Supporting Information

Selective Crystallization of Four Bis(phthalocyaninato)lanthanoid(III) Polymorphs

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Table S1. Crystallographic Parameters for the $LaPc_2$ Polymorphs

	α-Phase[a]	CH_2Cl_2 Solvate Phase
Chemical Formula	$C_{64}H_{32}N_{16}La$	$C_{64}H_{32}N_{16}La{\cdot}CH_2Cl_2$
Crystal System	Tetragonal	Orthorhombic
Z	2	4
Space Group	*P*4/*nnc*	*Pnma*
a (Å)	19.9227(6)	28.0409(9)
b (Å)	19.9227(6)	22.9440(7)
c (Å)	6.3925(4)	7.8783(2)
α (°)	90.0	90.0
β (°)	90.0	90.0
γ (°)	90.0	90.0
V ($Å^3$)	2537.27	5068.67
Density (g/cm^3)	1.524	1.637
R-factor (%)	8.03	3.01
CCDC Number	2096854	2096857

[a] There is a small residual electronic density peak at coordinates (¼, ¼, ¾), mirroring the La center with respect to the phthalocyanine ring. This suggests some La disorder between two positions shifted along the $LaPc_2$ stack by the Pc-Pc distance, as was observed in the neodymium case. Attempts to refine this model, however, converged to occupancy factors of less than 1% for the additional La site with no significant improvement of the R-factors, and where thus abandoned.

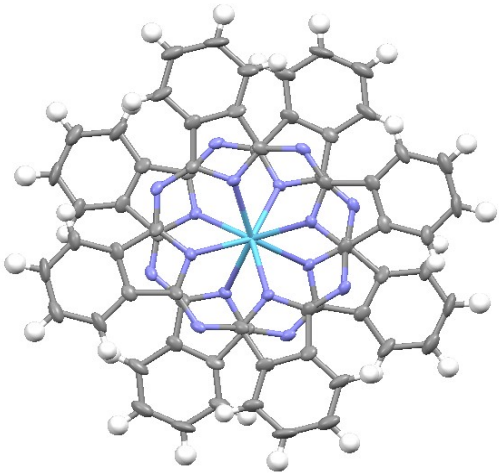


Figure S1. Thermal ellipsoid plot for the $LaPc_2$ α-phase. Ellipsoids shown at 50% probablilty (La: light blue, C: grey, N: blue, H: white).

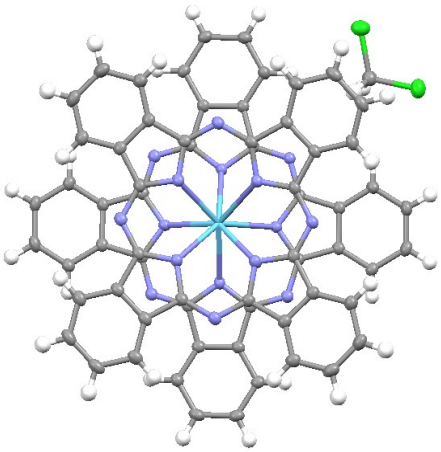


Figure S2. Thermal ellipsoid plot for the $LaPc_2{\cdot}CH_2Cl_2$ phase. Ellipsoids shown at 50% probablilty (La: light blue, C: grey, N: blue, Cl: bright green, H: white).

Table S2. Crystallographic Parameters for $PrPc_2$ Polymorphs

	δ-Phase	CH_2Cl_2 Solvate Phase
Chemical Formula	$C_{64}H_{32}N_{16}Pr$	$C_{64}H_{32}N_{16}Pr{\cdot}CH_2Cl_2$
Crystal System	Monoclinic	Orthorhombic
Z	4	4
Space Group	*C*2/*c*	*Pnma*
a (Å)	28.106(3)	28.1128(16)
b (Å)	14.1593(10)	22.9663(14)
c (Å)	13.1975(8)	7.8883(5)
α (°)	90.0	90.0
β (°)	115.551(4)	90.0
γ (°)	90.0	90.0
V ($Å^3$)	4738.45	5093.06
Density (g/cm^3)	1.634	1.631
R-factor (%)	2.68	2.94
CCDC Number	2096858	2096859

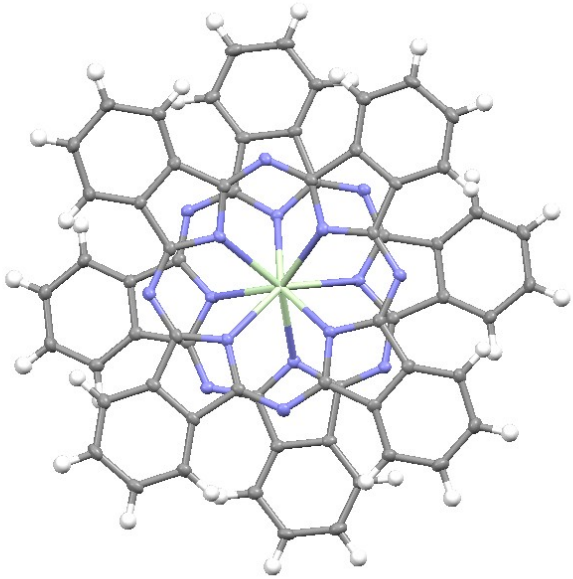


Figure S3. Thermal ellipsoid plot for the $PrPc_2$ δ-phase. Ellipsoids shown at 50% probablilty (Pr: yellow-green, C: grey, N: blue, H: white).

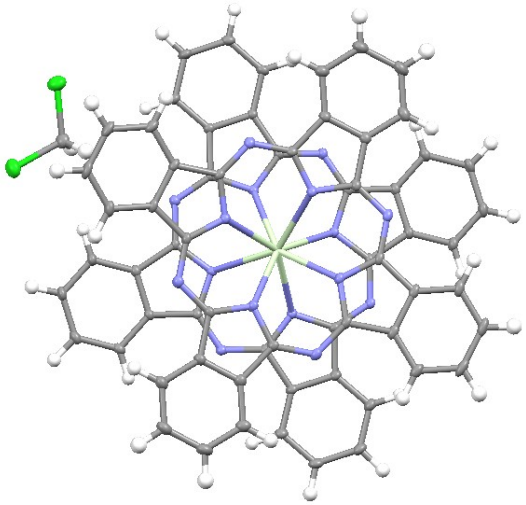
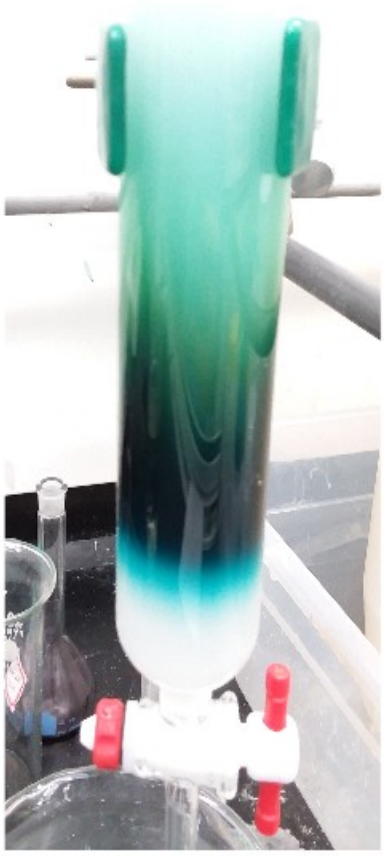


Figure S4. Thermal ellipsoid plot for the $PrPc_2{\cdot}CH_2Cl_2$ solvate phase. Ellipsoids shown at 50% probability (Pr: yellow-green, C: grey, N: blue, Cl: bright green, H: white).

a)



b)

Figure S5. a) Purification of $NdPc_2$ and $NdPc_2^-$ by column chromatography showing blue ($NdPc_2^-$) and green ($NdPc_2$) bands b) Resulting fractions.

Table S3. Crystallographic parameters for the $NdPc_2$ polymorphs

	α-Phase[a]	β-Phase[b]	γ-Phase[c]	δ-Phase	CH_2Cl_2 Solvate Phase
Chemical Formula	$C_{64}H_{32}N_{16}Nd$	$C_{64}H_{32}N_{16}Nd$	$C_{64}H_{32}N_{16}Nd$	$C_{64}H_{32}N_{16}Nd$	$C_{64}H_{32}N_{16}Nd{\cdot}CH_2Cl_2$
Crystal System	Tetragonal	Monoclinic	Orthorhombic	Monoclinic	Orthorhombic
Z	2	4	4	4	4
Space Group	*P*4/*nnc*	*C*2/*c*	$P2_12_12_1$	*C*2/*c*	*Pnma*
a (Å)	19.937(5)	19.010	8.852(2)	28.103(3)	28.085(16)
b (Å)	19.937(5)	19.066	10.604(2)	14.175(13)	22.964(13)
c (Å)	6.420(16)	15.538	50.844(12)	13.185(12)	7.890(4)
α (°)	90.0	90.0	90.0	90.0	90.0
β (°)	90.0	116.1	90.0	115.596(2)	90.0
γ (°)	90.0	90.0	90.0	90.0	90.0
V ($Å^3$)	2551.93	5057.39	4772.5(19)	4737.0(8)	5088.3(5)
Density (g/cm^3)	1.522	1.536	1.627	1.640	1.637
R-factor (%)	6.47	5.2	3.07	3.55	2.66
CCDC Number	2016007	N/A	2016008	2016006	2016009

a. Platon (Spek, A. L. *Acta Cryst*., **2009**, D65, 148-155) was used to transform the space group from P4/nnc to the suggested P4/mcc, which includes an additional mirror through the phthalocyanine ring, and therefore imposes a 50:50 disorder between the two Nd sites. Refinement of the structure in the new space group did not yield any appreciable improvement of the model or R-factors (P4/nnc: R_1=6.47%, wR_2=18.00%; P4/mcc: R_1=5.78%, wR_2=22.55%). Given that the Nd disorder refines away from a 50:50 ratio in the P4/nnc space group, and that the curvature observed for the phthalocyanine rings (convexity toward the major Nd site) is consistent with the structure of the $NdPc_2$ molecules in all other phases, P4/nnc was determined to be the correct space group. The OMIT command was used to omit reflections affected by the beam stop.

b. Parameters taken from the following reference: Darovskikh, A.N.; Tsytsenko, A.K.; Frank-Kamenetskaya, O.V.; Fundamenskii, V.S.; Moskalev, P.N. Polymorphism of Diphthalocyanine-Neodymium. Molecular and Crystal Structure of the β-Phase. *Sov. Phys. Crystallogr.,* **1984,** *24*, 273-276.

c. The OMIT command was used to omit reflections affected by the beam stop.

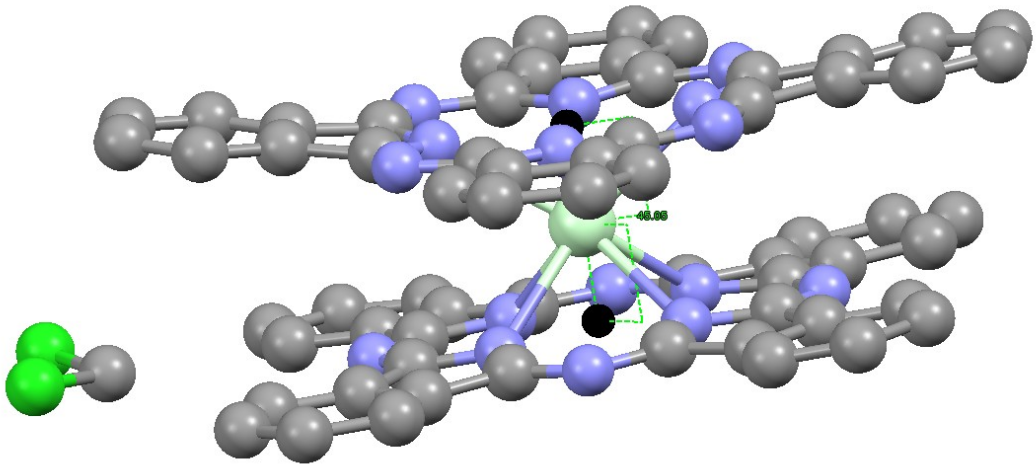


Figure S6. An example of how the skew angle is calculated using the CH_2Cl_2 solvate phase. Centroids are defined by the four isoindole nitrogens on each Pc ligand (Nd: green, N: blue, C: grey, Cl: bright green). Hydrogens are omitted for clarity.

Table S4. Geometric parameters of the different $NdPc_2$ polymorphs.

	α-Phase	β-Phase	γ-Phase	δ-Phase	CH_2Cl_2 Solvate Phase
Skew angle (°)	40.9	39.0	40.8	42.7	45
Shortest Nd-Nd Distance (Å)	6.4202(16)	8.458	8.852(2)	7.0782(6)	7.8897(4)
Slip angle (°)	90	49.5	47.3	67	55.3
Vertical intermolecular Pc-Pc Distance (Å)	3.45	3.45	3.57	3.57	3.54

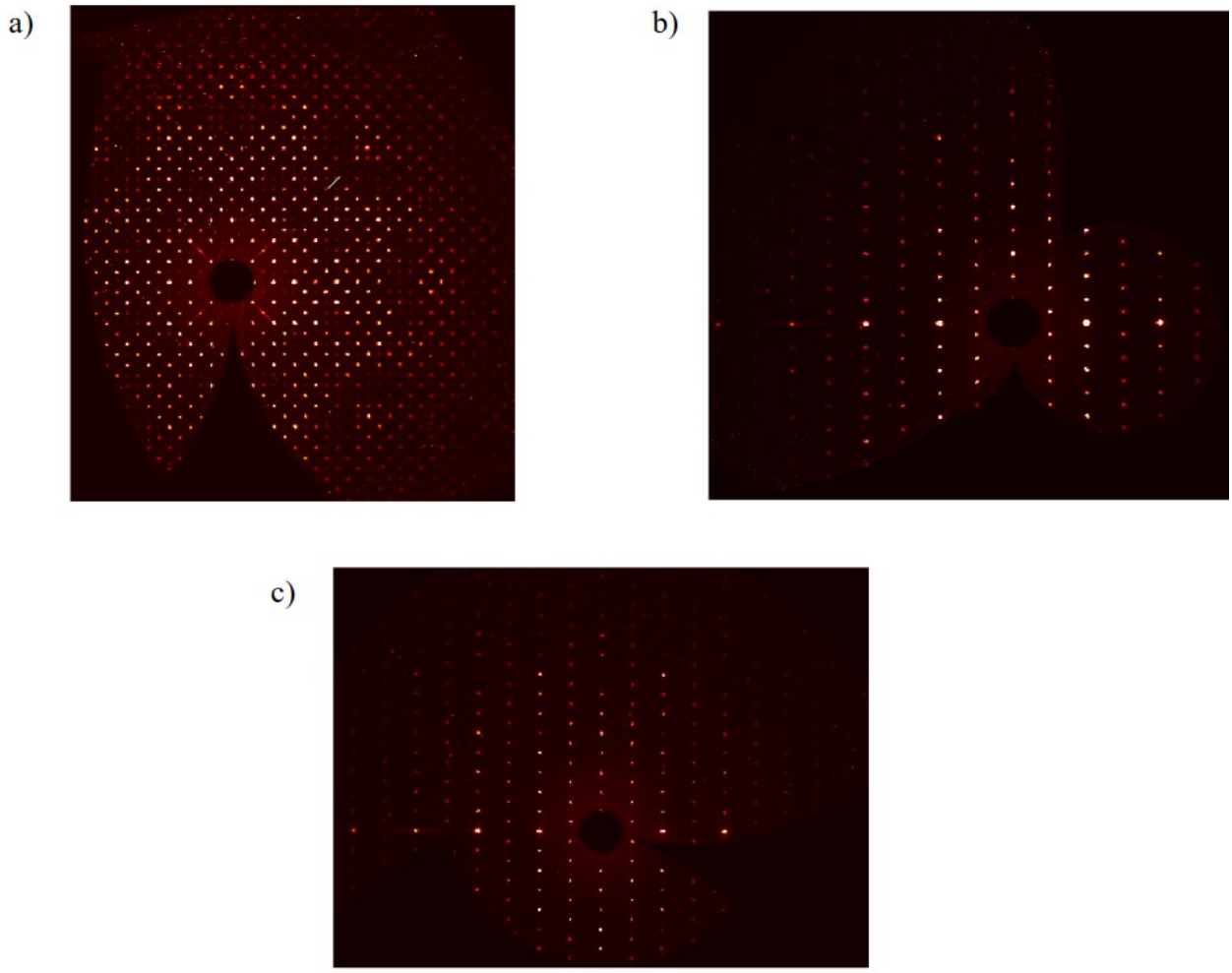


Figure S7. Reflection data for the $NdPc_2$ α-phase showing the lack of a supercell or superperiod in the directions a) 0kl b) h0l c) hk0.

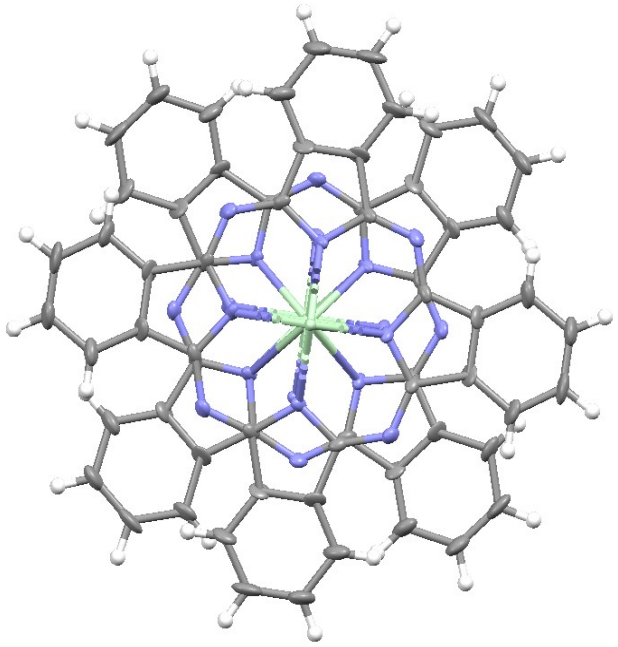


Figure S8. Thermal ellipsoid plot for the $NdPc_2$ α-phase. Ellipsoids shown at 50% probability (Nd: green, C: grey, N: blue, H: white).

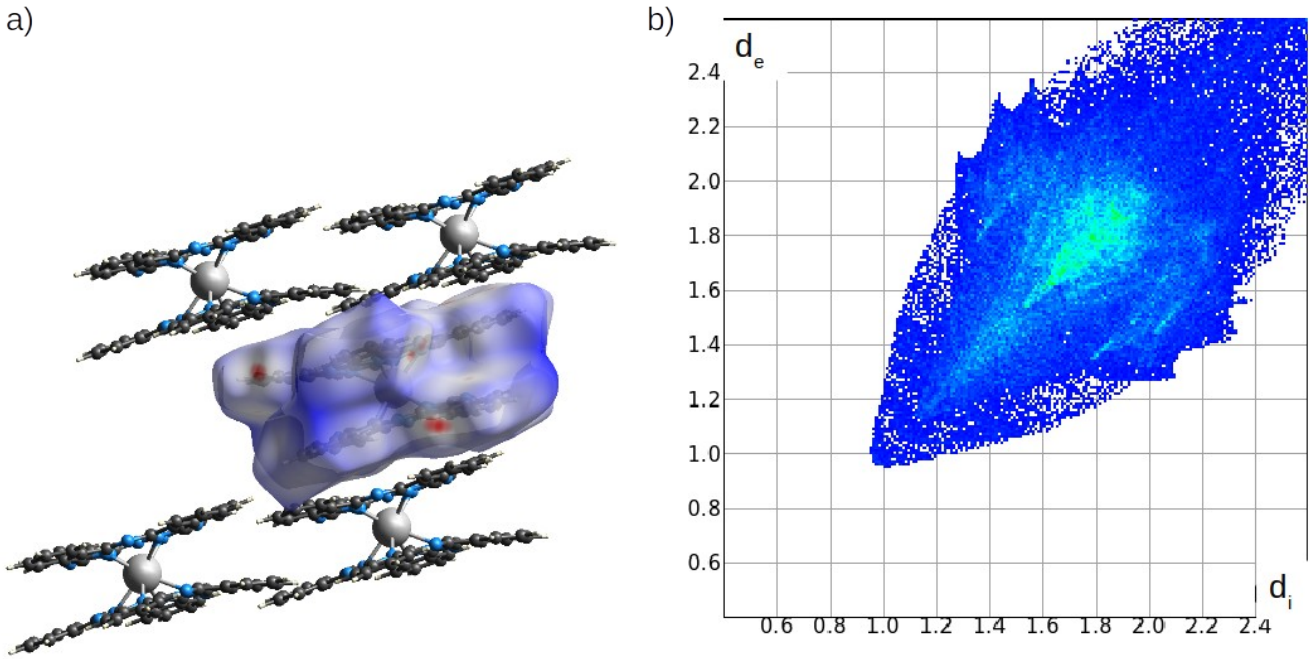


Figure S9. Hirshfeld plot (a) and corresponding fingerprint plot (b) for the $NdPc_2$ β-phase.

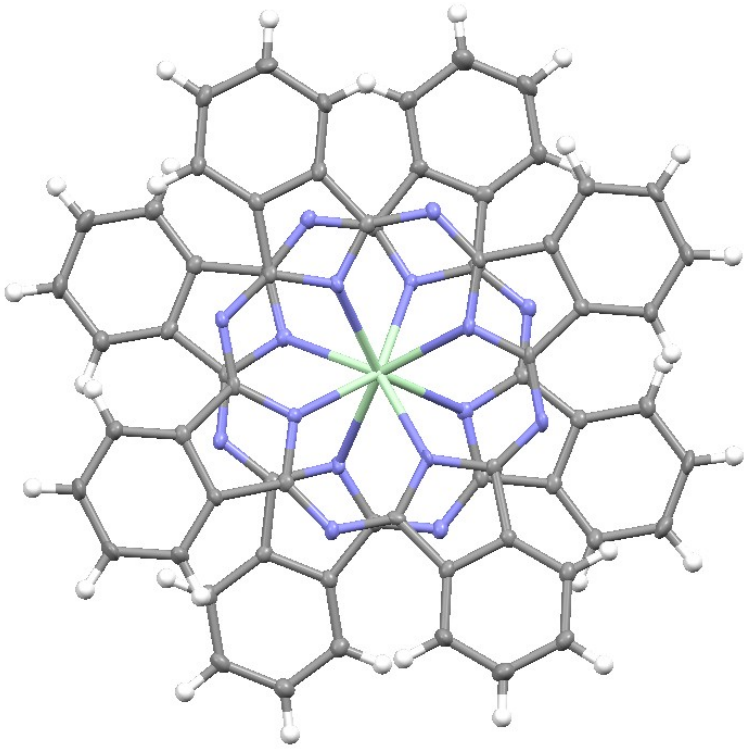


Figure S10. Thermal ellipsoid plot for the $NdPc_2$ γ-phase. Ellipsoids shown at a 50% probability (Nd: green, N: blue, C: grey, H: white).

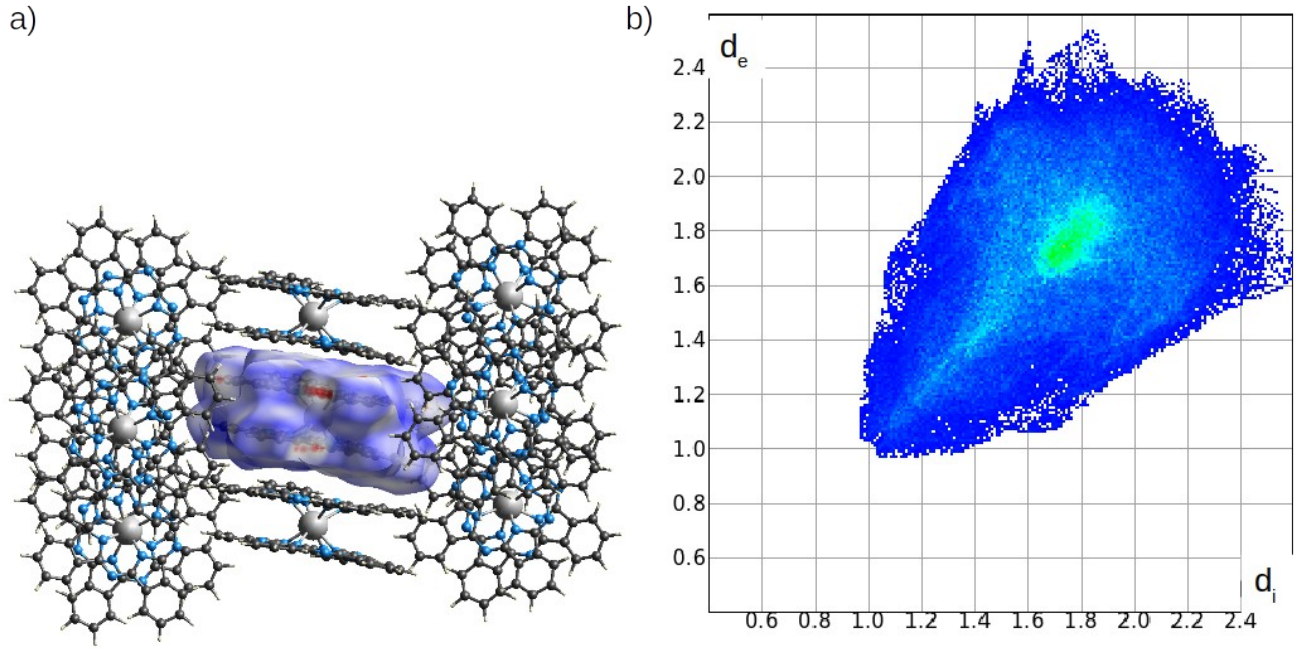


Figure S11. The Hirshfeld surface (a) and corresponding fingerprint plot (b) for the $NdPc_2$ γ-phase.

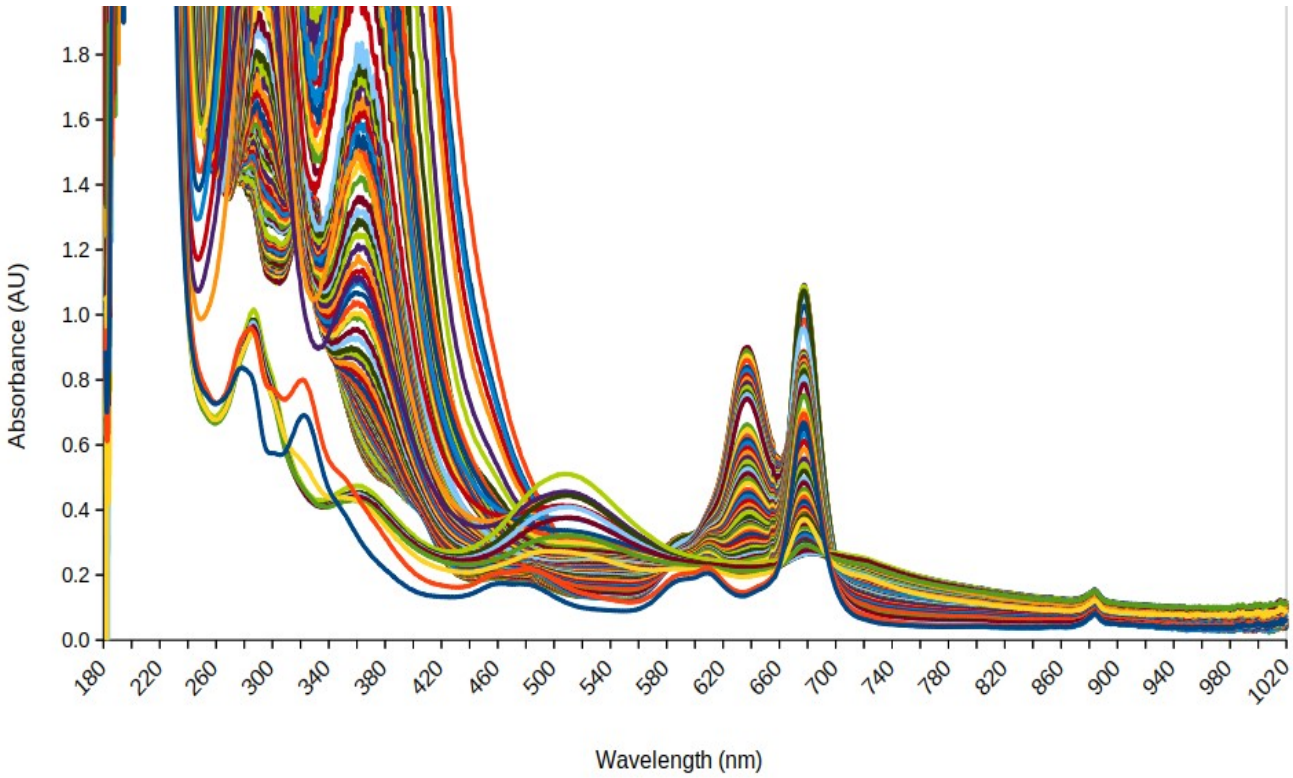


Figure S12. Redox titration of $NdPc_2$ γ-phase crystals, re-dissolved in CH_2Cl_2.

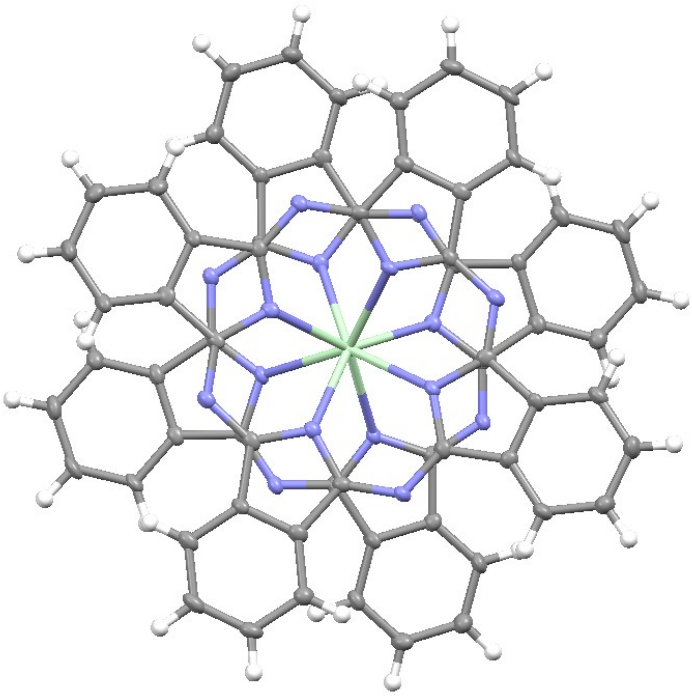


Figure S13. Thermal ellipsoid plot for the $NdPc_2$ δ-phase. Ellipsoids shown at a 50% probability (Nd: green, N: blue, C: grey, H: white).

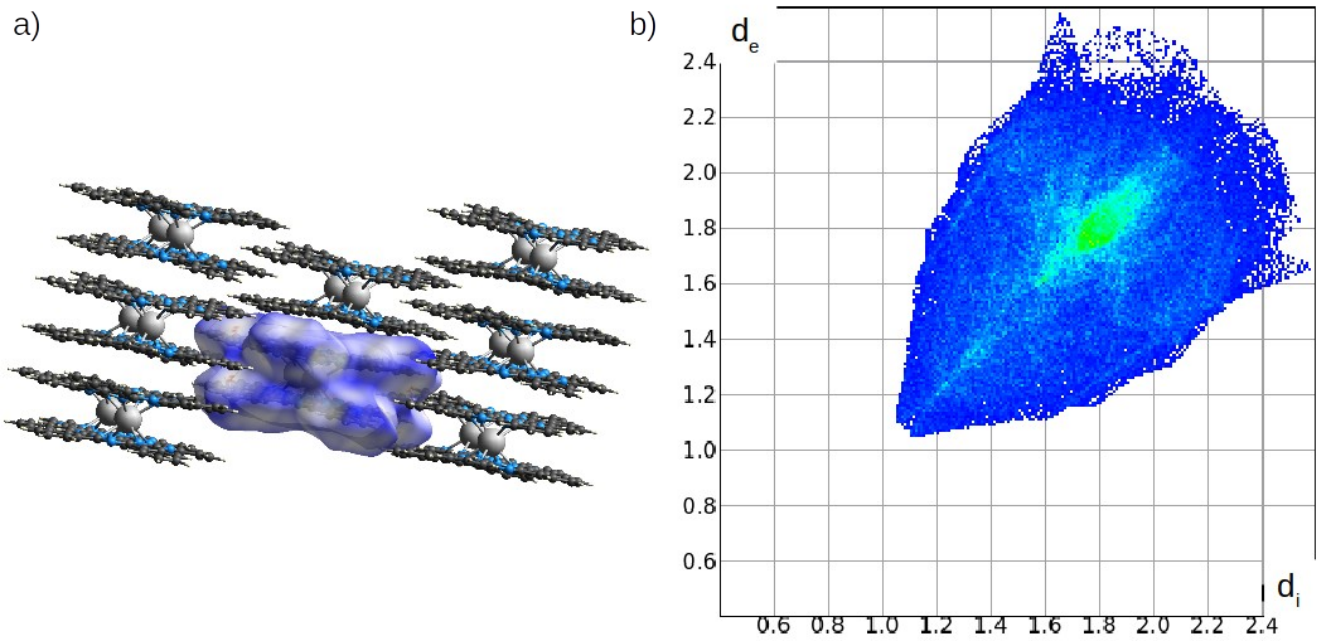


Figure S14: The Hirshfeld surface (a) and corresponding fingerprint plot (b) for the $NdPc_2$ δ-phase.

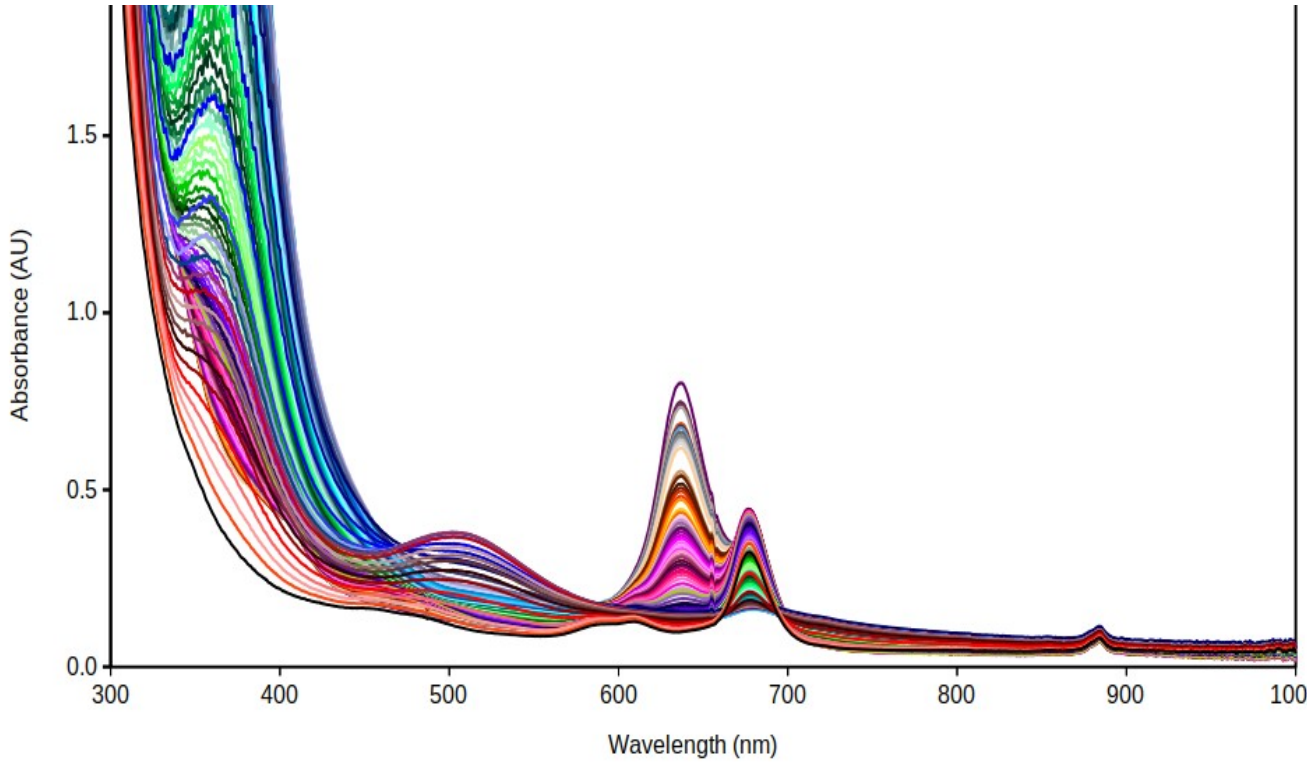


Figure S15. Redox titration of $NdPc_2$ δ-phase crystals, re-dissolved in CH_2Cl_2.

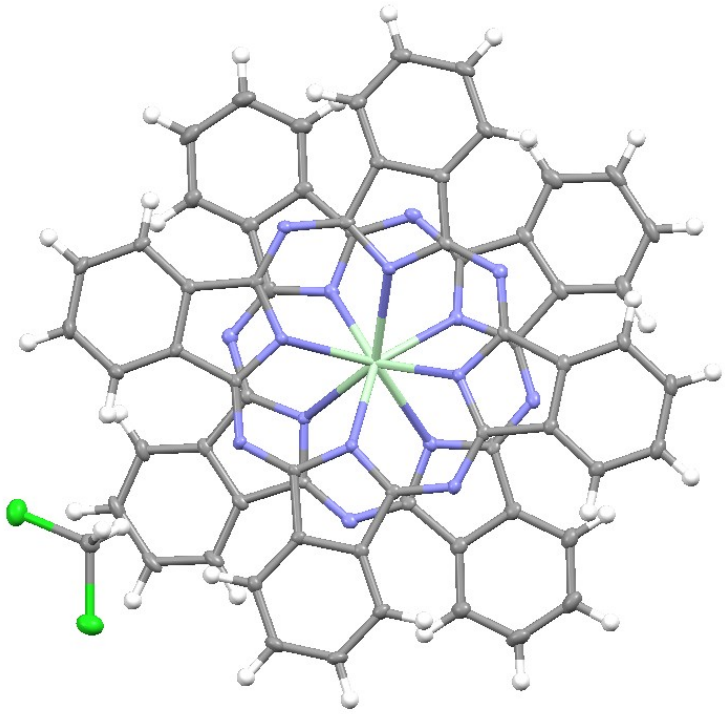


Figure S16. Thermal ellipsoid plot for the $NdPc_2$ CH_2Cl_2 solvate phase. Ellipsoids shown at a 50% probability (Nd: green, N: blue, C: grey, H: white).

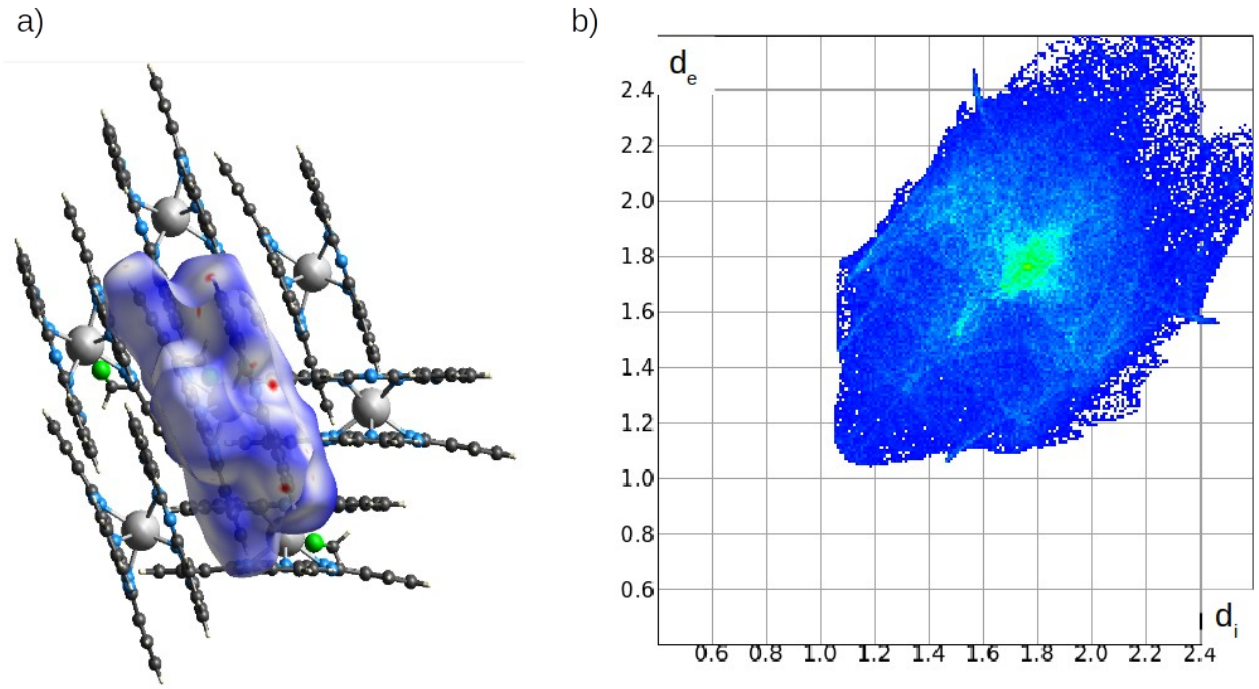


Figure S17. The Hirshfeld surface (a) and corresponding fingerprint plot (b) for the $NdPc_2$ CH_2Cl_2 solvate phase.

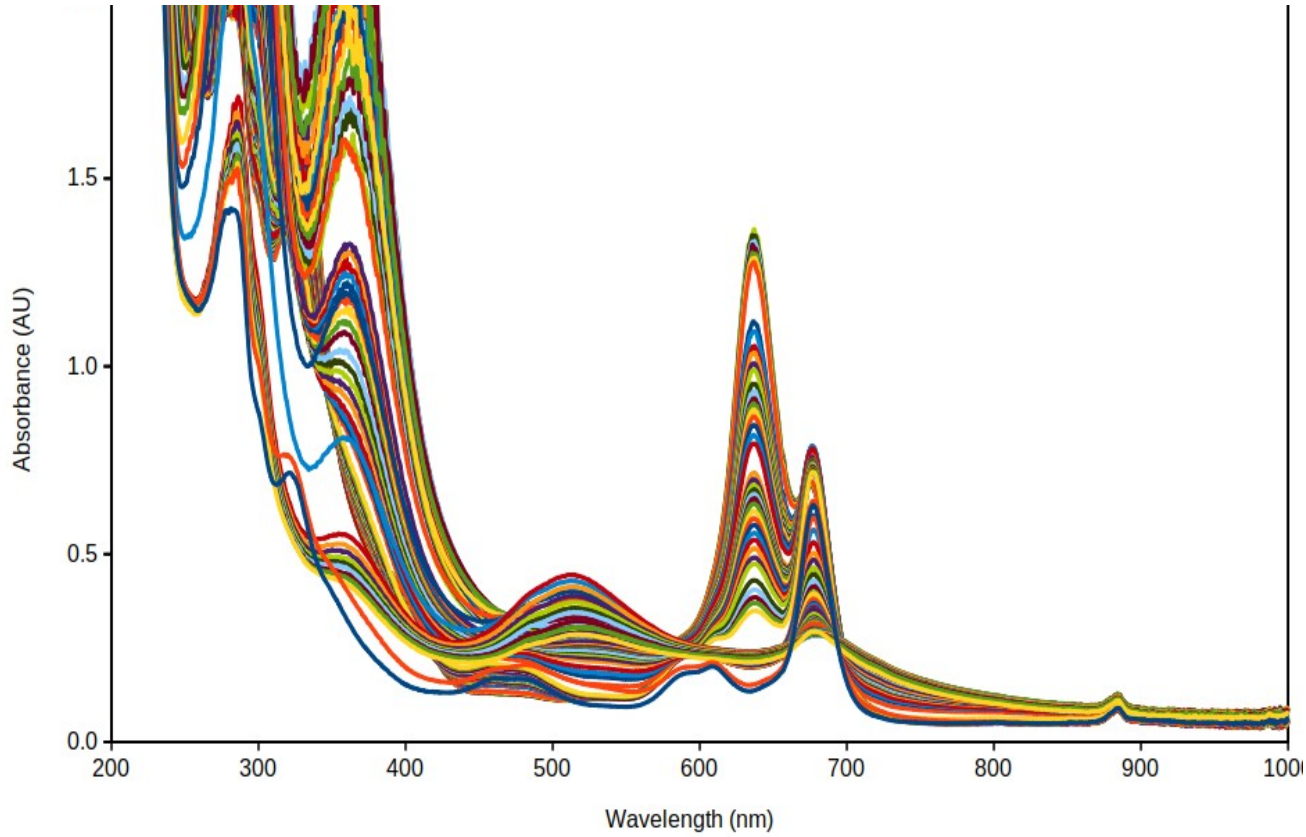


Figure S18. Redox titration of $NdPc_2{\cdot}CH_2Cl_2$ solvate phase crystals, re-dissolved in CH_2Cl_2.

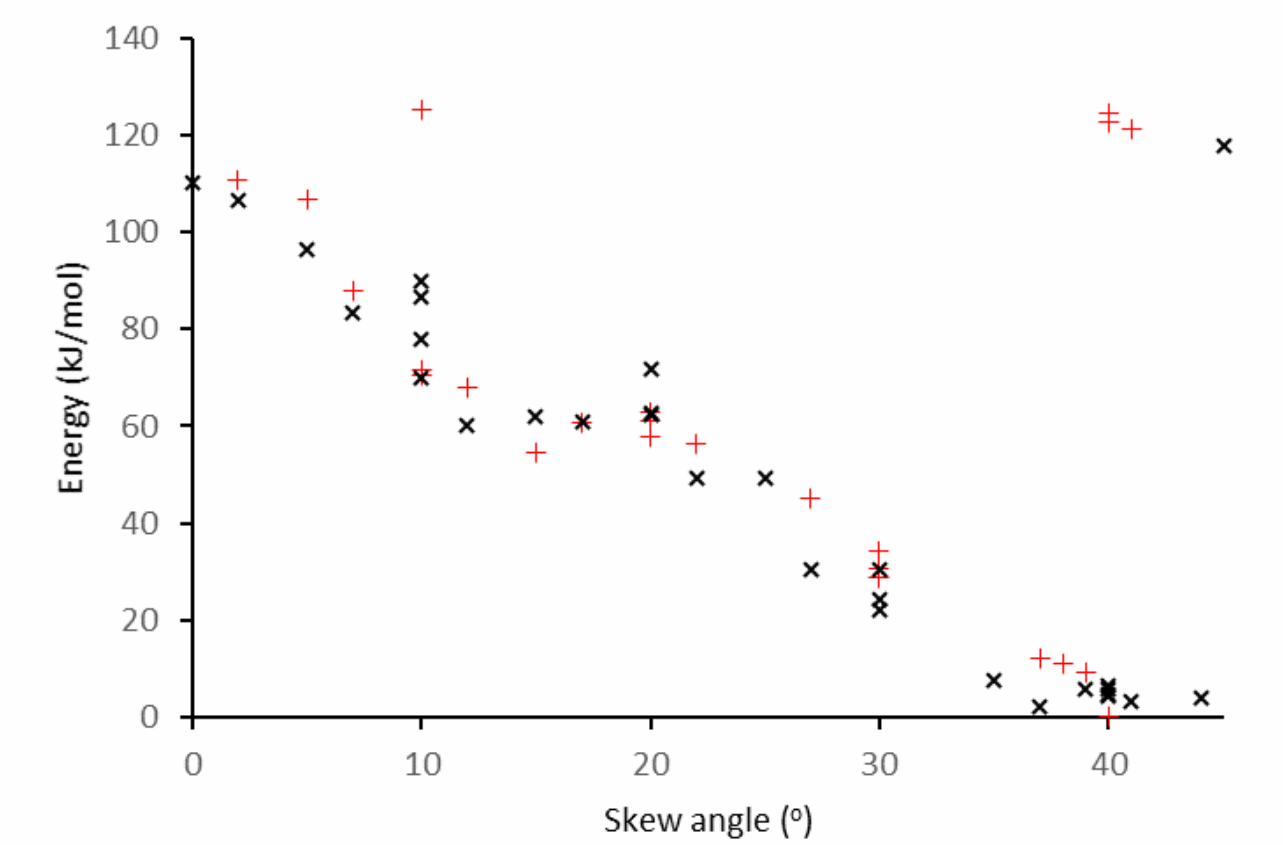


Figure S19. Influence of the skew angle of a $NdPc_2$ molecule on the energies of its quintet (ferromagnetic coupling between the Nd^{3+} center and the phthalocyanine radical, ×) and triplet states (antiferromagnetic coupling, +).

Table S5. Crystallographic Parameters for the $SmPc_2$ Polymorphs

	γ-Phase	δ-Phase	CH_2Cl_2 Solvate Phase
Chemical Formula	$C_{64}H_{32}N_{16}Sm$	$C_{64}H_{32}N_{16}Sm$	$C_{64}H_{32}N_{16}Sm{\cdot}CH_2Cl_2$
Crystal System	Orthorhombic	Monoclinic	Orthorhombic
Z	4	4	4
Space Group	$P2_12_12_1$	$C2/c$	$Pnma$
a (Å)	8.8201(2)	28.1112(14)	28.1354(6)
b (Å)	10.6092(3)	14.2031(12)	22.9450(6)
c (Å)	50.7567(11)	13.1654(5)	7.8933(2)
α (°)	90.0	90.0	90.0
β (°)	90.0	115.574(2)	90.0
γ (°)	90.0	90.0	90.0
V ($Å^3$)	4749.52	4741.51	5095.65
Density (g/cm^3)	1.644	1.647	1.643
R-factor (%)	3.8	1.73	3.1
CCDC Number	2096866	2096862	2096863

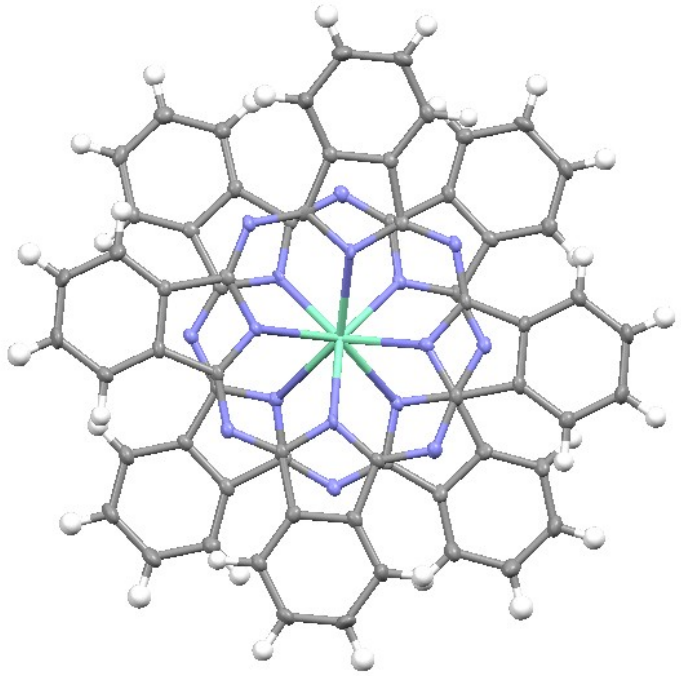


Figure S20. Thermal ellipsoid plot for the $SmPc_2$ γ-phase. Ellipsoids shown at 50% probablilty (Sm: teal, C: grey, N: blue, H: white).

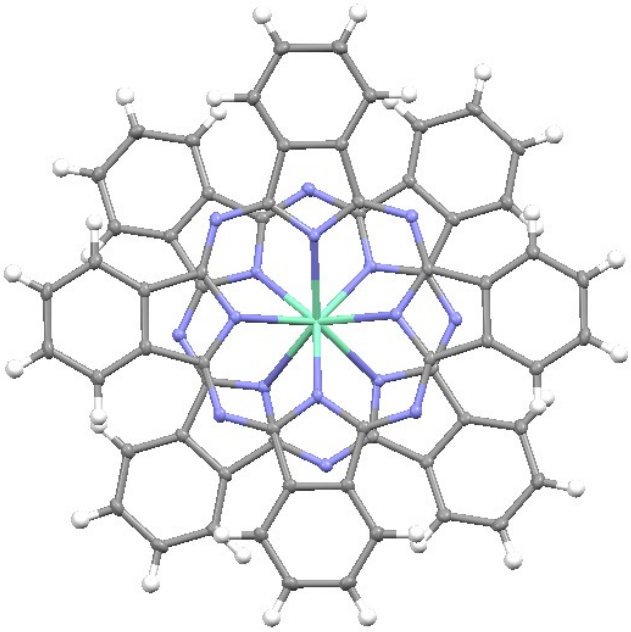


Figure S21. Thermal ellipsoid plot for the $SmPc_2$ δ-phase. Ellipsoids shown at 50% probablilty (Sm: teal, C: grey, N: blue, H: white).

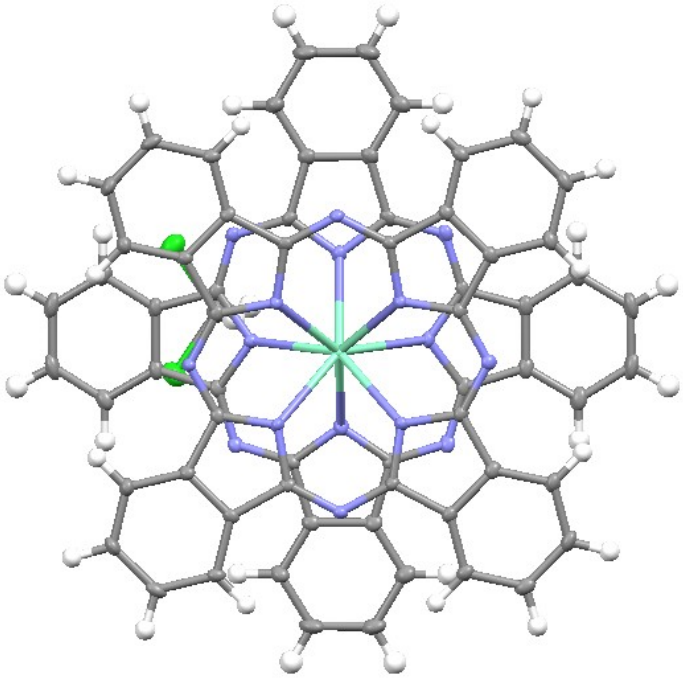


Figure S22. Thermal ellipsoid plot for the $SmPc_2 \cdot CH_2Cl_2$ phase. Ellipsoids shown at 50% probablilty (Sm: teal, C: grey, N: blue, H: white).

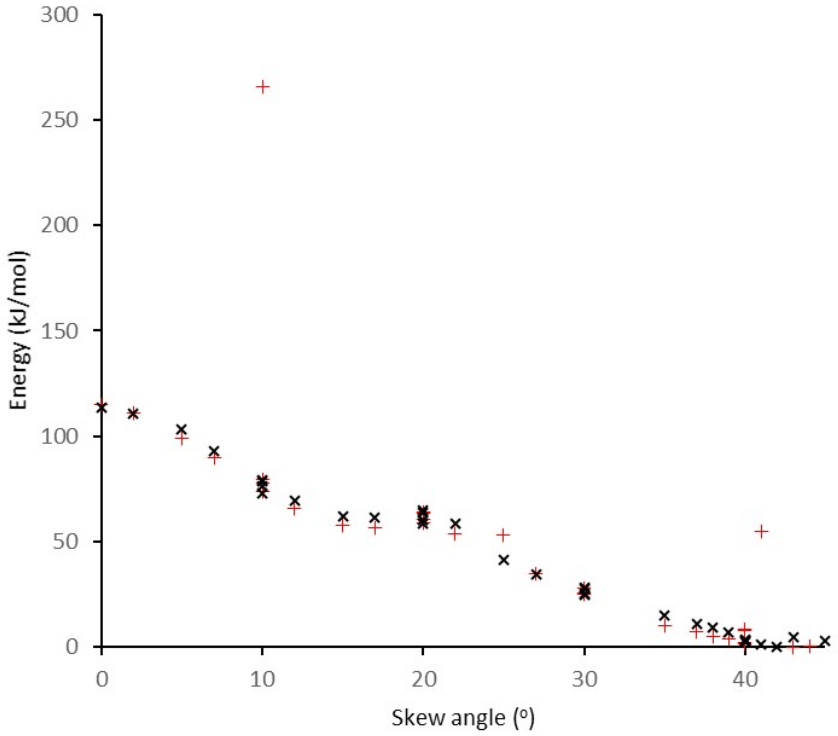


Figure S23. Influence of the skew angle of a $SmPc_2$ molecule on the energies of its septet (ferromagnetic coupling between the Sm^{3+} center and the phthalocyanine radical, ×) and quintet states (antiferromagnetic coupling, +).

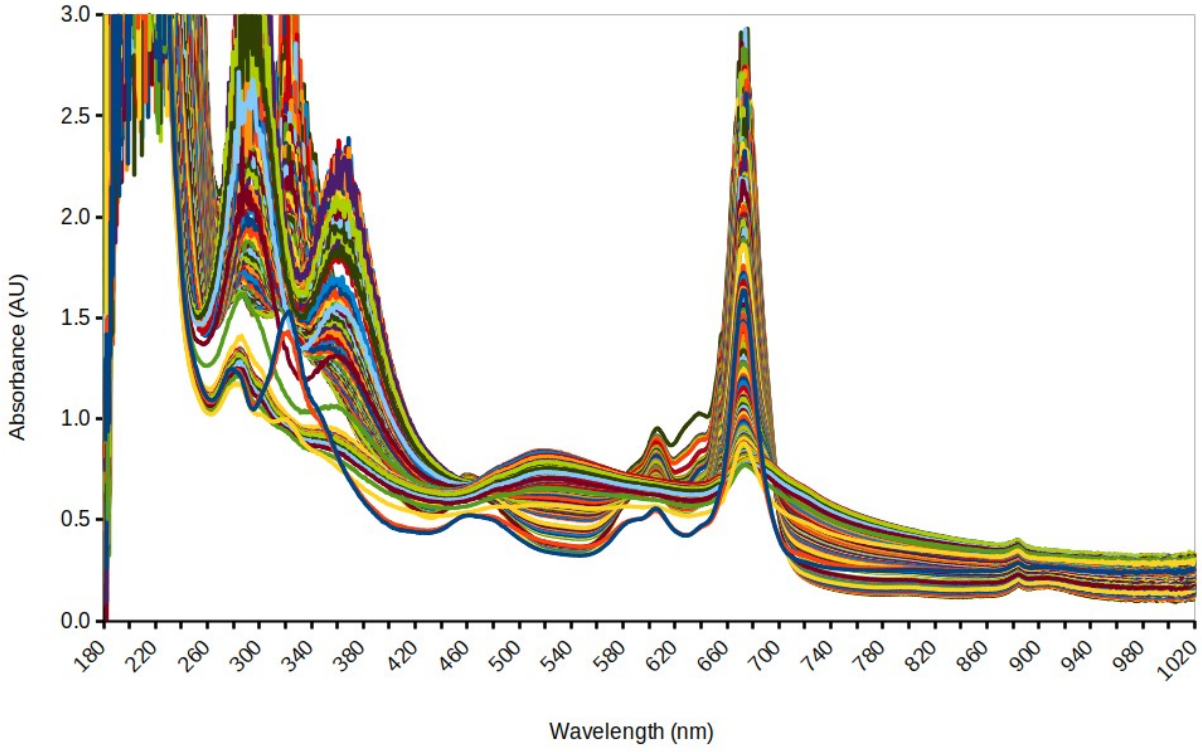


Figure S24. Redox titration of $SmPc_2 \cdot CH_2Cl_2$ solvate phase crystals, re-dissolved in CH_2Cl_2.

Table S6. Crystallographic Parameters for $GdPc_2$ Polymorphs

	γ-Phase[a]	δ-Phase	CH_2Cl_2 Solvate Phase
Chemical Formula	$C_{64}H_{32}N_{16}Gd$	$C_{64}H_{32}N_{16}Gd$	$C_{64}H_{32}N_{16}Gd{\cdot}CH_2Cl_2$
Crystal System	Orthorhombic	Monoclinic	Orthorhombic
Z	4	4	4
Space Group	$P2_12_12_1$	$C2/c$	$Pnma$
a (Å)	8.8412(14)	28.125(3)	28.356(3)
b (Å)	10.5892(15)	14.1663(14)	22.882(3)
c (Å)	50.762(8)	13.1416(14)	8.0460(10)
α (°)	90.0	90.0	90.0
β (°)	90.0	115.688(4)	90.0
γ (°)	90.0	90.0	90.0
V ($Å^3$)	4752.4	4718.49	5220.58
Density (g/cm^3)	1.653	1.664	1.612
R-factor (%)	5.38	5.12	4.45
CCDC Number	2096860	2096855	2096853

[a]The γ-phase crystals are often twinned, resulting in residual electron density along the Gd-Gd directions.

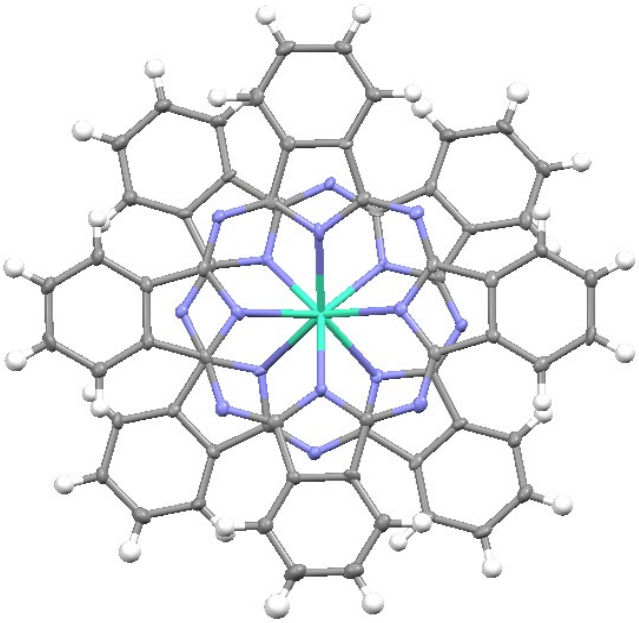


Figure S25. Thermal ellipsoid plot for the $GdPc_2$ γ-phase. Ellipsoids shown at 50% probablilty (Gd: blue-green, C: grey, N: blue, H: white).

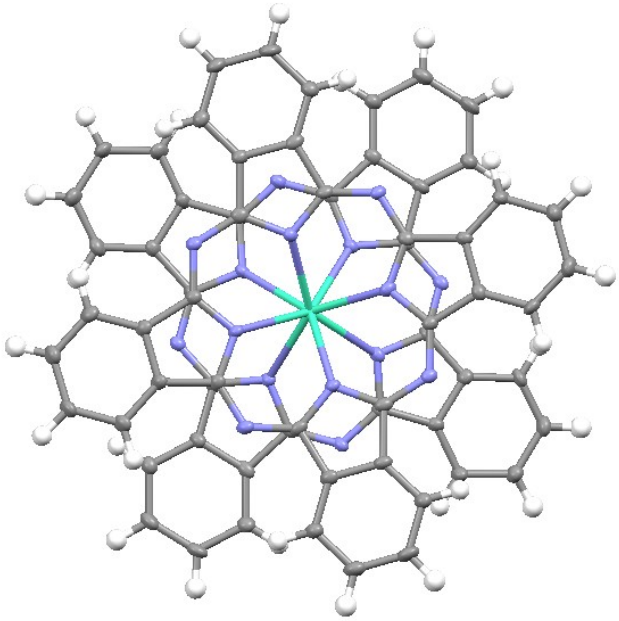


Figure S26. Thermal ellipsoid plot for the $GdPc_2$ δ-phase. Ellipsoids shown at 50% probablilty (Gd: blue-green, C: grey, N: blue, H: white).

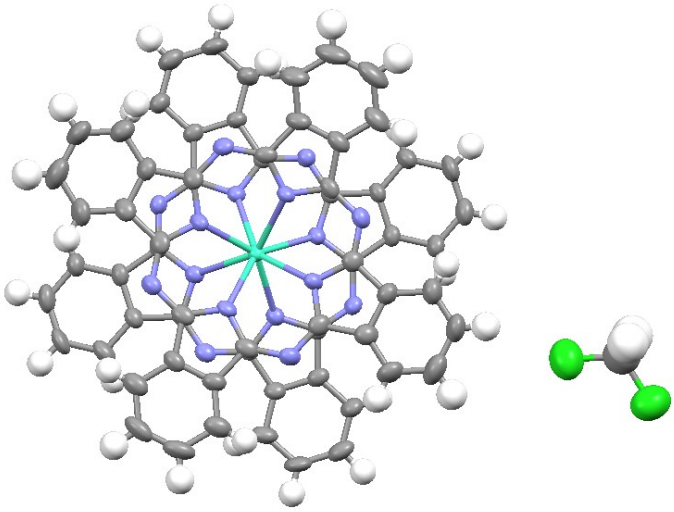


Figure S27. Thermal ellipsoid plot for the $GdPc_2 \cdot CH_2Cl_2$ phase. Ellipsoids shown at 50% probablilty (Gd: blue-green, C: grey, N: blue, Cl: bright green, H: white).

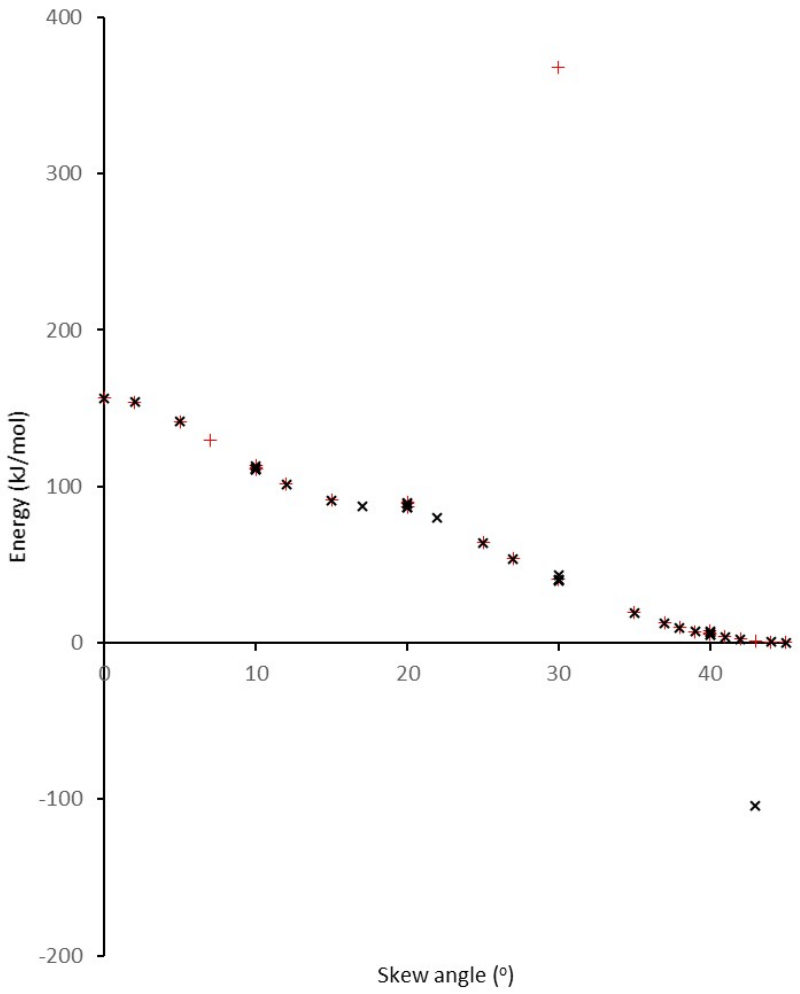


Figure S28. Influence of the skew angle of a $GdPc_2$ molecule on the energies of its nonet (ferromagnetic coupling between the Gd^{3+} center and the phthalocyanine radical, ×) and septet states (antiferromagnetic coupling, +).

Table S7. Crystallographic Parameters for $TbPc_2$ Polymorphs

	γ-Phase[a]	δ-Phase	CH_2Cl_2 Solvate Phase
Chemical Formula	$C_{64}H_{32}N_{16}Tb$	$C_{64}H_{32}N_{16}Tb$	$C_{64}H_{32}N_{16}Tb{\cdot}CH_2Cl_2$
Crystal System	Orthorhombic	Monoclinic	Orthorhombic
Z	4	4	4
Space Group	$P2_12_12_1$	$C2/c$	$Pnma$
a (Å)	8.8136(6)	28.086(3)	28.0516(7)
b (Å)	10.5756(7)	14.160(2)	22.9642(8)
c (Å)	50.713(3)	13.1416(14)	7.8827(2)
α (°)	90.0	90.0	90.0
β (°)	90.0	115.708(10)	90.0
γ (°)	90.0	90.0	90.0
V ($Å^3$)	4726.91	4709.06	5077.9
Density (g/cm^3)	1.664	1.670	1.660
R-factor (%)	5.01	4.62	2.39
CCDC Number	2108638	2096861	2096864

[a]The γ-phase crystals are often twinned, resulting in residual electron density along the Tb-Tb directions.

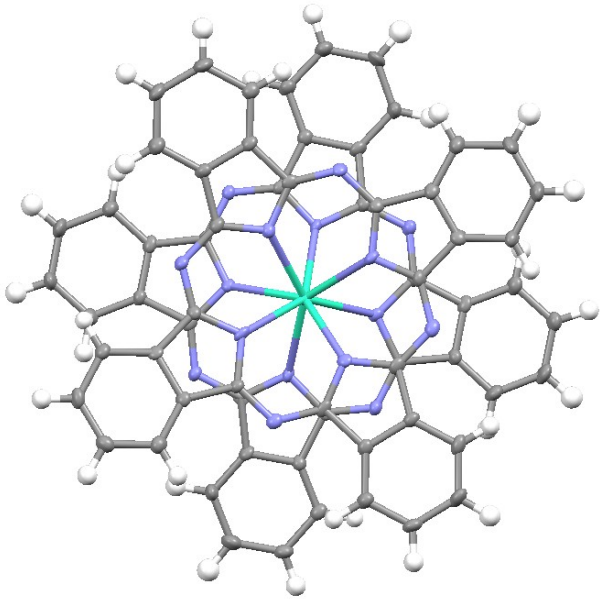


Figure S29. Thermal ellipsoid plot for the $TbPc_2$ γ-phase. Ellipsoids shown at 50% probablilty (Tb: blue-green, C: grey, N: blue, H: white).

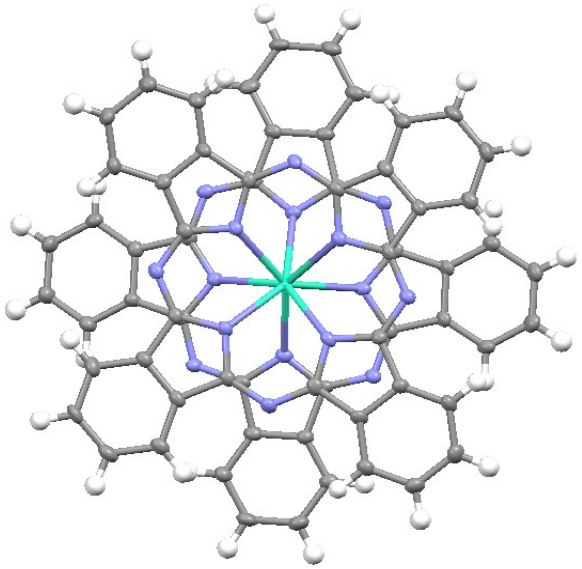


Figure S30. Thermal ellipsoid plot for the $TbPc_2$ δ-phase. Ellipsoids shown at 50% probablilty (Tb: blue-green, C: grey, N: blue, H: white).

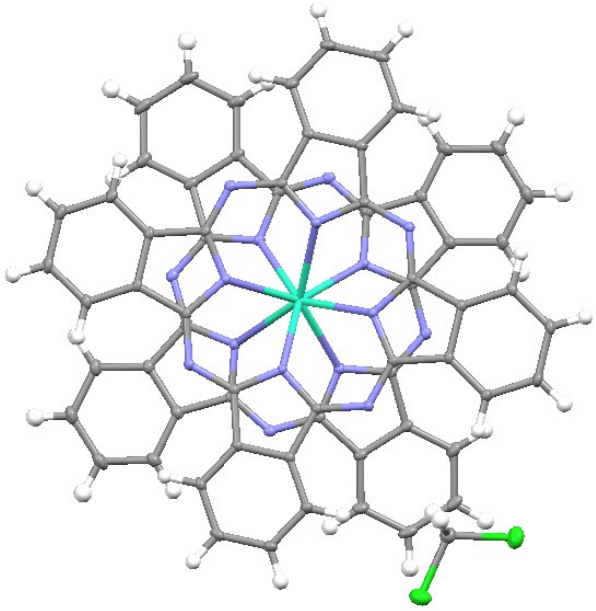


Figure S31. Thermal ellipsoid plot for the $TbPc_2 \cdot CH_2Cl_2$ phase. Ellipsoids shown at 50% probablilty (Tb: blue-green, C: grey, N: blue, Cl: bright green, H: white).

Table S8. Crystallographic Parameters for $DyPc_2$ Polymorphs

	α-Phase[a]	γ-Phase	CH_2Cl_2 Solvate Phase
Chemical Formula	$C_{64}H_{32}N_{16}Dy$	$C_{64}H_{32}N_{16}Dy$	$C_{64}H_{32}N_6Dy{\cdot}CH_2Cl_2$
Crystal System	Tetragonal	Orthorhombic	Orthorhombic
Z	2	4	4
Space Group	*P*4/*nnc*	$P2_12_12_1$	*Pnma*
a (Å)	19.548(4)	8.8171(11)	28.030(3)
b (Å)	19.548(4)	10.5671(12)	22.902(3)
c (Å)	6.477(2)	50.658(6)	7.8972(8)
α (°)	90.0	90.0	90.0
β (°)	90.0	90.0	90.0
γ (°)	90.0	90.0	90.0
V ($Å^3$)	2475.02	4718.93	5069.55
Density (g/cm^3)	1.584	1.672	1.667
R-factor (%)	7.00	4.57	5.87
CCDC Number	2096850	2096851	2096852

[a] There is a small residual electronic density peak at coordinates (¼, ¼, ¾), mirroring the Dy center with respect to the phthalocyanine ring. This suggests some Dy disorder between two positions shifted along the $DyPc_2$ stack by the Pc-Pc distance, as was observed in the neodymium case. Attempts to refine this model, however, converged to occupancy factors of less than 1% for the additional Dy site with no significant improvement of the R-factors, and where thus abandoned.

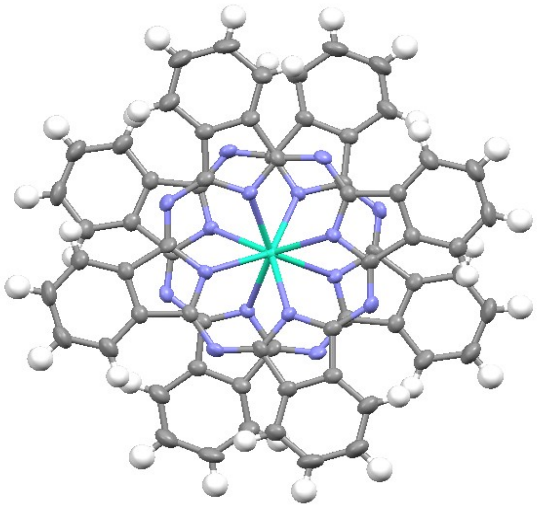


Figure S32. Thermal ellipsoid plot for the $DyPc_2$ α-phase. Ellipsoids shown at 50% probablilty (Dy: blue-green, C: grey, N: blue, H: white).

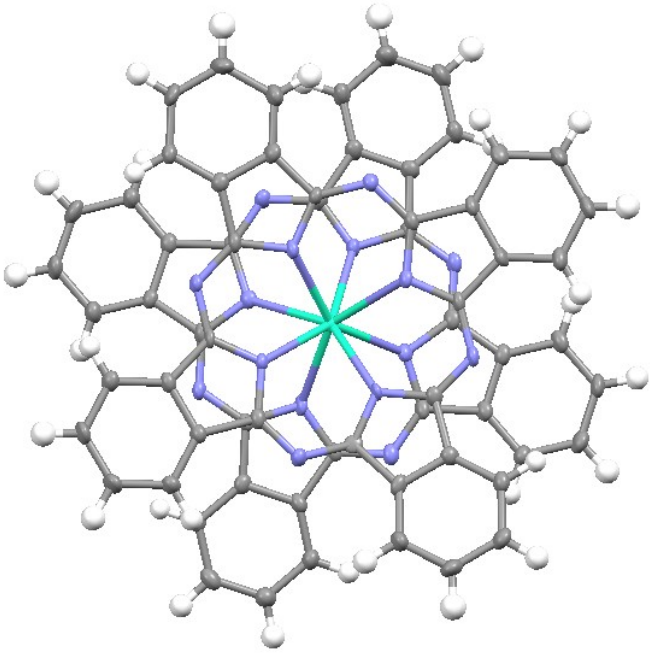


Figure S33. Thermal ellipsoid plot for the $DyPc_2$ γ-phase. Ellipsoids shown at 50% probablilty (Dy: blue-green, C: grey, N: blue, H: white).

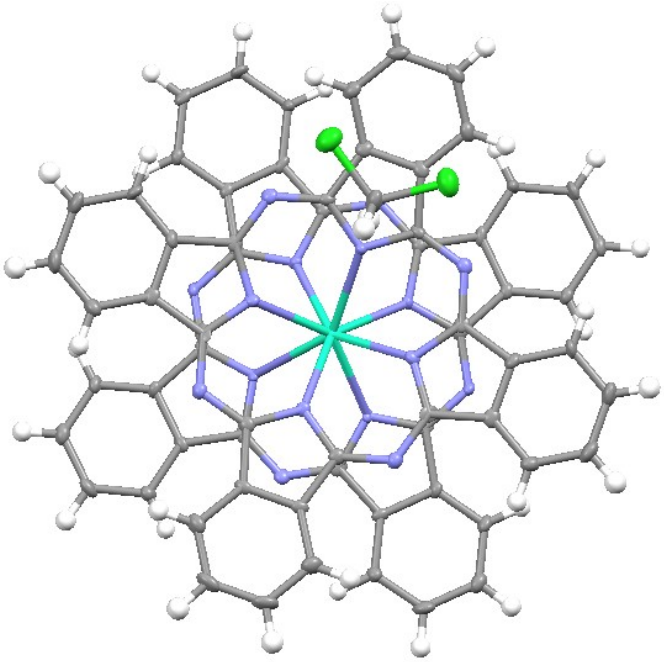


Figure S34. Thermal ellipsoid plot for the $DyPc_2 \cdot CH_2Cl_2$ phase. Ellipsoids shown at 50% probablilty (Dy: blue-green, C: grey, N: blue, Cl: bright green, H: white).

Table S9. Crystallographic Parameters for $ErPc_2$

	CH_2Cl_2·Phase
Chemical Formula	$C_{64}H_{32}N_{16}Er{\cdot}CH_2Cl_2$
Crystal System	Orthorhombic
Z	4
Space Group	*Pnma*
a (Å)	28.016(3)
b (Å)	22.942(3)
c (Å)	7.8678(7)
α (°)	90.0
β (°)	90.0
γ (°)	90.0
V ($Å^3$)	5056.97
Density (g/cm^3)	1.678
R-factor (%)	4.6
CCDC Number	2096856

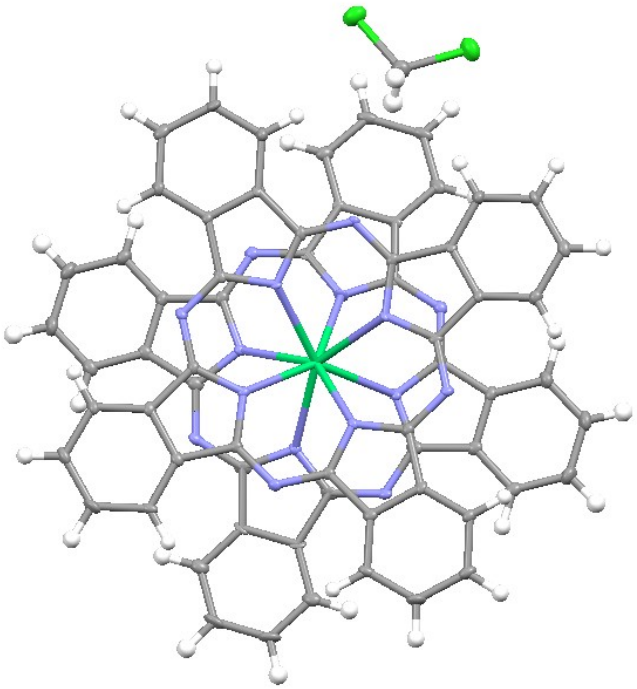


Figure S35. Thermal ellipsoid plot for the $ErPc_2{\cdot}CH_2Cl_2$ phase. Ellipsoids shown at 50% probablilty (Er: mint green, C: grey, N: blue, Cl: bright green, H: white).

Table S10. Crystallographic Parameters for $YbPc_2$ Polymorphs

	γ-Phase	CH_2Cl_2 Solvate Phase
Chemical Formula	$C_{64}H_{32}N_{16}Yb$	$C_{64}H_{32}N_{16}Yb{\cdot}CH_2Cl_2$
Crystal System	Orthorhombic	Orthorhombic
Z	4	4
Space Group	$P2_12_12_1$	*Pnma*
a (Å)	8.7901(6)	27.955(6)
b (Å)	10.5965(12)	22.921(5)
c (Å)	50.568(4)	7.8802(12)
α (°)	90.0	90.0
β (°)	90.0	90.0
γ (°)	90.0	90.0
V ($Å^3$)	4710.12	5049.29
Density (g/cm^3)	1.690	1.688
R-factor (%)	4.1	4.97
CCDC Number	2096867	2096865

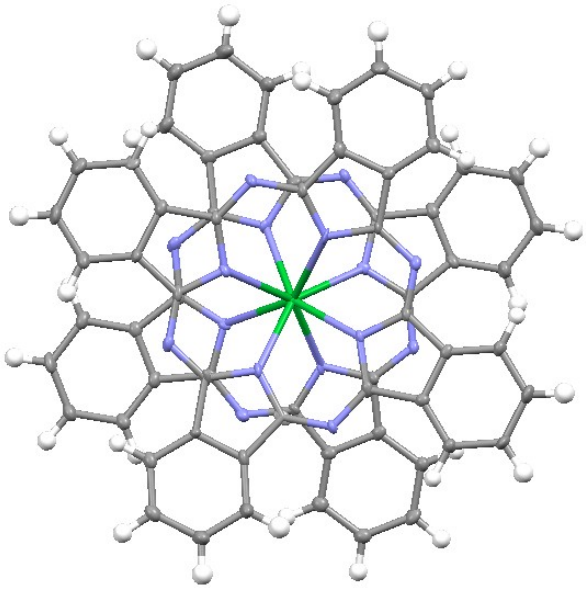


Figure S36. Thermal ellipsoid plot for the $YbPc_2$ γ-phase. Ellipsoids shown at 50% probablilty (Yb: green, C: grey, N: blue, H: white)

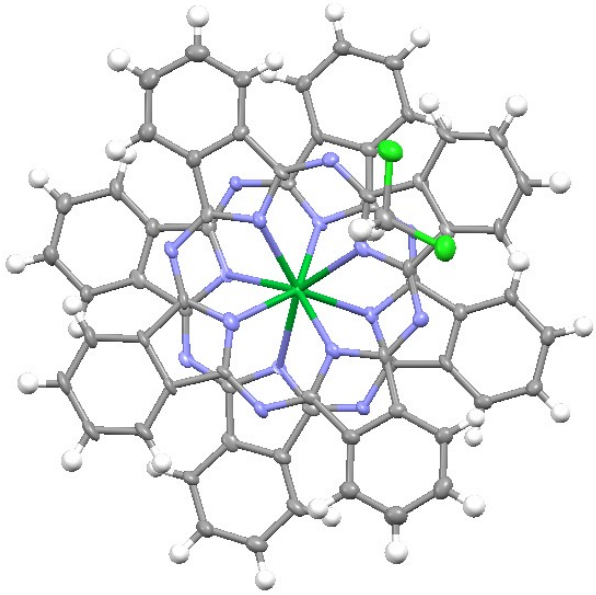


Figure S37. Thermal ellipsoid plot for the $YbPc_2{\cdot}CH_2Cl_2$ phase. Ellipsoids shown at 50% probablilty (La: green, C: grey, N: blue, Cl: bright green, H: white).

Table S11. Bond Lengths for α-$LnPc_2$

$LaPc_2$		$NdPc_2$		$DyPc_2$	
Atom 1 – Atom 2	Bond Length (Å)	Atom 1 – Atom 2	Bond Length (Å)	Atom 1 – Atom 2	Bond Length (Å)
La(1) - N(2)	2.421	Nd(1) – N(2)	2.467	Dy(1) - N(2)	2.408
C(1) - C(2)	1.471(1)	Nd(2) – N(2)	2.615	C(1) - C(2)	1.48(1)
C(1) - N(1)	1.32(1)	C(1) - C(4)	1.46(1)	C(1) - N(1)	1.31(1)
C(1) - N(2)	1.37(1)	C(1) - N(1)	1.33(1)	C(1) - N(2)	1.371(9)
C(2) - C(3)	1.371(1)	C(1) - N(2)	1.38(1)	C(2) - C(3)	1.38(1)
C(2) - C(7)	1.40(1)	C(2) - C(3)	1.45(1)	C(2) - C(7)	1.39(1)
C(3) - C(4)	1.38(2)	C(2) - N(1)	1.34(1)	C(3) - C(4)	1.38(1)
C(3) - H(3)	0.95	C(2) - N(2)	1.37(1)	C(3) - H(3)	0.931
C(4) - C(5)	1.40(2)	C(3) - C(4)	1.40(1)	C(4) - C(5)	1.40(1)
C(4) - H(4)	0.95	C(3) - C(8)	1.41(1)	C(4) - H(4)	0.93
C(5) - C(6)	1.40(1)	C(4) - C(5)	1.38(1)	C(5) - C(6)	1.38(1)
C(5) - H(5)	0.95	C(5) - C(6)	1.40(1)	C(5) - H(5)	0.93
C(6) - C(7)	1.38(1)	C(5) – H(5)	0.93	C(6) - C(7)	1.40(1)
C(6) - H(6)	0.95	C(6) - H(6)	0.93	C(6) - H(6)	0.93
C(7) - C(8)	1.46(1)	C(6) - C(7)	1.38(2)	C(7) - C(8)	1.46(1)
C(8) - N(1)	1.34(1)	C(7) - C(8)	1.40(1)	C(8) - N(1)	1.349(9)
C(8) - N(2)	1.37(1)	C(7) - H(7)	0.93	C(8) - N(2)	1.36(1)
		C(8) - H(8)	0.93		

Table S12. Bond Lengths for γ-$LnPc_2$

$NdPc_2$		$SmPc_2$		$GdPc_2$		$TbPc_2$		$DyPc_2$		$YbPc_2$	
Atom 1 – Atom 2	Bond Length (Å)	Atom 1 – Atom 2	Bond Length (Å)	Atom 1 – Atom 2	Bond Length (Å)	Atom 1 – Atom 2	Bond Length (Å)	Atom 1 – Atom 2	Bond Length (Å)	Atom 1 – Atom 2	Bond Length (Å)
Nd(1) - N(2)	2.459(3)	Sm(1) - N(1)	2.451(3)	Gd(1) - N(1)	2.439(7)	Tb(1) - N(1)	2.406(5)	Dy(1) - N(1)	2.420(5)	Yb(1) - N(1)	2.361(5)
Nd(1) - N(4)	2.458(4)	Sm(1) - N(3)	2.438(3)	Gd(1) - N(3)	2.424(7)	Tb(1) - N(3)	2.409(5)	Dy(1) - N(3)	2.412(4)	Yb(1) - N(3)	2.382(5)
Nd(1) - N(6)	2.474(4)	Sm(1) - N(5)	2.444(3)	Gd(1) - N(5)	2.414(7)	Tb(1) - N(5)	2.397(5)	Dy(1) - N(5)	2.403(4)	Yb(1) - N(5)	2.392(5)
Nd(1) - N(8)	2.470(3)	Sm(1) - N(7)	2.428(4)	Gd(1) - N(7)	2.440(7)	Tb(1) - N(7)	2.415(5)	Dy(1) - N(7)	2.395(4)	Yb(1) - N(7)	2.362(5)
Nd(1) - N(10)	2.476(3)	Sm(1) - N(9)	2.439(3)	Gd(1) - N(9)	2.433(8)	Tb(1) - N(9)	2.401(5)	Dy(1) - N(9)	2.402(5)	Yb(1) - N(9)	2.386(5)
Nd(1) - N(12)	2.462(3)	Sm(1) - N(11)	2.431(3)	Gd(1) - N(11)	2.420(8)	Tb(1) - N(11)	2.426(5)	Dy(1) - N(11)	2.398(4)	Yb(1) - N(11)	2.368(5)
Nd(1) - N(14)	2.470(4)	Sm(1) - N(13)	2.454(3)	Gd(1) - N(13)	2.444(7)	Tb(1) - N(13)	2.418(4)	Dy(1) - N(13)	2.397(4)	Yb(1) - N(13)	2.376(5)
Nd(1) - N(16)	2.458(4)	Sm(1) - N(15)	2.448(3)	Gd(1) - N(15)	2.417(7)	Tb(1) - N(15)	2.403(4)	Dy(1) - N(15)	2.411(4)	Yb(1) - N(15)	2.375(5)
C(1) - C(2)	1.466(6)	C(1) - C(2)	1.470(6)	C(1) - C(2)	1.47(1)	C(1) - C(2)	1.475(8)	C(1) - C(2)	1.485(8)	C(1) - C(2)	1.455(8)
C(1) - N(1)	1.341(5)	C(1) - N(1)	1.369(5)	C(1) - N(1)	1.37(1)	C(1) - N(1)	1.370(8)	C(1) - N(1)	1.376(7)	C(1) - N(1)	1.364(7)
C(1) - N(2)	1.368(5)	C(1) - N(8)	1.338(5)	C(1) - N(8)	1.33(1)	C(1) - N(8)	1.335(8)	C(1) - N(8)	1.328(7)	C(1) - N(8)	1.347(8)
C(2) - C(3)	1.384(6)	C(2) - C(3)	1.389(6)	C(2) - C(3)	1.38(1)	C(2) - C(3)	1.365(8)	C(2) - C(3)	1.385(8)	C(2) - C(3)	1.386(8)
C(2) - C(7)	1.407(6)	C(2) - C(7)	1.394(6)	C(2) - C(7)	1.41(1)	C(2) - C(7)	1.397(8)	C(2) - C(7)	1.388(8)	C(2) - C(7)	1.404(9)
C(3) - C(4)	1.395(6)	C(3) - C(4)	1.396(6)	C(3) - C(4)	1.38(1)	C(3) - C(4)	1.396(9)	C(3) - C(4)	1.404(8)	C(3) - C(4)	1.40(1)
C(3) - H(3)	0.93	C(3) - H(3)	0.95	C(3) - H(3)	0.95	C(3) - H(3)	0.95	C(3) - H(3)	0.95	C(3) - H(3)	0.95
C(4) - C(5)	1.392(7)	C(4) - C(5)	1.379(6)	C(4) - C(5)	1.40(1)	C(4) - C(5)	1.380(1)	C(4) - C(5)	1.365(9)	C(4) - C(5)	1.40(1)
C(4) - H(4)	0.93	C(4) - H(4)	0.95	C(4) - H(4)	0.95	C(4) - H(4)	0.95	C(4) - H(4)	0.95	C(4) - H(4)	0.95
C(5) - C(6)	1.395(7)	C(5) - C(6)	1.399(6)	C(5) - C(6)	1.39(1)	C(5) - C(6)	1.388(9)	C(5) - C(6)	1.395(9)	C(5) - C(6)	1.398(9)
C(5) - H(5)	0.93	C(5) - H(5)	0.95	C(5) - H(5)	0.95	C(5) - H(5)	0.95	C(5) - H(5)	0.95	C(5) - H(5)	0.95

C(6) - C(7)	1.379(5)	C(6) - C(7)	1.390(6)	C(6) - C(7)	1.39(1)	C(6) - C(7)	1.390(8)	C(6) - C(7)	1.389(9)	C(6) - C(7)	1.389(9)
C(6) - H(6)	0.93	C(6) - H(6)	0.95	C(6) - H(6)	0.95	C(6) - H(6)	0.95	C(6) - H(6)	0.95	C(6) - H(6)	0.95
C(7) - C(8)	1.460(6)	C(7) - C(8)	1.474(5)	C(7) - C(8)	1.47(1)	C(7) - C(8)	1.467(8)	C(7) - C(8)	1.464(8)	C(7) - C(8)	1.470(8)
C(8) - N(2)	1.370(5)	C(8) - N(1)	1.371(5)	C(8) - N(1)	1.38(1)	C(8) - N(1)	1.366(8)	C(8) - N(1)	1.363(7)	C(8) - N(1)	1.378(8)
C(8) - N(3)	1.339(5)	C(8) - N(2)	1.332(5)	C(8) - N(2)	1.31(1)	C(8) - N(2)	1.336(8)	C(8) - N(2)	1.333(7)	C(8) - N(2)	1.328(8)
C(9) - C(10)	1.464(6)	C(9) - C(10)	1.470(6)	C(9) - C(10)	1.47(1)	C(9) - C(10)	1.453(8)	C(9) - C(10)	1.479(8)	C(9) - C(10)	1.477(9)
C(9) - N(3)	1.336(5)	C(9) - N(2)	1.333(5)	C(9) - N(2)	1.35(1)	C(9) - N(2)	1.333(8)	C(9) - N(2)	1.319(8)	C(9) - N(2)	1.317(8)
C(9) - N(4)	1.374(5)	C(9) - N(3)	1.373(5)	C(9) - N(3)	1.37(1)	C(9) - N(3)	1.376(7)	C(9) - N(3)	1.372(7)	C(9) - N(3)	1.383(8)
C(10) - C(11)	1.391(6)	C(10) - C(11)	1.374(6)	C(10) - C(11)	1.39(1)	C(10) - C(11)	1.394(8)	C(10) - C(11)	1.372(8)	C(10) - C(11)	1.37(1)
C(10) - C(15)	1.402(6)	C(10) - C(15)	1.402(6)	C(10) - C(15)	1.41(1)	C(10) - C(15)	1.394(9)	C(10) - C(15)	1.399(8)	C(10) - C(15)	1.411(8)
C(11) - C(12)	1.388(6)	C(11) - C(12)	1.404(6)	C(11) - C(12)	1.39(1)	C(11) - C(12)	1.380(1)	C(11) - C(12)	1.380(9)	C(11) - C(12)	1.39(1)
C(11) - H(11)	0.93	C(11) - H(11)	0.95	C(11) - H(11)	0.95	C(11) - H(11)	0.95	C(11) - H(11)	0.95	C(11) - H(11)	0.95
C(12) - C(13)	1.400(6)	C(12) - C(13)	1.389(6)	C(12) - C(13)	1.40(2)	C(12) - C(13)	1.392(9)	C(12) - C(13)	1.386(9)	C(12) - C(13)	1.40(1)
C(12) - H(12)	0.93	C(12) - H(12)	0.95	C(12) - H(12)	0.95	C(12) - H(12)	0.95	C(12) - H(12)	0.95	C(12) - H(12)	0.95
C(13) - C(14)	1.393(7)	C(13) - C(14)	1.384(6)	C(13) - C(14)	1.39(1)	C(13) - C(14)	1.395(9)	C(13) - C(14)	1.40(1)	C(13) - C(14)	1.39(1)
C(13) - H(13)	0.93	C(13) - H(13)	0.95	C(13) - H(13)	0.95	C(13) - H(13)	0.95	C(13) - H(13)	0.95	C(13) - H(13)	0.95
C(14) - C(15)	1.376(7)	C(14) - C(15)	1.384(6)	C(14) - C(15)	1.38(1)	C(14) - C(15)	1.380(9)	C(14) - C(15)	1.370(9)	C(14) - C(15)	1.380(9)
C(14) - H(14)	0.93	C(14) - H(14)	0.95	C(14) - H(14)	0.95	C(14) - H(14)	0.95	C(14) - H(14)	0.95	C(14) - H(14)	0.95
C(15) - C(16)	1.462(6)	C(15) - C(16)	1.468(6)	C(15) - C(16)	1.46(1)	C(15) - C(16)	1.481(8)	C(15) - C(16)	1.470(8)	C(15) - C(16)	1.473(8)
C(16) - N(4)	1.367(5)	C(16) - N(3)	1.367(5)	C(16) - N(3)	1.36(1)	C(16) - N(3)	1.376(8)	C(16) - N(3)	1.377(7)	C(16) - N(3)	1.386(7)
C(16) - N(5)	1.344(5)	C(16) - N(4)	1.338(5)	C(16) - N(4)	1.33(1)	C(16) - N(4)	1.327(8)	C(16) - N(4)	1.330(7)	C(16) - N(4)	1.309(8)
C(17) -	1.481(6)	C(17) -	1.467(5)	C(17) -	1.47(1)	C(17) -	1.462(8)	C(17) -	1.472(7)	C(17) -	1.460(9)

C(18)		C(18)		C(18)		C(18)		C(18)		C(18)	
C(17) - N(5)	1.331(5)	C(17) - N(4)	1.332(5)	C(17) - N(4)	1.34(1)	C(17) - N(4)	1.336(8)	C(17) - N(4)	1.337(7)	C(17) - N(4)	1.329(8)
C(17) - N(6)	1.371(5)	C(17) - N(5)	1.372(5)	C(17) - N(5)	1.37(1)	C(17) - N(5)	1.377(7)	C(17) - N(5)	1.368(7)	C(17) - N(5)	1.367(8)
C(18) - C(19)	1.379(6)	C(18) - C(19)	1.390(5)	C(18) - C(19)	1.38(1)	C(18) - C(19)	1.368(8)	C(18) - C(19)	1.380(8)	C(18) - C(19)	1.390(9)
C(18) - C(23)	1.405(6)	C(18) - C(23)	1.400(5)	C(18) - C(23)	1.41(1)	C(18) - C(23)	1.409(8)	C(18) - C(23)	1.408(8)	C(18) - C(23)	1.395(9)
C(19) - C(20)	1.395(6)	C(19) - C(20)	1.389(6)	C(19) - C(20)	1.40(1)	C(19) - C(20)	1.395(9)	C(19) - C(20)	1.383(8)	C(19) - C(20)	1.39(1)
C(19) - H(19)	0.93	C(19) - H(19)	0.95	C(19) - H(19)	0.95	C(19) - H(19)	0.95	C(19) - H(19)	0.95	C(19) - H(19)	0.95
C(20) - C(21)	1.388(6)	C(20) - C(21)	1.389(6)	C(20) - C(21)	1.38(1)	C(20) - C(21)	1.385(9)	C(20) - C(21)	1.387(9)	C(20) - C(21)	1.39(1)
C(20) - H(20)	0.93	C(20) - H(20)	0.95	C(20) - H(20)	0.95	C(20) - H(20)	0.95	C(20) - H(20)	0.95	C(20) - H(20)	0.95
C(21) - C(22)	1.388(6)	C(21) - C(22)	1.395(6)	C(21) - C(22)	1.41(1)	C(21) - C(22)	1.392(9)	C(21) - C(22)	1.401(8)	C(21) - C(22)	1.397(9)
C(21) - H(21)	0.93	C(21) - H(21)	0.95	C(21) - H(21)	0.95	C(21) - H(21)	0.95	C(21) - H(21)	0.95	C(21) - H(21)	0.95
C(22) - C(23)	1.382(6)	C(22) - C(23)	1.384(6)	C(22) - C(23)	1.37(1)	C(22) - C(23)	1.384(8)	C(22) - C(23)	1.378(7)	C(22) - C(23)	1.397(9)
C(22) - H(22)	0.93	C(22) - H(22)	0.95	C(22) - H(22)	0.95	C(22) - H(22)	0.95	C(22) - H(22)	0.95	C(22) - H(22)	0.95
C(23) - C(24)	1.468(6)	C(23) - C(24)	1.476(6)	C(23) - C(24)	1.46(1)	C(23) - C(24)	1.465(8)	C(23) - C(24)	1.454(7)	C(23) - C(24)	1.467(8)
C(24) - N(6)	1.364(5)	C(24) - N(5)	1.372(5)	C(24) - N(5)	1.38(1)	C(24) - N(5)	1.373(8)	C(24) - N(5)	1.370(7)	C(24) - N(5)	1.381(8)
C(24) - N(7)	1.331(6)	C(24) - N(6)	1.329(5)	C(24) - N(6)	1.33(1)	C(24) - N(6)	1.327(8)	C(24) - N(6)	1.335(7)	C(24) - N(6)	1.328(8)
C(25) - C(26)	1.466(6)	C(25) - C(26)	1.462(5)	C(25) - C(26)	1.48(1)	C(25) - C(26)	1.463(9)	C(25) - C(26)	1.462(8)	C(25) - C(26)	1.447(9)
C(25) - N(7)	1.331(6)	C(25) - N(6)	1.339(5)	C(25) - N(6)	1.33(1)	C(25) - N(6)	1.343(8)	C(25) - N(6)	1.335(7)	C(25) - N(6)	1.338(8)
C(25) - N(8)	1.365(5)	C(25) - N(7)	1.373(5)	C(25) - N(7)	1.37(1)	C(25) - N(7)	1.363(8)	C(25) - N(7)	1.382(7)	C(25) - N(7)	1.370(8)
C(26) - C(27)	1.381(6)	C(26) - C(27)	1.380(6)	C(26) - C(27)	1.39(1)	C(26) - C(27)	1.388(9)	C(26) - C(27)	1.376(8)	C(26) - C(27)	1.39(1)
C(26) - C(31)	1.395(6)	C(26) - C(31)	1.406(5)	C(26) - C(31)	1.40(1)	C(26) - C(31)	1.396(9)	C(26) - C(31)	1.414(8)	C(26) - C(31)	1.399(8)
C(27) - H(27)	0.93	C(27) - C(28)	1.390(6)	C(27) - C(28)	1.39(1)	C(27) - C(28)	1.393(9)	C(27) - C(28)	1.395(8)	C(27) - C(28)	1.40(1)

C(27) - C(28)	1.392(6)	C(27) - H(27)	0.95	C(27) - H(27)	0.95	C(27) - H(27)	0.95	C(27) - H(27)	0.95	C(27) - H(27)	0.95
C(28) - C(29)	1.402(7)	C(28) - C(29)	1.391(6)	C(28) - C(29)	1.40(1)	C(28) - C(29)	1.380(1)	C(28) - C(29)	1.376(8)	C(28) - C(29)	1.384(9)
C(28) - H(28)	0.93	C(28) - H(28)	0.951	C(28) - H(28)	0.95	C(28) - H(28)	0.95	C(28) - H(28)	0.95	C(28) - H(28)	0.95
C(29) - H(30)	1.384(7)	C(29) – C(30)	1.389(6)	C(29) - C(30)	1.38(1)	C(29) - C(30)	1.406(9)	C(29) - C(30)	1.414(9)	C(29) - C(30)	1.40(1)
C(29) - H(29)	0.929	C(29) - H(29)	0.95	C(29) - H(29)	0.95	C(29) - H(29)	0.95	C(29) - H(29)	0.95	C(29) - H(29)	0.95
C(30) - C(31)	1.386(6)	C(30) - C(31)	1.385(5)	C(30) - C(31)	1.39(1)	C(30) - C(31)	1.381(8)	C(30) - C(31)	1.372(9)	C(30) - C(31)	1.379(9)
C(30) - H(30)	0.93	C(30) - H(30)	0.95	C(30) - H(30)	0.95	C(30) - H(30)	0.95	C(30) - H(30)	0.95	C(30) - H(30)	0.95
C(31) - C(32)	1.476(6)	C(31) - C(32)	1.472(5)	C(31) - C(32)	1.47(1)	C(31) - C(32)	1.475(8)	C(31) - C(32)	1.446(7)	C(31) - C(32)	1.470(9)
C(32) - N(1)	1.330(5)	C(32) - N(7)	1.372(5)	C(32) - N(7)	1.35(1)	C(32) - N(7)	1.376(8)	C(32) - N(7)	1.377(7)	C(32) - N(7)	1.394(7)
C(32) - N(8)	1.370(5)	C(32) - N(8)	1.332(5)	C(32) - N(8)	1.34(1)	C(32) - N(8)	1.329(8)	C(32) - N(8)	1.340(7)	C(32) - N(8)	1.325(7)
C(33) - C(34)	1.472(6)	C(33) - C(34)	1.469(5)	C(33) - C(34)	1.47(1)	C(33) - C(34)	1.466(9)	C(33) - C(34)	1.475(8)	C(33) - C(34)	1.481(8)
C(33) - N(9)	1.335(5)	C(33) - N(9)	1.369(5)	C(33) - N(9)	1.37(1)	C(33) - N(9)	1.379(7)	C(33) - N(9)	1.371(7)	C(33) - N(9)	1.379(8)
C(33) - N(10)	1.366(5)	C(33) - N(16)	1.340(5)	C(33) - N(16)	1.33(1)	C(33) - N(16)	1.334(8)	C(33) - N(16)	1.343(7)	C(33) - N(16)	1.322(8)
C(34) - C(35)	1.384(6)	C(34) - C(35)	1.380(6)	C(34) - C(35)	1.39(1)	C(34) - C(35)	1.384(9)	C(34) - C(35)	1.346(8)	C(34) - C(35)	1.389(9)
C(34) - C(39)	1.397(6)	C(34) - C(39)	1.402(6)	C(34) - C(39)	1.41(1)	C(34) - C(39)	1.406(8)	C(34) - C(39)	1.404(8)	C(34) - C(39)	1.392(9)
C(35) - C(36)	1.393(6)	C(35) - C(36)	1.389(6)	C(35) - C(36)	1.39(1)	C(35) - C(36)	1.389(9)	C(35) - C(36)	1.417(9)	C(35) - C(36)	1.406(9)
C(35) - H(35)	0.93	C(35) - H(35)	0.95	C(35) - H(35)	0.95	C(35) - H(35)	0.95	C(35) - H(35)	0.95	C(35) - H(35)	0.95
C(36) - C(37)	1.391(7)	C(36) - C(37)	1.393(6)	C(36) - C(37)	1.40(1)	C(36) - C(37)	1.388(9)	C(36) - C(37)	1.379(9)	C(36) - C(37)	1.40(1)
C(36) - H(36)	0.93	C(36) - H(36)	0.95	C(36) - H(36)	0.95	C(36) - H(36)	0.95	C(36) - H(36)	0.95	C(36) - H(36)	0.95
C(37) - C(38)	1.400(7)	C(37) - C(38)	1.399(6)	C(37) - C(38)	1.40(1)	C(37) - C(38)	1.402(9)	C(37) - C(38)	1.386(9)	C(37) - C(38)	1.42(1)
C(37) - H(37)	0.93	C(37) - H(37)	0.95	C(37) - H(37)	0.95	C(37) - H(37)	0.95	C(37) - H(37)	0.95	C(37) - H(37)	0.95
C(38) -	1.388(6)	C(38) -	1.378(5)	C(38) -	1.40(1)	C(38) -	1.376(9)	C(38) -	1.389(8)	C(38) -	1.376(9)

C(39)		C(39)		C(39)		C(39)		C(39)		C(39)	
C(38) - H(38)	0.93	C(38) - H(38)	0.95	C(38) - H(38)	0.95	C(38) - H(38)	0.95	C(38) - H(38)	0.95	C(38) - H(38)	0.95
C(39) - C(40)	1.470(5)	C(39) - C(40)	1.463(5)	C(39) - C(40)	1.47(1)	C(39) - C(40)	1.457(8)	C(39) - C(40)	1.470(8)	C(39) - C(40)	1.471(9)
C(40) - N(10)	1.371(6)	C(40) - N(9)	1.372(5)	C(40) - N(9)	1.47(1)	C(40) - N(9)	1.371(8)	C(40) - N(9)	1.375(7)	C(40) - N(9)	1.372(7)
C(40) - N(11)	1.337(6)	C(40) - N(10)	1.331(5)	C(40) - N(10)	1.34(1)	C(40) - N(10)	1.346(7)	C(40) - N(10)	1.328(7)	C(41) - C(42)	1.462(9)
C(41) - C(42)	1.468(6)	C(41) - C(42)	1.465(5)	C(41) - C(42)	1.46(1)	C(41) - C(42)	1.483(8)	C(41) - C(42)	1.463(8)	C(41) - N(10)	1.326(8)
C(41) - N(11)	1.343(5)	C(41) - N(10)	1.336(5)	C(41) - N(10)	1.33(1)	C(41) - N(10)	1.318(8)	C(41) - N(10)	1.329(7)	C(41) - N(11)	1.382(8)
C(41) - N(12)	1.365(5)	C(41) - N(11)	1.385(5)	C(41) - N(11)	1.37(1)	C(41) - N(11)	1.374(8)	C(41) - N(11)	1.383(7)	C(42) - C(43)	1.390(9)
C(42) - C(43)	1.382(6)	C(42) - C(43)	1.381(6)	C(42) - C(43)	1.39(1)	C(42) - C(43)	1.389(8)	C(42) - C(43)	1.395(8)	C(42) - C(47)	1.397(9)
C(42) - C(47)	1.397(6)	C(42) - C(47)	1.409(5)	C(42) - C(47)	1.41(1)	C(42) - C(47)	1.392(8)	C(42) - C(47)	1.399(8)	C(43) - C(44)	1.39(1)
C(43) - C(44)	1.397(7)	C(43) - C(44)	1.382(6)	C(43) - C(44)	1.39(1)	C(43) - C(44)	1.393(9)	C(43) - C(44)	1.381(9)	C(43) - H(43)	0.95
C(43) - H(43)	0.93	C(43) - H(43)	0.95	C(43) - H(43)	0.95	C(43) - H(43)	0.95	C(43) - H(43)	0.95	C(44) - C(45)	1.400(9)
C(44) - C(45)	1.395(7)	C(44) - C(45)	1.386(6)	C(44) - C(45)	1.39(1)	C(45) - C(45)	1.390(1)	C(44) - C(45)	1.389(9)	C(44) - H(44)	0.95
C(44) - H(44)	0.929	C(44) - H(44)	0.95	C(44) - H(44)	0.95	C(44) - H(44)	0.95	C(44) - H(44)	0.95	C(45) - C(46)	1.381(9)
C(45) - C(46)	1.380(6)	C(45) - C(46)	1.402(6)	C(45) - C(46)	1.40(1)	C(45) - C(46)	1.390(9)	C(45) - C(46)	1.401(8)	C(45) - H(45)	0.95
C(45) - H(45)	0.93	C(45) - H(45)	0.95	C(45) - H(45)	0.95	C(45) - H(45)	0.95	C(45) - H(45)	0.95	C(46) - C(47)	1.388(9)
C(46) - C(47)	1.394(6)	C(46) - C(47)	1.375(6)	C(46) - C(47)	1.39(1)	C(46) - C(47)	1.391(9)	C(46) - C(47)	1.382(8)	C(46) - H(46)	0.95
C(46) - H(46)	0.93	C(46) - H(46)	0.95	C(46) - H(46)	0.95	C(46) - H(46)	0.95	C(46) - H(46)	0.95	C(47) - C(48)	1.461(9)
C(47) - C(48)	1.464(6)	C(47) - C(48)	1.455(6)	C(47) - C(48)	1.48(1)	C(47) - C(48)	1.463(8)	C(47) - C(48)	1.477(8)	C(48) - N(11)	1.368(8)
C(48) - N(12)	1.364(5)	C(48) - N(11)	1.368(5)	C(48) - N(11)	1.38(1)	C(48) - N(11)	1.360(7)	C(48) - N(11)	1.372(8)	C(48) - N(12)	1.342(8)
C(48) - N(13)	1.335(5)	C(48) - N(12)	1.347(5)	C(48) - N(12)	1.33(1)	C(48) - N(12)	1.328(8)	C(48) - N(12)	1.324(7)	C(49) - C(50)	1.457(8)
C(49) - C(50)	1.459(6)	C(49) - C(50)	1.485(5)	C(49) - C(50)	1.47(1)	C(49) - C(50)	1.479(8)	C(49) - C(50)	1.468(7)	C(49) - N(12)	1.340(8)

C(49) - N(13)	1.343(6)	C(49) - N(12)	1.326(5)	C(49) - N(12)	1.35(1)	C(49) - N(12)	1.321(8)	C(49) - N(12)	1.339(7)	C(49) - N(13)	1.386(9)
C(49) - N(14)	1.372(5)	C(49) - N(13)	1.372(5)	C(49) - N(13)	1.36(1)	C(49) - N(13)	1.375(7)	C(49) - N(13)	1.376(7)	C(50) - C(51)	1.38(1)
C(50) - C(51)	1.392(6)	C(50) - C(51)	1.385(5)	C(50) - C(51)	1.38(1)	C(50) - C(51)	1.381(8)	C(50) - C(51)	1.370(8)	C(50) - C(55)	1.400(9)
C(50) - C(55)	1.395(6)	C(50) - C(55)	1.392(6)	C(50) - C(55)	1.41(1)	C(50) - C(55)	1.392(8)	C(50) - C(55)	1.404(8)	C(51) - C(52)	1.399(9)
C(51) - C(52)	1.391(6)	C(51) - C(52)	1.400(6)	C(51) - C(52)	1.40(1)	C(51) - C(52)	1.383(9)	C(51) - C(52)	1.391(8)	C(51) - H(51)	0.949
C(51) - H(51)	0.93	C(51) - H(51)	0.95	C(51) - H(51)	0.95	C(51) - H(51)	0.95	C(51) - H(51)	0.95	C(52) - C(53)	1.39(1)
C(52) - C(53)	1.390(6)	C(52) - C(53)	1.383(6)	C(52) - C(53)	1.40(1)	C(52) - C(53)	1.380(1)	C(52) - C(53)	1.381(9)	C(52) - H(52)	0.95
C(52) - H(52)	0.93	C(52) - H(52)	0.95	C(52) - H(52)	0.95	C(52) - H(52)	0.95	C(52) - H(52)	0.95	C(53) - C(54)	1.39(1)
C(53) - C(54)	1.408(6)	C(53) - C(54)	1.386(6)	C(53) - C(54)	1.39(1)	C(53) - C(54)	1.400(1)	C(53) - C(54)	1.390(8)	C(53) - H(53)	0.95
C(53) - H(53)	0.931	C(53) - H(53)	0.95	C(53) - H(53)	0.95	C(53) - H(53)	0.95	C(53) - H(53)	0.95	C(54) - C(55)	1.390(8)
C(54) - C(55)	1.391(6)	C(54) - C(55)	1.392(6)	C(54) - C(55)	1.38(1)	C(54) - C(55)	1.380(1)	C(54) - C(55)	1.388(8)	C(54) - H(54)	0.95
C(54) - H(54)	0.929	C(54) - H(54)	0.95	C(54) - H(54)	0.95	C(54) - H(54)	0.95	C(54) - H(54)	0.95	C(55) - C(56)	1.465(8)
C(55) - C(56)	1.477(6)	C(55) - C(56)	1.467(5)	C(55) - C(56)	1.47(1)	C(55) - C(56)	1.471(8)	C(55) - C(56)	1.470(7)	C(56) - N(13)	1.384(8)
C(56) - N(14)	1.368(5)	C(56) - N(13)	1.364(5)	C(56) - N(13)	1.37(1)	C(56) - N(13)	1.371(7)	C(56) - N(13)	1.369(7)	C(56) - N(14)	1.324(9)
C(56) - N(15)	1.333(6)	C(56) - N(14)	1.333(5)	C(56) - N(14)	1.34(1)	C(56) - N(14)	1.334(8)	C(56) - N(14)	1.336(7)	C(57) - C(58)	1.464(9)
C(57) - C(58)	1.460(6)	C(57) - C(58)	1.467(6)	C(57) - C(58)	1.46(1)	C(57) - C(58)	1.472(8)	C(57) - C(58)	1.475(8)	C(57) - N(14)	1.327(8)
C(57) - N(15)	1.340(6)	C(57) - N(14)	1.329(5)	C(57) - N(14)	1.33(1)	C(57) - N(14)	1.334(7)	C(57) - N(14)	1.336(8)	C(57) - N(15)	1.377(8)
C(57) - N(16)	1.373(5)	C(57) - N(15)	1.368(4)	C(57) - N(15)	1.37(1)	C(57) - N(15)	1.378(7)	C(57) - N(15)	1.365(7)	C(58) - C(59)	1.382(9)
C(58) - C(59)	1.389(7)	C(58) - C(59)	1.383(6)	C(58) - C(59)	1.38(1)	C(58) - C(59)	1.377(9)	C(58) - C(59)	1.379(8)	C(58) - C(63)	1.415(9)
C(58) - C(63)	1.402(6)	C(58) - C(63)	1.396(6)	C(58) - C(63)	1.41(1)	C(58) - C(63)	1.405(8)	C(58) - C(63)	1.393(8)	C(59) - C(60)	1.39(1)
C(59) - C(60)	1.391(6)	C(59) - C(60)	1.388(6)	C(59) - C(60)	1.40(2)	C(59) - C(60)	1.392(9)	C(59) - C(60)	1.401(9)	C(59) - H(59)	0.95
C(59) -	0.93	C(59) -	0.95	C(59) -	0.95	C(59) -	0.95	C(59) -	0.95	C(60) -	1.38(1)

H(59)		H(59)		H(59)		H(59)		H(59)		C(61)	
C(60) - C(61)	1.391(6)	C(60) - C(61)	1.393(6)	C(60) - C(61)	1.39(1)	C(60) - C(61)	1.390(1)	C(60) - C(61)	1.383(9)	C(60) - H(60)	0.95
C(60) - H(60)	0.93	C(60) - H(60)	0.95	C(60) - H(60)	0.95	C(60) - H(60)	0.95	C(60) - H(60)	0.95	C(61) - C(62)	1.42(1)
C(61) - C(62)	1.385(6)	C(61) - C(62)	1.385(6)	C(61) - C(62)	1.40(1)	C(61) - C(62)	1.401(9)	C(61) - C(62)	1.400(9)	C(61) - H(61)	0.95
C(61) - H(61)	0.93	C(61) - H(61)	0.95	C(61) - H(61)	0.95	C(61) - H(61)	0.95	C(61) - H(61)	0.95	C(62) - C(63)	1.37(1)
C(62) - C(63)	1.392(6)	C(62) - C(63)	1.382(7)	C(62) - C(63)	1.39(1)	C(62) - C(63)	1.389(7)	C(62) - C(63)	1.393(8)	C(62) - H(62)	0.95
C(62) - H(62)	0.93	C(62) - H(62)	0.95	C(62) - H(62)	0.95	C(62) - H(62)	0.95	C(62) - H(62)	0.95	C(62) - H(62)	0.95
C(63) - C(64)	1.475(6)	C(63) - C(64)	1.382(7)	C(63) - C(64)	1.47(1)	C(63) - C(64)	1.452(8)	C(63) - C(64)	1.475(7)	C(63) - C(64)	1.468(9)
C(64) - N(9)	1.334(5)	C(64) - N(15)	1.379(5)	C(64) - N(15)	1.37(1)	C(64) - N(15)	1.367(7)	C(64) - N(15)	1.361(7)	C(64) - N(15)	1.380(8)
C(64) - N(16)	1.366(5)	C(64) - N(16)	1.331(5)	C(64) - (N16)	1.33(1)	C(64) - N(16)	1.334(8)	C(64) - N(16)	1.325(7)	C(64) - N(16)	1.324(8)

Table S13. Bond Lengths for δ-$LnPc_2$

$PrPc_2$		$NdPc_2$		$SmPc_2$		$GdPc_2$		$TbPc_2$	
Atom 1 – Atom 2	Bond Lengths (Å)	Atom 1 – Atom 2	Bond Length (Å)	Atom 1 – Atom 2	Bond Length (Å)	Atom 1 – Atom 2	Bond Length (Å)	Atom 1 – Atom 2	Bond Length (Å)
Pr(1) - N(1)	2.476	Nd(1) - N(2)	2.473	Sm(1) - N(2)	2.457	Gd(1) - N(2)	2.431	Tb(1) - N(2)	2.426
Pr(1) - N(3)	2.481	Nd(1) - N(4)	2.471	Sm(1) - N(4)	2.444	Gd(1) - N(4)	2.436	Tb(1) - N(4)	2.424
Pr(1) - N(5)	2.487	Nd(1) - N(6)	2.468	Sm(1) - N(6)	2.445	Gd(1) - N(6)	2.422	Tb(1) - N(6)	2.417
Pr(1) - N(7)	2.473	Nd(1) - N(8)	2.466	Sm(1) - N(8)	2.451	Gd(1) - N(8)	2.431	Tb(1) - N(8)	2.425
C(1) - C(2)	1.460(3)	C(1) - C(2)	1.463(6)	C(1) - C(2)	1.465(2)	C(1) - C(2)	1.465(6)	C(1) - C(2)	1.460(6)
C(1) - N(1)	1.367(3)	C(1) - N(1)	1.343(5)	C(1) - N(1)	1.336(2)	C(1) - N(1)	1.339(5)	C(1) - N(1)	1.334(6)
C(1) - N(8)	1.335(3)	C(1) - N(2)	1.366(5)	C(1) - N(2)	1.369(2)	C(1) - N(2)	1.373(5)	C(1) - N(2)	1.361(6)
C(2) - C(3)	1.388(3)	C(2) - C(3)	1.383(6)	C(2) - C(3)	1.388(2)	C(2) - C(3)	1.382(6)	C(2) - C(3)	1.389(6)
C(2) - C(7)	1.400(3)	C(2) - C(7)	1.394(6)	C(2) - C(7)	1.401(2)	C(2) - C(7)	1.394(6)	C(2) - C(7)	1.406(6)
C(3) - C(4)	1.397(3)	C(3) - C(4)	1.388(6)	C(3) - C(4)	1.396(2)	C(3) - C(4)	1.395(6)	C(3) - C(4)	1.399(6)
C(3) - H(3)	0.95	C(3) - H(1)	0.93	C(3) - H(3)	0.95	C(3) - H(3)	0.95	C(3) - H(3)	0.95
C(4) -	1.398(3)	C(4) -	1.385(6)	C(4) -	1.403(2)	C(4) -	1.386(6)	C(4) -	1.395(7)

C(5)		C(5)		C(5)		C(5)		C(5)	
C(4) - H(4)	0.95	C(4) - H(2)	0.93	C(4) - H(4)	0.95	C(4) - H(4)	0.95	C(4) - H(4)	0.95
C(5) - C(6)	1.387(3)	C(5) - C(6)	1.382(6)	C(5) - C(6)	1.395(2)	C(5) - C(6)	1.395(6)	C(5) - C(6)	1.393(6)
C(5) - H(5)	0.95	C(5) - H(3)	0.93	C(5) - H(5)	0.95	C(5) - H(5)	0.95	C(5) - H(5)	0.949
C(6) - C(7)	1.390(3)	C(6) - C(7)	1.388(6)	C(6) - C(7)	1.392(2)	C(6) - C(7)	1.387(5)	C(6) - C(7)	1.377(6)
C(6) - H(6)	0.95	C(6) - H(4)	0.929	C(6) - H(6)	0.95	C(6) - H(6)	0.95	C(6) - H(6)	0.95
C(7) - C(8)	1.463(3)	C(7) - C(8)	1.458(6)	C(7) - C(8)	1.471(2)	C(7) - C(8)	0.95	C(7) - C(8)	1.471(6)
C(8) - N(1)	1.369(3)	C(8) - N(2)	1.375(5)	C(8) - N(2)	1.371(2)	C(8) - N(2)	1.370(5)	C(8) - N(2)	1.371(6)
C(8) - N(2)	1.336(3)	C(8) - N(3)	1.340(5)	C(8) - N(3)	1.339(2)	C(8) - N(3)	1.329(5)	C(8) - N(3)	1.339(6)
C(9) - C(10)	1.464(3)	C(9) - C(10)	1.462(6)	C(9) - C(10)	1.470(2)	C(9) - C(10)	1.461(6)	C(9) - C(10)	1.467(6)
C(9) - N(2)	1.337(3)	C(9) - N(3)	1.329(5)	C(9) - N(3)	1.338(2)	C(9) - N(3)	1.332(5)	C(9) - N(3)	1.337(5)
C(9) - N(3)	1.370(3)	C(9) - N(4)	1.370(5)	C(9) - N(4)	1.372(2)	C(9) - N(4)	1.368(5)	C(9) - N(4)	1.379(6)
C(10) - C(11)	1.391(3)	C(10) - C(11)	1.389(6)	C(10) - C(11)	1.388(2)	C(10) - C(11)	1.389(6)	C(10) - C(11)	1.383(6)
C(10) - C(15)	1.396(3)	C(10) - C(15)	1.399(6)	C(10) - C(15)	1.402(2)	C(10) - C(15)	1.404(5)	C(10) - C(15)	1.390(6)
C(11) -	1.393(3)	C(11) -	1.384(6)	C(11) -	1.397(2)	C(11) -	1.392(6)	C(11) -	1.402(7)

C(12)		C(12)		C(12)		C(12)		C(12)	
C(11) - H(11)	0.95	C(11) - H(5)	0.93	C(11) - H(11)	0.95	C(11) - H(11)	0.95	C(11) - H(11)	0.95
C(12) - C(13)	1.394(3)	C(12) - C(13)	1.391(6)	C(12) - C(13)	1.399(2)	C(12) - C(13)	1.398(6)	C(12) - C(13)	1.376(6)
C(12) - H(12)	0.95	C(12) - H(6)	0.93	C(12) - H(12)	0.95	C(12) - H(12)	0.95	C(12) - H(12)	0.95
C(13) - C(14)	1.392(3)	C(13) - C(14)	1.393(6)	C(13) - C(14)	1.393(2)	C(13) - C(14)	1.392(6)	C(13) - C(14)	1.387(6)
C(13) - H(13)	0.95	C(13) - H(7)	0.93	C(13) - H(13)	0.95	C(13) - H(13)	0.95	C(13) - H(13)	0.95
C(14) - C(15)	1.389(3)	C(14) - C(15)	1.387(6)	C(14) - C(15)	1.390(2)	C(14) - C(15)	1.388(6)	C(14) - C(15)	1.386(6)
C(14) - H(14)	0.95	C(14) - H(8)	0.93	C(14) - H(14)		C(14) - H(14)	0.95	C(14) - H(14)	0.95
C(15) - C(16)	1.464(3)	C(15) - C(16)	1.476(6)	C(15) - C(16)	1.463(2)	C(15) - C(16)	1.465(6)	C(15) - C(16)	1.451(6)
C(16) - N(3)	1.369(3)	C(16) - N(4)	1.368(5)	C(16) - N(4)	1.372(2)	C(16) - N(4)	1.362(5)	C(16) - N(4)	1.361(5)
C(16) - N(4)	1.336(3)	C(16) - N(5)	1.335(5)	C(16) - N(5)	1.337(2)	C(16) - N(5)	1.341(5)	C(16) - N(5)	1.339(6)
C(17) - C(18)	1.463(3)	C(17) - C(18)	1.466(6)	C(17) - C(18)	1.467(2)	C(17) - C(18)	1.742(5)	C(17) - C(18)	1.460(6)
C(17) - N(4)	1.336(3)	C(17) – N(5)	1.340(5)	C(17) - N(5)	1.334(2)	C(17) - N(5)	1.342(5)	C(17) - N(5)	1.337(6)
C(17) - N(5)	1.365(3)	C(17) - N(6)	1.365(5)	C(17) - N(6)	1.372(2)	C(17) - N(6)	1.370(5)	C(17) - N(6)	1.373(5)

C(18) - C(19)	1.388(3)	C(18) - C(19)	1.382(6)	C(18) - C(19)	1.392(2)	C(18) - C(19)	1.369(5)	C(18) - C(19)	1.388(6)
C(18) - C(23)	1.400(3)	C(18) - C(23)	1.395(6)	C(18) - C(23)	1.400(2)	C(18) - C(23)	1.406(5)	C(18) - C(23)	1.394(6)
C(19) - C(20)	1.391(3)	C(19) - C(20)	1.391(6)	C(19) - C(20)	1.394(2)	C(19) - C(20)	1.396(6)	C(19) - C(20)	1.391(6)
C(19) - H(19)	0.95	C(19) - H(9)	0.931	C(19) - H(19)	0.95	C(19) - H(19)	0.95	C(19) - H(19)	0.95
C(20) - C(21)	1.399(3)	C(20) - C(21)	1.388(6)	C(20) - C(21)	1.404(2)	C(20) - C(21)	1.388(6)	C(20) - C(21)	1.396(7)
C(20) - H(20)	0.95	C(20) - H(10)	0.93	C(20) - H(20)	0.95	C(20) - H(20)	0.95	C(20) - H(20)	0.95
C(21) - C(22)	1.393(3)	C(21) - C(22)	1.384(6)	C(21) - C(22)	1.391(2)	C(21) - C(22)	1.393(6)	C(21) - C(22)	1.383(6)
C(21) - H(21)	0.95	C(21) - H(11)	0.93	C(21) - H(21)	0.95	C(21) - H(21)	0.95	C(21) - H(21)	0.95
C(22) - C(23)	1.390(3)	C(22) - C(23)	1.382(6)	C(22) - C(23)	1.389(2)	C(22) - C(23)	1.386(5)	C(22) - C(23)	1.386(6)
C(22) - H(22)	0.95	C(22) - H(12)	0.93	C(22) - H(22)	0.95	C(22) - H(22)	0.95	C(22) - H(22)	0.95
C(23) - C(24)	1.470(3)	C(23) - C(24)	1.460(6)	C(23) - C(24)	1.469(2)	C(23) - C(24)	1.464(5)	C(23) - C(24)	1.473(6)
C(24) - N(5)	1.369(3)	C(24) - N(6)	1.365(5)	C(24) - N(6)	1.369(2)	C(24) - N(6)	1.369(5)	C(24) - N(6)	1.365(5)
C(24) - N(6)	1.337(3)	C(24) - N(7)	1.336(5)	C(24) - N(7)	1.337(2)	C(24) - N(7)	1.336(5)	C(24) - N(7)	1.337(6)

C(25) - C(26)	1.471(3)	C(25) - C(26)	1.468(6)	C(25) - C(26)	1.470(2)	C(25) - C(26)	1.461(6)	C(25) - C(26)	1.466(6)
C(25) - N(6)	1.338(3)	C(25) - N(7)	1.335(5)	C(25) - N(7)	1.337(2)	C(25) - N(7)	1.332(5)	C(25) - N(7)	1.334(6)
C(25) - N(7)	1.374(3)	C(25) - N(8)	1.367(5)	C(25) - N(8)	1.370(2)	C(25) - N(8)	1.368(5)	C(25) - N(8)	1.369(5)
C(26) - C(27)	1.384(3)	C(26) - C(27)	1.384(6)	C(26) - C(27)	1.391(2)	C(26) - C(27)	1.384(5)	C(26) - C(27)	1.393(6)
C(26) - C(31)	1.397(3)	C(26) - C(31)	1.387(6)	C(26) - C(31)	1.399(2)	C(26) - C(31)	1.398(5)	C(26) - C(31)	1.385(6)
C(27) - C(28)	1.395(3)	C(27) - C(28)	1.376(6)	C(27) - C(28)	1.398(2)	C(27) - C(28)	1.402(6)	C(27) - C(28)	1.391(7)
C(27) - H(27)	0.95	C(27) - H(13)	0.93	C(27) - H(27)	0.95	C(27) - H(27)	0.95	C(27) - H(27)	0.949
C(28) - C(29)	1.393(3)	C(28) - C(29)	1.394(6)	C(28) - C(29)	1.399(2)	C(28) - C(29)	1.400(6)	C(28) - C(29)	1.388(7)
C(28) - H(28)	0.95	C(28) - H(14)	0.93	C(28) - H(28)	0.95	C(28) - H(28)	0.95	C(28) - H(28)	0.95
C(29) - C(30)	1.393(3)	C(29) - C(30)	1.379(6)	C(29) - C(30)	1.369(2)	C(29) - C(30)	1.374(6)	C(29) - C(30)	1.396(7)
C(29) - H(29)	0.95	C(29) - H(15)	0.931	C(29) - H(29)	0.95	C(29) - H(29)	0.95	C(29) - H(29)	0.95
C(30) - C(31)	1.388(3)	C(30) - C(31)	1.383(5)	C(30) - C(31)	1.389(2)	C(30) - C(31)	1.382(6)	C(30) - C(31)	1.385(6)
C(30) - H(30)	0.95	C(30) - H(16)	0.93	C(30) - H(30)	0.95	C(30) - H(30)	0.95	C(30) - H(30)	0.95

C(31) - C(32)	1.458(3)	C(31) - C(32)	1.475(5)	C(31) - C(32)	1.466(2)	C(31) - C(32)	1.459(6)	C(31) - C(32)	1.462(6)
C(32) - N(7)	1.368(3)	C(32) - N(1)	1.334(5)	C(32) - N(1)	1.336(2)	C(32) - N(1)	1.334(5)	C(32) - N(1)	1.327(6)
C(32) - N(8)	1.337(3)	C(32) - N(8)	1.369(5)	C(32) - N(8)	1.370(2)	C(32) - N(8)	1.368(5)	C(32) - N(8)	1.371(6)

Table S14. Bond Lengths for $LnPc_2 \cdot CH_2Cl_2$

$LaPc_2$		$PrPc_2$		$NdPc_2$		$SmPc_2$		$GdPc_2$		$TbPc_2$		$DyPc_2$		$ErPc_2$		$YbPc_2$	
Atom 1 – Atom 2	Bond Length (Å)	Atom 1 – Atom 2	Bond Length (Å)	Atom 1 – Atom 2	Bond Length (Å)	Atom 1 – Atom 2	Bond Length (Å)	Atom 1 – Atom 2	Bond Length (Å)	Atom 1 – Atom 2	Bond Length (Å)	Atom 1 – Atom 2	Bond Length (Å)	Atom 1 – Atom 2	Bond Length (Å)	Atom 1 – Atom 2	Bond Length (Å)
La(1) - N(1)	2.442	Pr(1) - N(1)	2.458	Nd(1) - N(2)	2.463	Sm(1) - N(1)	2.481	Gd(1) - N(1)	2.438	Tb(1) - N(1)	2.438	Dy(1) - N(3)	2.408	Er(1) - N(2)	2.384	Yb(1) - N(1)	2.384
La(1) - N(3)	2.426	Pr(1) - N(3)	2.476	Nd(1) - N(4)	2.470	Sm(1) - N(3)	2.462	Gd(1) - N(3)	2.422	Tb(1) - N(3)	2.428	Dy(1) - N(5)	2.415	Er(1) - N(4)	2.390	Yb(1) - N(3)	2.371
La(1) - N(5)	2.440	Pr(1) - N(5)	2.486	Nd(1) - N(6)	2.477	Sm(1) - N(5)	2.476	Gd(1) - N(5)	2.431	Tb(1) - N(5)	2.439	Dy(1) - N(7)	2.410	Er(1) - N(6)	2.403	Yb(1) - N(5)	2.394
La(1) - N(7)	2.431	Pr(1) - N(6)	2.475	Nd(1) - N(8)	2.462	Sm(1) - N(7)	2.471	Gd(1) - N(7)	2.430	Tb(1) - N(7)	2.433	Dy(1) - N(8)	2.426	Er(1) - N(8)	2.388	Yb(1) - N(7)	2.384
La(1) - N(9)	2.430	Pr(1) - N(9)	2.480	Nd(1) - N(10)	2.477	Sm(1) - N(9)	2.465	Gd(1) - N(9)	2.427	Tb(1) - N(10)	2.432	Dy(1) - N(9)	2.407	Er(1) - N(10)	2.395	Yb(1) - N(9)	2.379
C(1) - C(1)	1.399(5)	C(1) - C(1)	1.392(4)	C(1) - C(2)	1.459(3)	C(1) - C(1)	1.375(6)	C(1) - C(1)	1.390(1)	C(1) - C(1)	1.398(3)	C(10) - C(12)	1.400(7)	C(1) - C(2)	1.465(6)	C(1) - C(1)	1.390(1)
C(1) - C(2)	1.396(5)	C(1) - C(2)	1.394(3)	C(1) - N(1)	1.339	C(1) - C(2)	1.403(5)	C(1) - C(2)	1.382(8)	C(1) - C(2)	1.396(2)	C(10) - C(G)	1.394(7)	C(1) - N(1)	1.335	C(1) - C(2)	1.385(9)
C(1) - H(1)	0.95	C(1) - H(1)	0.95	C(1) - N(2)	1.368(3)	C(1) - H(1)	0.95	C(1) - H(1)	0.931	C(1) - H(1)	0.95	C(10) - H(10)	0.929	C(1) - N(2)	1.367(6)	C(1) - H(1)	0.95
C(2) - C(3)	1.386(4)	C(2) - C(3)	1.391(3)	C(2) - C(3)	1.393(3)	C(2) - C(3)	1.381(5)	C(2) - C(3)	1.390(8)	C(2) - C(3)	1.389(2)	C(11) - C(16)	1.376(7)	C(2) - C(3)	1.387(6)	C(2) - C(3)	1.386(9)
C(2) - H(2)	0.95	C(2) - H(2)	0.95	C(2) - C(7)	1.401(3)	C(2) - H(2)	0.95	C(2) - H(2)	0.929	C(2) - H(2)	0.95	C(11) - C(R)	1.387(7)	C(2) - C(7)	1.391(6)	C(2) - H(2)	0.949
C(3) - C(3)	1.409(3)	C(3) - C(3)	1.399(3)	C(3) - C(4)	1.391(4)	C(3) - C(3)	1.403(5)	C(3) - C(3)	1.382(6)	C(3) - C(3)	1.402(2)	C(11) - H(11)	0.93	C(3) - C(4)	1.391(6)	C(3) - C(3)	1.400(1)
C(3) - C(4)	1.467(4)	C(3) - C(4)	1.464(3)	C(3) - H(3)	0.95	C(3) - C(4)	1.470(4)	C(3) - C(4)	1.464(7)	C(3) - C(4)	1.468(2)	C(12) - C(K)	1.380(7)	C(3) - H(3)	0.95	C(3) - C(4)	1.470(8)
C(4) - N(1)	1.367	C(4) - N(1)	1.368	C(4) - C(5)	1.403(4)	C(4) - N(1)	1.365	C(4) - N(1)	1.369	C(4) - N(1)	1.371	C(12) - H(12)	0.93	C(4) - C(5)	1.397(6)	C(4) - N(1)	1.363

C(4) - N(2)	1.337(4)	C(4) - N(2)	1.340(3)	C(4) - H(4)	0.95	C(4) - N(2)	1.338(4)	C(4) - N(2)	1.333(6)	C(4) - N(2)	1.338(2)	C(13) - C(15)	1.393(7)	C(4) - H(4)	0.95	C(4) - N(2)	1.341(8)
C(5) - C(6)	1.456(4)	C(5) - C(6)	1.469(3)	C(5) - C(6)	1.391(3)	C(5) - C(6)	1.470(5)	C(5) - C(6)	1.465(7)	C(5) - C(6)	1.468(2)	C(13) - C(U)	1.379(7)	C(5) - C(6)	1.395(6)	C(5) - C(6)	1.470(1)
C(5) - N(2)	1.337(4)	C(5) - N(2)	1.342(2)	C(5) - H(5)	0.95	C(5) - N(2)	1.335(4)	C(5) - N(2)	1.355(7)	C(5) - N(2)	1.338(2)	C(13) - H(13)	0.93	C(5) - H(5)	0.949	C(5) - N(2)	1.340(7)
C(5) - N(3)	1.372(4)	C(5) - N(3)	1.364(2)	C(6) - C(7)	1.388(3)	C(5) - N(3)	1.368(4)	C(5) - N(3)	1.368(6)	C(5) - N(3)	1.368(2)	C(14) - C(16)	1.407(8)	C(6) - C(7)	1.394(6)	C(5) - N(3)	1.361(8)
C(6) - C(7)	1.392(5)	C(6) - C(7)	1.387(3)	C(6) - H(6)	0.95	C(6) - C(7)	1.384(5)	C(6) - C(7)	1.386(8)	C(6) - C(7)	1.387(2)	C(14) - C(Q)	1.386(7)	C(6) - H(6)	0.95	C(6) - C(7)	1.390(1)
C(6) - C(11)	1.398(4)	C(6) - C(11)	1.402(3)	C(7) - C(8)	1.471(3)	C(6) - C(11)	1.399(5)	C(6) - C(11)	1.413(8)	C(6) - C(11)	1.399(2)	C(14) - H(14)	0.931	C(7) - C(8)	1.458(6)	C(6) - C(11)	1.405(8)
C(7) - C(8)	1.395(4)	C(7) - C(8)	1.395(3)	C(8) - N(2)	1.369(3)	C(7) - C(8)	1.395(5)	C(7) - C(8)	1.339(9)	C(7) - C(8)	1.398(2)	C(15) - C(X)	1.387(7)	C(8) - N(2)	1.383(5)	C(7) - C(8)	1.380(1)
C(7) - H(7)	0.95	C(7) - H(7)	0.95	C(8) - N(3)	1.339(3)	C(7) - H(7)	0.95	C(7) - H(7)	0.93	C(7) - H(7)	0.95	C(15) - H(15)	0.931	C(8) - N(3)	1.333(6)	C(7) - H(7)	0.95
C(8) - C(9)	1.401(5)	C(8) - C(9)	1.400(3)	C(9) - C(10)	1.466(3)	C(8) - C(9)	1.399(6)	C(8) - C(9)	1.420(1)	C(8) - C(9)	1.401(2)	C(16) - H(16)	0.931	C(9) - C(10)	1.475(6)	C(8) - C(9)	1.420(1)
C(8) - H(8)	0.95	C(8) - H(8)	0.95	C(9) - N(3)	1.340(3)	C(8) - H(8)	0.95	C(8) - H(8)	0.93	C(8) - H(8)	0.95	C(17) - C(17)	1.389(6)	C(9) - N(3)	1.342(6)	C(8) - H(8)	0.951
C(9) - C(10)	1.389(5)	C(9) - C(10)	1.939(3)	C(9) - N(4)	1.371(3)	C(9) - C(10)	1.390(5)	C(9) - C(10)	1.390(1)	C(9) - C(10)	1.396(2)	C(17) - C(T)	1.379(7)	C(9) - N(4)	1.362(6)	C(9) - C(10)	1.360(1)
C(9) - H(9)	0.95	C(9) - H(9)	0.95	C(10) - C(11)	1.390(3)	C(9) - H(9)	0.95	C(9) - H(9)	0.93	C(9) - H(9)	0.95	C(17) - H(17)	0.93	C(10) - C(11)	1.387(6)	C(9) - H(9)	0.951
C(10) - C(11)	1.389(5)	C(10) - C(11)	1.386(3)	C(10) - C(15)	1.395(3)	C(10) - C(11)	1.387(5)	C(10) - C(11)	1.376(9)	C(10) - C(11)	1.385(2)	C(18) - C(18)	1.398(6)	C(10) - C(15)	1.395(6)	C(10) - C(11)	1.390(1)
C(10) - H(10)	0.95	C(10) - H(10)	0.95	C(11) - C(12)	1.390(3)	C(10) - H(10)	0.95	C(10) - H(10)	0.929	C(10) - H(10)	0.95	C(18) - C(Z)	1.384(8)	C(11) - C(12)	1.392(6)	C(10) - H(10)	0.95
C(11) - C(12)	1.469(4)	C(11) - C(12)	1.468(3)	C(11) - H(11)	0.95	C(11) - C(12)	1.462(5)	C(11) - C(12)	1.476(8)	C(11) - C(12)	1.467(2)	C(18) - H(18)	0.93	C(11) - H(11)	0.95	C(11) - C(12)	1.460(1)
C(12) -	1.367(4	C(12) -	1.371(2	C(12) -	1.394(4	C(12) -	1.375(4	C(12) -	1.360(6	C(12) -	1.371(2	C(D) -	1.385(6	C(12) -	1.402(6	C(12) -	1.386(8

N(3)	)	N(3)	)	C(13)	)	N(3)	)	N(3)	)	N(3)	)	C(D)	)	C(13)	)	N(3)	)
C(12) - N(4)	1.340(4)	C(12) - N(4)	1.335(2)	C(12) - H(12)	0.95	C(12) - N(4)	1.334(4)	C(12) - N(4)	1.335(6)	C(12) - N(4)	1.336(2)	C(D) - C(N)	1.471(7)	C(12) - H(12)	0.95	C(12) - N(4)	1.325(8)
C(13) - C(14)	1.468(4)	C(13) - C(14)	1.466(3)	C(13) - C(14)	1.388(4)	C(13) - C(14)	1.469(4)	C(13) - C(14)	1.466(7)	C(13) - C(14)	1.467(2)	C(D) - C(Z)	1.389(8)	C(13) - C(14)	1.394(6)	C(13) - C(14)	1.464(8)
C(13) - N(4)	1.337(4)	C(13) - N(4)	1.339(2)	C(13) - H(13)	0.95	C(13) - N(4)	1.333(4)	C(13) - N(4)	1.337(8)	C(13) - N(4)	1.335(2)	C(E) - C(G)	1.386(7)	C(13) - H(13)	0.95	C(13) - N(4)	1.347(8)
C(13) - N(5)	1.366	C(13) - N(5)	1.370	C(14) - C(15)	1.381(3)	C(13) - N(5)	1.368	C(13) - N(5)	1.376	C(13) - N(5)	1.371	C(E) - C(S)	1.404(7)	C(14) - C(15)	1.388(6)	C(13) - N(5)	1.367
C(14) - C(15)	1.390(4)	C(14) - C(15)	1.392(3)	C(14) - H(14)	0.95	C(14) - C(14)	1.406(5)	C(14) - C(14)	1.387(6)	C(14) - C(14)	1.405(2)	C(E) - C(O)	1.458(7)	C(14) - H(14)	0.95	C(14) - C(14)	1.420(1)
C(14) - C(14)	1.393(5)	C(14) - C(14)	1.405(3)	C(15) - C(16)	1.468(3)	C(14) - C(15)	1.389(5)	C(14) - C(15)	1.393(8)	C(14) - C(15)	1.391(2)	C(F) - C(R)	1.457(7)	C(15) - C(16)	1.465(6)	C(14) - C(15)	1.393(9)
C(15) - C(16)	1.401(5)	C(15) - C(16)	1.391(3)	C(16) - N(4)	1.366(3)	C(15) - C(16)	1.387(5)	C(15) - C(16)	1.388(8)	C(15) - C(16)	1.397(2)	C(F) - N(3)	1.381(6)	C(16) – N(4)	1.373(5)	C(15) - C(16)	1.375(9)
C(15) - H(15)	0.95	C(15) - H(15)	0.95	C(16) - N(5)	1.335	C(15) - H(15)	0.95	C(15) - H(15)	0.931	C(15) - H(15)	0.95	C(F) - N(A)	1.339(6)	C(16) - (N(5)	1.338	C(15) - H(15)	0.949
C(16) - C(16)	1.396(5)	C(16) - C(16)	1.399(4)	C(17) - C(18)	1.467(3)	C(16) - C(16)	1.398(6)	C(16) - C(16)	1.390(1)	C(16) - C(16)	1.399(3)	C(G) - H(G)	0.93	C(17) - C(18)	1.470(6)	C(16) - C(16)	1.380(1)
C(16) - H(16)	0.95	C(16) - H(16)	0.95	C(17) - N(6)	1.370	C(16) - H(16)	0.95	C(16) - H(16)	0.93	C(16) - H(16)	0.95	C(H) - C(J)	1.460(7)	C(17) - N(6)	1.361	C(16) - H(16)	0.949
C(17) - C(18)	1.465(4)	C(17) - C(18)	1.468(2)	C(17) - N(7)	1.334(3)	C(17) - C(18)	1.470(5)	C(17) - C(18)	1.460(7)	C(17) - C(18)	1.469(2)	C(H) - C(M)	1.398(7)	C(17) - N(7)	1.337(6)	C(17) - C(18)	1.463(9)
C(17) - N(6)	1.338	C(17) - N(6)	1.374(2)	C(18) - C(18)	1.398(4)	C(17) - N(6)	1.326	C(17) - N(6)	1.323	C(17) - N(6)	1.334(2)	C(H) - C(U)	1.393(7)	C(18) - C(18)	1.394(6)	C(17) - N(6)	1.323
C(17) - N(7)	1.368(4)	C(17) - N(10)	1.333(2)	C(18) - C(19)	1.395(3)	C(17) - N(7)	1.365(4)	C(17) - N(7)	1.369(3)	C(17) - N(7)	1.372(2)	C(J) - N(4)	1.323	C(18) - C(19)	1.394(6)	C(17) - N(7)	1.389(8)
C(18) - C(19)	1.389(4)	C(18) - C(19)	1.389(3)	C(19) - C(20)	1.389(4)	C(18) - C(19)	1.389(4)	C(18) - C(19)	1.394(7)	C(18) - C(19)	1.392(2)	C(J) - N(7)	1.377(6)	C(19) - C(20)	1.391(6)	C(18) - C(19)	1.393(8)

C(18) - C(23)	1.397(4)	C(18) - C(23)	1.402(3)	C(19) - H(19)	0.95	C(18) - C(23)	1.399(4)	C(18) - C(23)	1.391(7)	C(18) - C(23)	1.399(2)	C(I) – C(L)	1.458(7)	C(19) - H(19)	0.95	C(18) - C(23)	1.395(9)
C(19) - C(20)	1.389(5)	C(19) - C(20)	1.390(3)	C(20) - C(20)	1.392(4)	C(19) - C(20)	1.389(5)	C(19) - C(20)	1.370(1)	C(19) - C(20)	1.392(2)	C(I) - C(I)	1.385(6)	C(20) - C(20)	1.395(6)	C(19) - C(20)	1.370(1)
C(19) - H(19)	0.95	C(19) - H(19)	0.95	C(20) - H(20)	0.95	C(19) - H(19)	0.95	C(19) - H(19)	0.931	C(19) - H(19)	0.95	C(I) - C(T)	1.394(7)	C(20) - H(20)	0.95	C(19) - H(19)	0.95
C(20) - C(21)	1.399(5)	C(20) - C(21)	1.402(3)	C(21) - C(22)	1.465(3)	C(20) - C(21)	1.395(5)	C(20) - C(21)	1.389(9)	C(20) - C(21)	1.400(2)	C(K) - C(S)	1.379(7)	C(21) - C(22)	1.461(6)	C(20) - C(21)	1.405(9)
C(20) - H(20)	0.95	C(20) - H(20)	0.95	C(21) - N(7)	1.332(3)	C(20) - H(20)	0.95	C(20) - H(20)	0.931	C(20) - H(20)	0.95	C(K) - H(K)	0.93	C(21) - N(7)	1.343(6)	C(20) - H(20)	0.95
C(21) - C(22)	1.392(4)	C(21) - C(22)	1.395(3)	C(21) - N(8)	1.374(3)	C(21) - C(22)	1.389(5)	C(21) - C(22)	1.375(8)	C(21) - C(22)	1.393(2)	C(L) - N(5)	1.381	C(21) - N(8)	1.373(6)	C(21) - C(22)	1.412(9)
C(21) - H(21)	0.95	C(21) - H(21)	0.95	C(22) - C(23)	1.388(4)	C(21) - H(21)	0.95	C(21) - H(21)	0.931	C(21) - H(21)	0.95	C(L) - N(A)	1.336(6)	C(22) - C(23)	1.391(6)	C(21) - H(21)	0.949
C(22) - C(23)	1.392(5)	C(22) - C(23)	1.385(3)	C(22) - C(27)	1.398(4)	C(22) - C(23)	1.389(5)	C(22) - C(23)	1.391(7)	C(22) - C(23)	1.390(2)	C(M) - C(W)	1.465(7)	C(22) - C(27)	1.396(6)	C(22) - C(23)	1.380(1)
C(22) - H(22)	0.95	C(22) - H(22)	0.95	C(23) - C(24)	1.389(4)	C(22) - H(22)	0.95	C(22) - H(22)	0.93	C(22) - H(22)	0.95	C(M) - C(X)	1.385(7)	C(23) - C(24)	1.397(7)	C(22) - H(22)	0.951
C(23) - C(24)	1.468(4)	C(23) - C(24)	1.465(3)	C(23) - H(23)	0.95	C(23) - C(24)	1.464(4)	C(23) - C(24)	1.461(7)	C(23) - C(24)	1.461(2)	C(N) - N(8)	1.366	C(23) - H(23)	0.95	C(23) - C(24)	1.469(9)
C(24) - N(7)	1.361(4)	C(24) - N(6)	1.369(2)	C(24) - C(25)	1.399(4)	C(24) - N(7)	1.367(4)	C(24) - N(7)	1.372(6)	C(24) - N(7)	1.369(2)	C(N) - N(30)	1.337(6)	C(24) - C(25)	1.413(7)	C(24) - N(7)	1.356(8)
C(24) - N(8)	1.347(4)	C(24) - N(7)	1.338	C(24) - H(24)	0.95	C(24) - N(8)	1.339(4)	C(24) - N(8)	1.336(6)	C(24) - N(8)	1.335	C(O) - N(6)	1.330(6)	C(24) - H(24)	0.951	C(24) - N(8)	1.343(8)
C(25) - C(26)	1.459(4)	C(25) - C(26)	1.463(3)	C(25) - C(26)	1.391(4)	C(25) – C(26)	1.468(4)	C(25) - C(26)	1.459(7)	C(25) - C(26)	1.463(2)	C(O) - N(9)	1.380(6)	C(25) - C(26)	1.382(7)	C(25) - C(26)	1.471(9)
C(25) - N(8)	1.336(4)	C(25) - N(8)	1.338	C(25) - H(25)	0.95	C(25) - N(8)	1.336(4)	C(25) - N(8)	1.333(6)	C(25) - N(9)	1.334	C(P) - C(Y)	1.463(7)	C(25) - H(25)	0.95	C(25) - N(8)	1.364(8)
C(25) - N(9)	1.373(4)	C(25) - N(9)	1.368(2)	C(26) - C(27)	1.386(4)	C(25) - N(9)	1.370(4)	C(25) - N(9)	1.366(6)	C(25) - N(10)	1.371(2)	C(P) - N(3)	1.367(6)	C(26) - C(27)	1.388(6)	C(25) - N(9)	1.361(8)
C(26) -	1.389(4	C(26) -	1.391(3	C(26) -	0.95	C(26) -	1.385(5	C(26) -	1.385(7	C(26) -	1.392(2	C(P) -	1.338(7	C(26) -	0.95	C(26) -	1.390(1

C(27)	)	C(27)	)	H(26)		C(27)	)	C(27)	)	C(27)	)	N(30)	)	H(26)		C(27)	)
C(26) - C(31)	1.396(4)	C(26) - C(31)	1.401(3)	C(27) - C(28)	1.464(3)	C(26) - C(31)	1.398(4)	C(26) - C(31)	1.392(7)	C(26) - C(31)	1.401(2)	C(Q) - C(Y)	1.385(7)	C(27) - C(28)	1.464(6)	C(26) - C(31)	1.396(9)
C(27) - C(28)	1.393(4)	C(27) - C(28)	1.391(3)	C(28) - N(8)	1.366(3)	C(27) - C(28)	1.396(5)	C(27) - C(28)	1.381(8)	C(27) - C(28)	1.392(2)	C(Q) - H(Q)	0.93	C(28) - N(8)	1.378(6)	C(27) - C(28)	1.389(8)
C(27) - H(27)	0.95	C(27) - H(27)	0.95	C(28) - N(9)	1.342(3)	C(27) - H(27)	0.95	C(27) - H(27)	0.93	C(27) - C(28)	0.95	C(R) - C(Y)	1.399(7)	C(28) - N(9)	1.338(6)	C(27) - H(27)	0.949
C(28) - C(29)	1.398(4)	C(28) - C(29)	1.402(3)	C(29) - C(30)	1.468(3)	C(28) - C(29)	1.408(5)	C(28) - C(29)	1.387(9)	C(28) - C(29)	1.403(2)	C(S) - C(V)	1.454(7)	C(29) - C(30)	1.470(6)	C(28) - C(29)	1.399(9)
C(28) - H(28)	0.95	C(28) - H(28)	0.95	C(29) - N(9)	1.340(3)	C(28) - H(28)	0.95	C(28) - H(28)	0.93	C(28) - H(28)	0.95	C(T) - H(T)	0.931	C(29) - N(9)	1.333(6)	C(28) - H(28)	0.949
C(29) - C(30)	1.389(5)	C(29) - C(30)	1.398(3)	C(29) - N(10)	1.368	C(29) - C(30)	1.390(5)	C(29) - C(30)	1.378(8)	C(29) - C(30)	1.396(2)	C(U) - H(U)	0.93	C(29) - N(10)	1.375	C(29) - C(30)	1.390(1)
C(29) - H(29)	0.95	C(29) - H(29)	0.95	C(30) - C(30)	1.398(4)	C(29) - H(29)	0.95	C(29) - H(29)	0.93	C(29) - H(29)	0.95	C(V) - N(9)	1.369(6)	C(30) - C(30)	1.402(6)	C(29) - H(29)	0.95
C(30) - C(31)	1.383(4)	C(30) - C(31)	1.391(3)	C(30) - C(31)	1.384(4)	C(30) - C(31)	1.392(4)	C(30) - C(31)	1.381(7)	C(30) - C(31)	1.391(2)	C(V) - N(40)	1.330	C(30) - C(31)	1.397(6)	C(30) - C(31)	1.388(8)
C(30) - H(30)	0.95	C(30) - H(30)	0.95	C(31) - C(32)	1.395(4)	C(30) - H(30)	0.95	C(30) - H(30)	0.93	C(30) - H(30)	0.95	C(W) - N(6)	1.354(6)	C(31) - C(32)	1.394(6)	C(30) - H(30)	0.949
C(31) - C(32)	1.460(4)	C(31) - C(32)	1.468(3)	C(31) - H(31)	0.95	C(31) - C(32)	1.461(5)	C(31) - C(32)	1.466(7)	C(31) - C(32)	1.469(2)	C(W) - N(7)	1.355(6)	C(31) - H(31)	0.95	C(31) - C(32)	1.455(9)
C(32) - N(9)	1.371(4)	C(32) - N(9)	1.369(2)	C(32) - C(32)	1.384(4)	C(32) - N(9)	1.369(4)	C(32) - N(9)	1.364(6)	C(32) - N(6)	1.338(2)	C(X) - H(X)	0.93	C(32) - C(32)	1.395(6)	C(32) - N(9)	1.392(8)
C(32) - N(10)	1.336	C(32) - N(10)	1.342(2)	C(32) - H(32)	0.95	C(32) - N(10)	1.339	C(32) - N(10)	1.333	C(32) - N(10)	1.368(2)	C(Z) - H(Z)	0.93	C32 - H(32)	0.951	C(32) - N(10)	1.317
C(33) - Cl(1)	1.769	C(33) - Cl(1)	1.768	C(33) - Cl(1)	1.768	C(33) - Cl(1)	1.769	C33 – Cl(1)	1.702	C(33) - Cl(2)	1.768	C(19) - Cl(1)	1.765	C(33) - Cl(1)	1.772	C(33) - Cl	1.763
C(33) - H(33)	0.99	C(33) - H(33)	0.99	C(33) - H(33)	0.99	C(33) - H(33)	0.99	C(33) - H(33)	0.97	C(33) - H(33)	0.99	C(19) - H(19)	0.971	C(33) - H(33)	0.99	C(33) - H(33)	0.99