0.173865	-2.305498
H	-1.369694	-0.108848	1.979224
H	-2.595432	0.029954	-1.938648

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