Synthesis and antiproliferative activity of hindered, chiral 1,2-diaminodiamantane platinum(II) complexes

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Supplementary information

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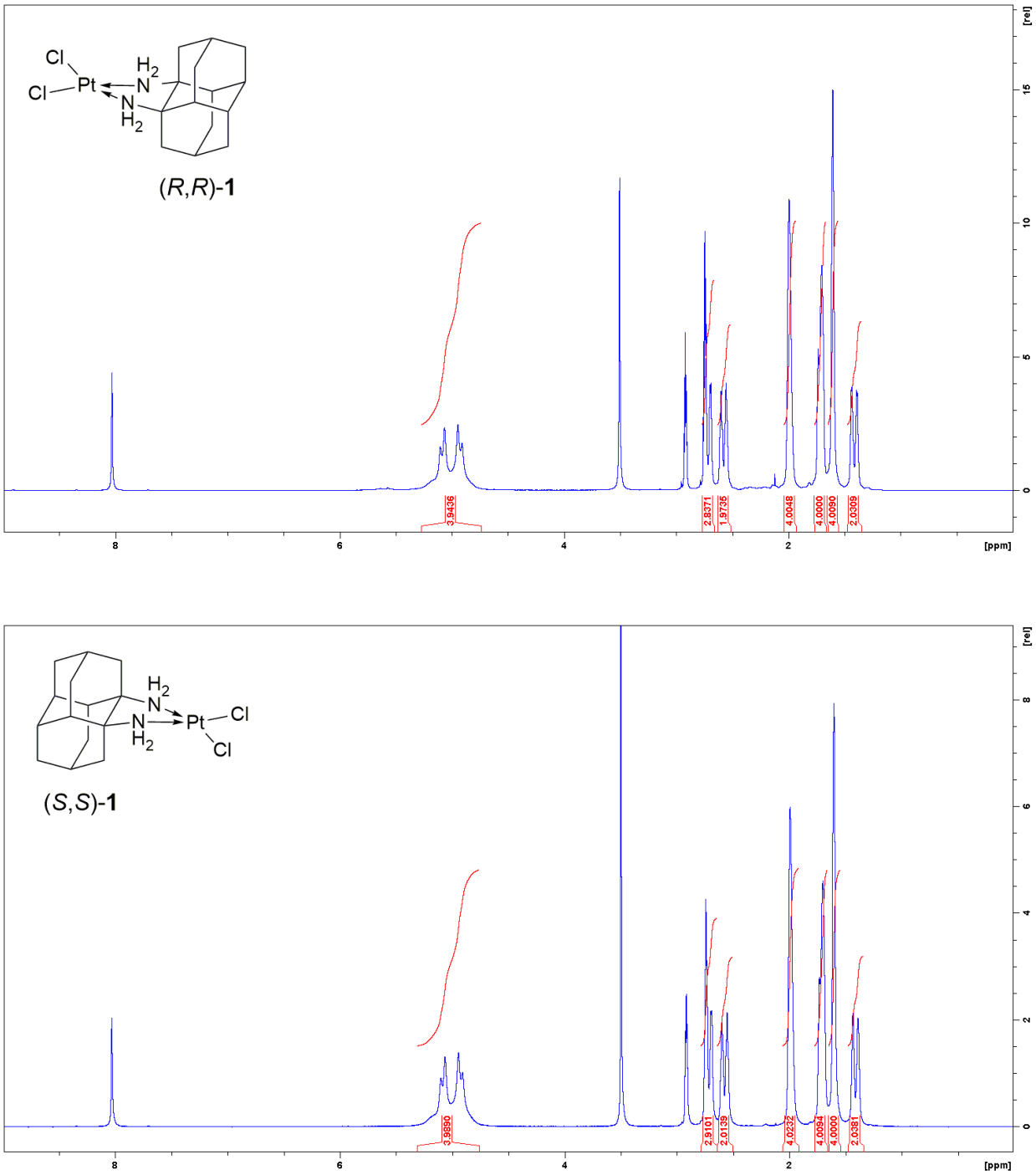


Figure S1 ^{1}H NMR spectra of (*R*,*R*)-**1** and (*S*,*S*)-**1**.

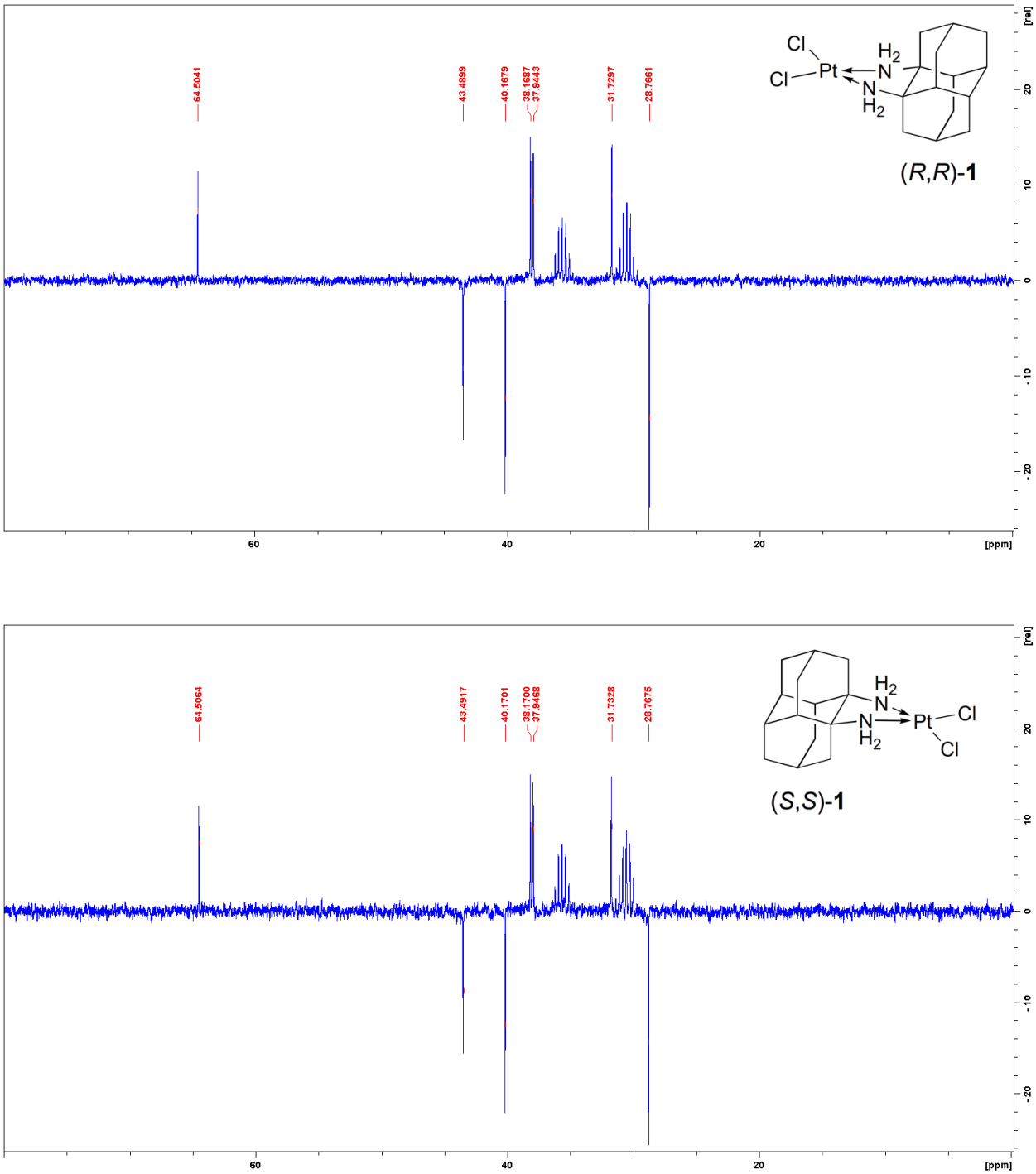
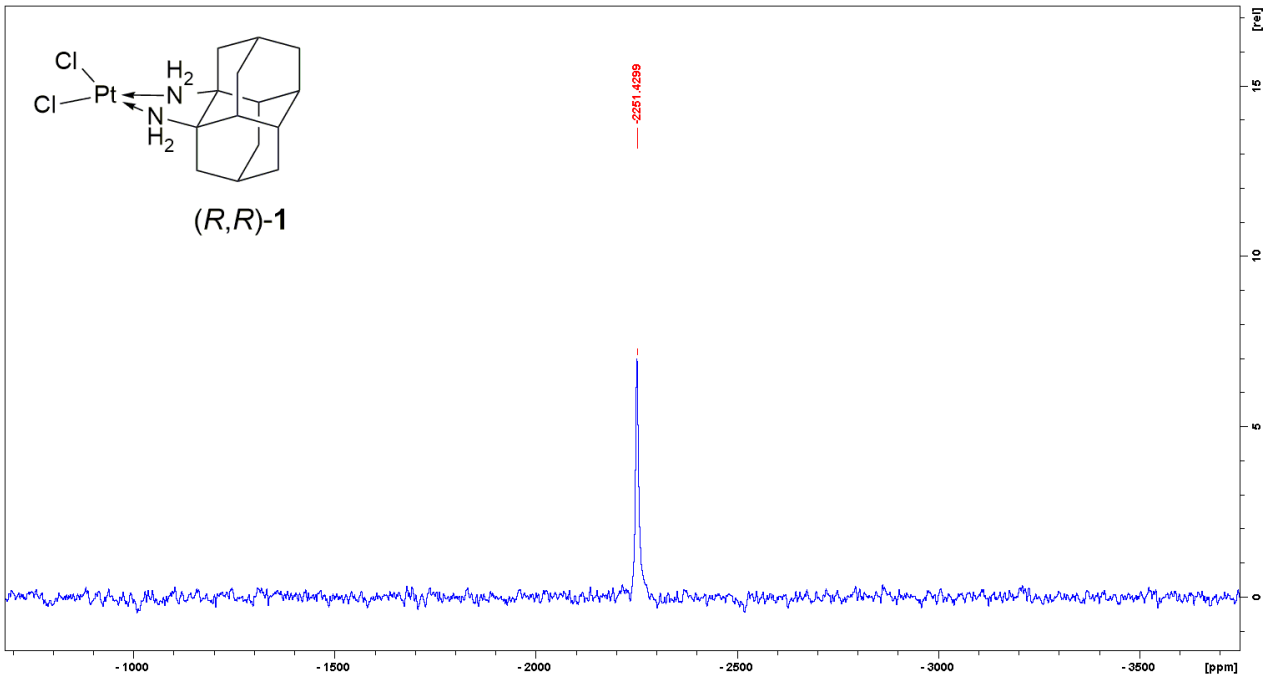


Figure S2 ^{13}C NMR spectra of (*R*,*R*)-**1** and (*S*,*S*)-**1**.



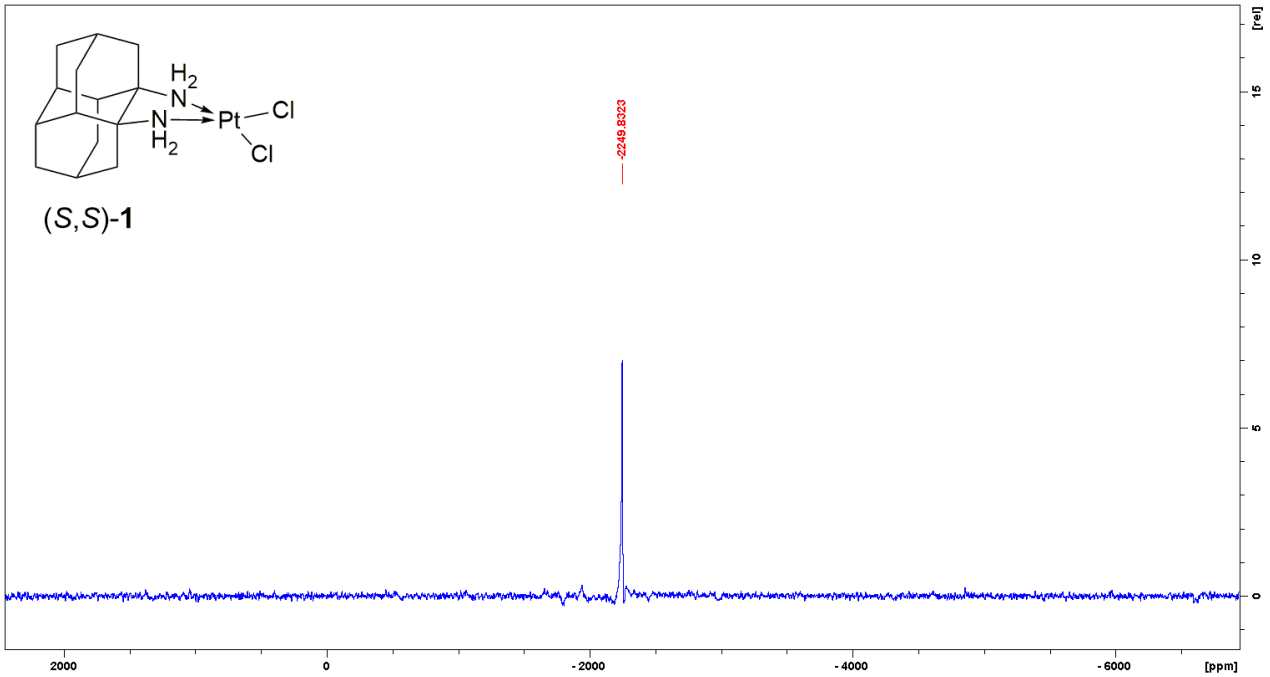


Figure S3 ^{195}Pt NMR spectra of (*R*,*R*)-**1** and (*S*,*S*)-**1**.

Crystallographic data for (*S*,*S*)-1,2-diaminodiamantane

The unit cell of (*S*,*S*)-1,2-diaminodiamantane was determined using 9978 reflections and the structure was solved in the monoclinic space group $P2_1$. The asymmetric unit contains the cation, two chloride anions and a methanol molecule. The absolute configuration of the structure could be successfully determined utilizing the anomalous dispersion effect and using the improved Flack method[1] with a Flack x of 0.004(4).

Table S1 Crystal data and structure refinement for (*S*,*S*)-1,2-diaminodiamantane.

CCDC No	1956841	
Empirical formula	$C_{15}H_{28}Cl_2N_2O$	
Formula weight	323.29	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1$	
Unit cell dimensions	a = 9.7449(3) Å	α= 90°.
	b = 8.4127(3) Å	β= 92.4679(15)°.
	c = 9.7717(3) Å	γ = 90°.
Volume	800.35(5) $Å^3$	
Z	2	
Density (calculated)	1.342 Mg/m^3	
Absorption coefficient	0.404 mm^{-1}	
F(000)	348	
Crystal size	0.560 x 0.335 x 0.260 mm^3	
Theta range for data collection	2.890 to 49.117°.	
Index ranges	-20<=h<=20, -17<=k<=17, -20<=l<=20	
Reflections collected	272934	
Independent reflections	16136 [R(int) = 0.0480]	
Completeness to theta = 25.242°	99.4 %	
Absorption correction	Semi-empirical from equivalents	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	16136 / 8 / 203	
Goodness-of-fit on F^2	1.078	
Final R indices [I>2sigma(I)]	R1 = 0.0189, wR2 = 0.0511	
R indices (all data)	R1 = 0.0207, wR2 = 0.0516	
Absolute structure parameter	0.004(4)	
Largest diff. peak and hole	0.265 and -0.296 $e.Å^{-3}$	

Table S2 Atomic coordinates *(× 10^4)* and equivalent isotropic displacement parameters *(Å^2 × 10^3)* for (*S*,*S*)-1,2-diaminodiamantane. *U(eq)* is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	x	y	z	U(eq)
Cl(1)	8282(1)	659(1)	5790(1)	12(1)
Cl(2)	9303(1)	9342(1)	640(1)	13(1)
O(1)	9067(1)	5838(1)	6829(1)	20(1)
N(1)	8820(1)	3941(1)	4413(1)	10(1)
N(2)	9346(1)	5951(1)	1926(1)	9(1)
C(1)	7778(1)	4140(1)	3237(1)	8(1)
C(2)	7944(1)	5753(1)	2498(1)	7(1)
C(3)	6865(1)	5805(1)	1287(1)	10(1)
C(4)	5422(1)	5771(1)	1874(1)	12(1)
C(5)	5248(1)	4178(1)	2630(1)	11(1)
C(6)	6325(1)	4108(1)	3829(1)	9(1)
C(7)	7946(1)	2739(1)	2257(1)	11(1)
C(8)	6858(1)	2826(1)	1081(1)	13(1)
C(9)	7024(1)	4394(1)	306(1)	13(1)
C(10)	5423(1)	2767(1)	1663(1)	14(1)
C(11)	7734(1)	7149(1)	3481(1)	10(1)
C(12)	6288(1)	7077(1)	4041(1)	12(1)
C(13)	5225(1)	7180(1)	2841(1)	14(1)
C(14)	6095(1)	5502(1)	4801(1)	11(1)
C(15)	8186(1)	6835(1)	7579(1)	16(1)

Table S3 Bond lengths *(Å)* and angles *(°)* for (*S*,*S*)-1,2-diaminodiamantane.

		N(2)-H(2A)	0.858(10)
O(1)-C(15)	1.4257(7)	N(2)-H(2B)	0.893(10)
O(1)-H(1)	0.864(13)	N(2)-H(2C)	0.847(10)
N(1)-C(1)	1.5098(5)	C(1)-C(7)	1.5312(5)
N(1)-H(1A)	0.963(10)	C(1)-C(2)	1.5487(5)
N(1)-H(1B)	0.908(11)	C(1)-C(6)	1.5519(5)
N(1)-H(1C)	0.835(10)	C(2)-C(11)	1.5363(6)
N(2)-C(2)	1.5078(5)	C(2)-C(3)	1.5489(5)

C(3)-C(9)	1.5377(7)	C(1)-N(1)-H(1B)	104.3(6)
C(3)-C(4)	1.5413(6)	H(1A)-N(1)-H(1B)	106.7(9)
C(3)-H(3)	1.0000	C(1)-N(1)-H(1C)	110.6(7)
C(4)-C(13)	1.5335(7)	H(1A)-N(1)-H(1C)	114.0(10)
C(4)-C(5)	1.5429(6)	H(1B)-N(1)-H(1C)	107.5(10)
C(4)-H(4)	1.0000	C(2)-N(2)-H(2A)	109.1(7)
C(5)-C(10)	1.5313(7)	C(2)-N(2)-H(2B)	111.4(7)
C(5)-C(6)	1.5404(6)	H(2A)-N(2)-H(2B)	103.6(10)
C(5)-H(5)	1.0000	C(2)-N(2)-H(2C)	115.0(7)
C(6)-C(14)	1.5324(6)	H(2A)-N(2)-H(2C)	105.3(10)
C(6)-H(6)	1.0000	H(2B)-N(2)-H(2C)	111.6(10)
C(7)-C(8)	1.5319(6)	N(1)-C(1)-C(7)	107.66(3)
C(7)-H(7A)	0.9900	N(1)-C(1)-C(2)	111.80(3)
C(7)-H(7AB)	0.9900	C(7)-C(1)-C(2)	111.51(3)
C(8)-C(10)	1.5328(7)	N(1)-C(1)-C(6)	108.00(3)
C(8)-C(9)	1.5329(7)	C(7)-C(1)-C(6)	110.10(3)
C(8)-H(8)	1.0000	C(2)-C(1)-C(6)	107.71(3)
C(9)-H(9A)	0.9900	N(2)-C(2)-C(11)	107.12(3)
C(9)-H(9AB)	0.9900	N(2)-C(2)-C(1)	112.59(3)
C(10)-H(10A)	0.9900	C(11)-C(2)-C(1)	111.04(3)
C(10)-H(10B)	0.9900	N(2)-C(2)-C(3)	108.04(3)
C(11)-C(12)	1.5349(6)	C(11)-C(2)-C(3)	110.59(3)
C(11)-H(11A)	0.9900	C(1)-C(2)-C(3)	107.45(3)
C(11)-H(11B)	0.9900	C(9)-C(3)-C(4)	109.58(4)
C(12)-C(13)	1.5334(7)	C(9)-C(3)-C(2)	111.79(3)
C(12)-C(14)	1.5343(6)	C(4)-C(3)-C(2)	108.38(3)
C(12)-H(12)	1.0000	C(9)-C(3)-H(3)	109.0
C(13)-H(13A)	0.9900	C(4)-C(3)-H(3)	109.0
C(13)-H(13B)	0.9900	C(2)-C(3)-H(3)	109.0
C(14)-H(14A)	0.9900	C(13)-C(4)-C(3)	110.82(4)
C(14)-H(14B)	0.9900	C(13)-C(4)-C(5)	110.92(4)
C(15)-H(15A)	0.9800	C(3)-C(4)-C(5)	108.39(3)
C(15)-H(15B)	0.9800	C(13)-C(4)-H(4)	108.9
C(15)-H(15C)	0.9800	C(3)-C(4)-H(4)	108.9
		C(5)-C(4)-H(4)	108.9
C(15)-O(1)-H(1)	108.1(9)	C(10)-C(5)-C(6)	110.42(4)
C(1)-N(1)-H(1A)	113.1(6)	C(10)-C(5)-C(4)	111.10(4)

C(6)-C(5)-C(4)	108.18(3)
C(10)-C(5)-H(5)	109.0
C(6)-C(5)-H(5)	109.0
C(4)-C(5)-H(5)	109.0
C(14)-C(6)-C(5)	109.20(3)
C(14)-C(6)-C(1)	112.21(3)
C(5)-C(6)-C(1)	108.58(3)
C(14)-C(6)-H(6)	108.9
C(5)-C(6)-H(6)	108.9
C(1)-C(6)-H(6)	108.9
C(1)-C(7)-C(8)	110.05(3)
C(1)-C(7)-H(7A)	109.7
C(8)-C(7)-H(7A)	109.7
C(1)-C(7)-H(7AB)	109.7
C(8)-C(7)-H(7AB)	109.7
H(7A)-C(7)-H(7AB)	108.2
C(7)-C(8)-C(10)	109.47(4)
C(7)-C(8)-C(9)	109.11(4)
C(10)-C(8)-C(9)	109.15(4)
C(7)-C(8)-H(8)	109.7
C(10)-C(8)-H(8)	109.7
C(9)-C(8)-H(8)	109.7
C(8)-C(9)-C(3)	109.93(3)
C(8)-C(9)-H(9A)	109.7
C(3)-C(9)-H(9A)	109.7
C(8)-C(9)-H(9AB)	109.7
C(3)-C(9)-H(9AB)	109.7
H(9A)-C(9)-H(9AB)	108.2
C(5)-C(10)-C(8)	109.37(4)
C(5)-C(10)-H(10A)	109.8
C(8)-C(10)-H(10A)	109.8
C(5)-C(10)-H(10B)	109.8
C(8)-C(10)-H(10B)	109.8
H(10A)-C(10)-H(10B)	108.2
C(12)-C(11)-C(2)	110.00(3)
C(12)-C(11)-H(11A)	109.7
C(2)-C(11)-H(11A)	109.7
C(12)-C(11)-H(11B)	109.7
C(2)-C(11)-H(11B)	109.7
H(11A)-C(11)-H(11B)	108.2
C(13)-C(12)-C(14)	109.05(4)
C(13)-C(12)-C(11)	108.98(4)
C(14)-C(12)-C(11)	109.86(3)
C(13)-C(12)-H(12)	109.6
C(14)-C(12)-H(12)	109.6
C(11)-C(12)-H(12)	109.6
C(12)-C(13)-C(4)	109.22(3)
C(12)-C(13)-H(13A)	109.8
C(4)-C(13)-H(13A)	109.8
C(12)-C(13)-H(13B)	109.8
C(4)-C(13)-H(13B)	109.8
H(13A)-C(13)-H(13B)	108.3
C(6)-C(14)-C(12)	109.68(3)
C(6)-C(14)-H(14A)	109.7
C(12)-C(14)-H(14A)	109.7
C(6)-C(14)-H(14B)	109.7
C(12)-C(14)-H(14B)	109.7
H(14A)-C(14)-H(14B)	108.2
O(1)-C(15)-H(15A)	109.5
O(1)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
O(1)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5

Table S4 Anisotropic displacement parameters *(Å^2 × 10^3)* for (*S*,*S*)-1,2-diaminodiamantane. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cl(1)	9(1)	12(1)	16(1)	4(1)	-1(1)	0(1)
Cl(2)	16(1)	10(1)	12(1)	1(1)	3(1)	-2(1)
O(1)	17(1)	30(1)	13(1)	-6(1)	-3(1)	7(1)
N(1)	9(1)	11(1)	10(1)	2(1)	-2(1)	0(1)
N(2)	8(1)	10(1)	9(1)	0(1)	1(1)	-1(1)
C(1)	7(1)	8(1)	8(1)	1(1)	-1(1)	-1(1)
C(2)	7(1)	8(1)	8(1)	1(1)	1(1)	0(1)
C(3)	9(1)	13(1)	8(1)	2(1)	-1(1)	0(1)
C(4)	8(1)	15(1)	12(1)	2(1)	-1(1)	1(1)
C(5)	7(1)	14(1)	12(1)	0(1)	-1(1)	-2(1)
C(6)	8(1)	10(1)	9(1)	1(1)	1(1)	-2(1)
C(7)	11(1)	9(1)	12(1)	-2(1)	0(1)	0(1)
C(8)	12(1)	14(1)	12(1)	-4(1)	-1(1)	-3(1)
C(9)	12(1)	18(1)	8(1)	-1(1)	-1(1)	-2(1)
C(10)	11(1)	16(1)	15(1)	-3(1)	-1(1)	-5(1)
C(11)	10(1)	8(1)	12(1)	-1(1)	2(1)	0(1)
C(12)	10(1)	11(1)	14(1)	-1(1)	3(1)	1(1)
C(13)	10(1)	14(1)	18(1)	2(1)	2(1)	4(1)
C(14)	10(1)	14(1)	10(1)	-1(1)	3(1)	-1(1)
C(15)	17(1)	16(1)	14(1)	-1(1)	1(1)	1(1)

Table S5 Hydrogen coordinates *(× 10^4)* and isotropic displacement parameters *(Å^2 × 10^3)* for (*S*,*S*)-1,2-diaminodiamantane.

Atom	x	y	z	U(eq)
H(1)	9565(13)	5290(18)	7410(14)	30
H(1A)	8656(11)	4632(13)	5174(10)	12
H(1B)	8687(11)	2931(13)	4710(10)	12
H(1C)	9617(10)	3992(14)	4135(10)	12
H(2A)	9402(11)	6877(13)	1565(10)	11
H(2B)	10004(10)	5961(14)	2592(10)	11

H(2C)	9530(10)	5305(13)	1295(10)	11
H(3)	6978	6818	769	12
H(4)	4720	5836	1100	14
H(5)	4309	4137	3003	13
H(6)	6210	3089	4339	11
H(7A)	7850	1727	2761	13
H(7AB)	8874	2767	1884	13
H(8)	6975	1911	443	15
H(9A)	6320	4464	-453	15
H(9AB)	7941	4431	-91	15
H(10A)	4715	2813	906	17
H(10B)	5306	1759	2167	17
H(11A)	8429	7099	4249	12
H(11B)	7855	8166	2991	12
H(12)	6158	7987	4682	14
H(13A)	5341	8191	2340	17
H(13B)	4286	7157	3190	17
H(14A)	6757	5439	5597	14
H(14B)	5155	5449	5145	14
H(15A)	7883	7735	7005	24
H(15B)	8685	7231	8402	24
H(15C)	7384	6224	7846	24

Table S6 Hydrogen bonds for (*S*,*S*)-1,2-diaminodiamantane *(Å and °)*.

D-H...A	**d(D-H)**	**d(H...A)**	**d(D...A)**	**<(DHA)**
O(1)-H(1)...Cl(2)#1	0.864(13)	2.303(13)	3.1438(4)	164.5(13)
N(1)-H(1A)...O(1)	0.963(10)	1.937(10)	2.8517(6)	157.8(9)
N(1)-H(1B)...Cl(1)	0.908(11)	2.228(11)	3.1258(4)	169.8(9)
N(1)-H(1C)...Cl(1)#2	0.835(10)	2.480(10)	3.1864(4)	143.0(10)
N(2)-H(2A)...Cl(2)	0.858(10)	2.262(10)	3.1172(4)	173.8(10)
N(2)-H(2B)...Cl(1)#2	0.893(10)	2.265(10)	3.1527(4)	172.7(10)
N(2)-H(2C)...Cl(2)#3	0.847(10)	2.389(10)	3.1840(4)	156.5(9)

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,y-1/2,-z+1 #2 -x+2,y+1/2,-z+1 #3 -x+2,y-1/2,-z

Crystallographic data for (*S*,*S*)-1

The unit cell of (*S*,*S*)-**1** was determined using 9150 reflections and the structure was solved in the hexagonal space group *P*622. The asymmetric unit contains besides heavily disordered solvent molecules one molecule of (*S*,*S*)-**1**. The structure was modelled with the help similarity restrains on all anisotropic atomic displacement parameters[2]. The SQUEEZE[3] method as implemented in Platon[4] was used to include a model for the disordered solvent molecules. The obtained model was added as fab-file to the refinement using SHELXL. SQUEEZE found one independent void with disordered solvent, located at 0.0 0.0 0.0, with a volume of 2349 Å^3. The equivalent of 722 electrons were identified in the void.

Table S7 Crystal data and structure refinement for (*S*,*S*)-**1**

CCDC No	1956840	
Empirical formula	C_{14} H_{22} Cl_2 N_2 Pt	
Formula weight	484.32	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Hexagonal	
Space group	*P*622	
Unit cell dimensions	a = 24.8348(11) Å	α= 90°.
	b = 24.8348(11) Å	β= 90°.
	c = 12.1765(5) Å	γ = 120°.
Volume	6503.9(6) Å^3	
Z	12	
Density (calculated)	1.484 Mg/m^3	
Absorption coefficient	6.710 mm^{-1}	
F(000)	2784	
Crystal size	0.422 x 0.418 x 0.416 mm^3	
Theta range for data collection	2.343 to 27.874°.	
Index ranges	-32<=h<=32, -32<=k<=32, -16<=l<=16	
Reflections collected	580785	
Independent reflections	5199 [R(int) = 0.1440]	
Completeness to theta = 25.242°	99.7 %	
Absorption correction	Numerical	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5199 / 125 / 184	
Goodness-of-fit on F^2	1.047	
Final R indices [I>2sigma(I)]	R1 = 0.0271, wR2 = 0.0618	
R indices (all data)	R1 = 0.0323, wR2 = 0.0639	
Absolute structure parameter	0.024(10)	
Largest diff. peak and hole	1.242 and -3.050 e.Å^{-3}	

Table S8 Atomic coordinates *(× 10⁴)* and equivalent isotropic displacement parameters *(Å² × 10³)* for (*S*,*S*)-**1**. *U(eq)* is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	x	y	z	U(eq)
Pt(1)	4090(1)	4129(1)	2501(1)	20(1)
Cl(1)	3504(1)	4334(1)	3718(1)	31(1)
Cl(2)	4006(1)	4726(1)	1141(1)	25(1)
N(1)	4625(2)	3917(2)	1536(4)	23(1)
N(2)	4155(2)	3549(2)	3590(4)	27(1)
C(1)	4640(3)	3387(3)	3225(4)	23(1)
C(2)	4593(3)	3334(3)	1973(5)	25(1)
C(3)	5123(3)	3225(3)	1533(5)	31(1)
C(4)	5022(3)	2610(3)	2035(5)	33(2)
C(5)	5072(3)	2677(3)	3299(5)	28(1)
C(6)	4546(3)	2781(3)	3698(4)	25(1)
C(7)	5280(3)	3930(3)	3555(5)	31(1)
C(8)	5793(3)	3825(3)	3135(8)	46(2)
C(9)	5747(3)	3748(3)	1872(6)	42(2)
C(10)	5697(3)	3214(3)	3650(6)	39(2)
C(11)	3965(3)	2773(3)	1625(5)	31(1)
C(12)	3894(3)	2174(3)	2096(5)	33(2)
C(13)	3917(3)	2229(3)	3383(5)	31(1)
C(14)	4406(3)	2067(3)	1693(5)	40(2)

Table S9 Bond lengths *(Å)* and angles *(°)* for (*S*,*S*)-**1**.

		C(1)-C(2)	1.530(7)
Pt(1)-N(2)	2.022(5)	C(1)-C(7)	1.537(8)
Pt(1)-N(1)	2.031(4)	C(2)-C(11)	1.543(9)
Pt(1)-Cl(2)	2.3014(12)	C(2)-C(3)	1.566(8)
Pt(1)-Cl(1)	2.3057(13)	C(3)-C(9)	1.498(10)
N(1)-C(2)	1.507(8)	C(3)-C(4)	1.546(9)
N(1)-H(1A)	0.90(2)	C(3)-H(3)	1.0000
N(1)-H(1B)	0.89(3)	C(4)-C(14)	1.506(10)
N(2)-C(1)	1.514(8)	C(4)-C(5)	1.546(9)
N(2)-H(2A)	0.87(2)	C(4)-H(4)	1.0000
N(2)-H(2B)	0.89(3)	C(5)-C(10)	1.515(9)
C(1)-C(6)	1.517(8)	C(5)-C(6)	1.534(8)

C(5)-H(5)	1.0000
C(6)-C(13)	1.525(8)
C(6)-H(6)	1.0000
C(7)-C(8)	1.513(9)
C(7)-H(7A)	0.9900
C(7)-H(7AB)	0.9900
C(8)-C(10)	1.546(9)
C(8)-C(9)	1.548(10)
C(8)-H(8)	1.0000
C(9)-H(9A)	0.9900
C(9)-H(9AB)	0.9900
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-C(12)	1.519(8)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-C(14)	1.506(10)
C(12)-C(13)	1.572(9)
C(12)-H(12)	1.0000
C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
N(2)-Pt(1)-N(1)	84.25(19)
N(2)-Pt(1)-Cl(2)	174.86(14)
N(1)-Pt(1)-Cl(2)	91.88(13)
N(2)-Pt(1)-Cl(1)	91.10(14)
N(1)-Pt(1)-Cl(1)	175.20(13)
Cl(2)-Pt(1)-Cl(1)	92.83(5)
C(2)-N(1)-Pt(1)	108.5(3)
C(2)-N(1)-H(1A)	115(4)
Pt(1)-N(1)-H(1A)	114(4)
C(2)-N(1)-H(1B)	121(4)
Pt(1)-N(1)-H(1B)	102(4)
H(1A)-N(1)-H(1B)	95(5)
C(1)-N(2)-Pt(1)	110.7(3)
C(1)-N(2)-H(2A)	106(4)
Pt(1)-N(2)-H(2A)	123(4)
C(1)-N(2)-H(2B)	119(4)
Pt(1)-N(2)-H(2B)	102(4)
H(2A)-N(2)-H(2B)	97(5)
N(2)-C(1)-C(6)	113.8(5)
N(2)-C(1)-C(2)	106.2(5)
C(6)-C(1)-C(2)	109.0(5)
N(2)-C(1)-C(7)	107.6(5)
C(6)-C(1)-C(7)	110.4(5)
C(2)-C(1)-C(7)	109.7(6)
N(1)-C(2)-C(1)	107.7(5)
N(1)-C(2)-C(11)	108.4(5)
C(1)-C(2)-C(11)	110.5(6)
N(1)-C(2)-C(3)	113.5(5)
C(1)-C(2)-C(3)	108.8(6)
C(11)-C(2)-C(3)	107.9(5)
C(9)-C(3)-C(4)	109.5(5)
C(9)-C(3)-C(2)	110.6(5)
C(4)-C(3)-C(2)	107.5(5)
C(9)-C(3)-H(3)	109.7
C(4)-C(3)-H(3)	109.7
C(2)-C(3)-H(3)	109.7
C(14)-C(4)-C(3)	111.5(6)
C(14)-C(4)-C(5)	111.3(6)
C(3)-C(4)-C(5)	108.8(6)
C(14)-C(4)-H(4)	108.4
C(3)-C(4)-H(4)	108.4
C(5)-C(4)-H(4)	108.4
C(10)-C(5)-C(6)	110.3(5)
C(10)-C(5)-C(4)	111.6(6)
C(6)-C(5)-C(4)	107.7(5)
C(10)-C(5)-H(5)	109.1
C(6)-C(5)-H(5)	109.1
C(4)-C(5)-H(5)	109.1
C(1)-C(6)-C(13)	112.2(5)
C(1)-C(6)-C(5)	109.0(5)

C(13)-C(6)-C(5)	110.1(5)	H(10A)-C(10)-H(10B)	108.2
C(1)-C(6)-H(6)	108.5	C(12)-C(11)-C(2)	110.5(5)
C(13)-C(6)-H(6)	108.5	C(12)-C(11)-H(11A)	109.5
C(5)-C(6)-H(6)	108.5	C(2)-C(11)-H(11A)	109.5
C(8)-C(7)-C(1)	110.6(5)	C(12)-C(11)-H(11B)	109.5
C(8)-C(7)-H(7A)	109.5	C(2)-C(11)-H(11B)	109.5
C(1)-C(7)-H(7A)	109.5	H(11A)-C(11)-H(11B)	108.1
C(8)-C(7)-H(7AB)	109.5	C(14)-C(12)-C(11)	110.8(6)
C(1)-C(7)-H(7AB)	109.5	C(14)-C(12)-C(13)	110.0(5)
H(7A)-C(7)-H(7AB)	108.1	C(11)-C(12)-C(13)	108.1(5)
C(7)-C(8)-C(10)	107.6(6)	C(14)-C(12)-H(12)	109.3
C(7)-C(8)-C(9)	110.0(6)	C(11)-C(12)-H(12)	109.3
C(10)-C(8)-C(9)	108.4(7)	C(13)-C(12)-H(12)	109.3
C(7)-C(8)-H(8)	110.3	C(6)-C(13)-C(12)	107.8(5)
C(10)-C(8)-H(8)	110.3	C(6)-C(13)-H(13A)	110.1
C(9)-C(8)-H(8)	110.3	C(12)-C(13)-H(13A)	110.1
C(3)-C(9)-C(8)	111.2(6)	C(6)-C(13)-H(13B)	110.1
C(3)-C(9)-H(9A)	109.4	C(12)-C(13)-H(13B)	110.1
C(8)-C(9)-H(9A)	109.4	H(13A)-C(13)-H(13B)	108.5
C(3)-C(9)-H(9AB)	109.4	C(12)-C(14)-C(4)	108.7(5)
C(8)-C(9)-H(9AB)	109.4	C(12)-C(14)-H(14A)	109.9
H(9A)-C(9)-H(9AB)	108.0	C(4)-C(14)-H(14A)	109.9
C(5)-C(10)-C(8)	109.7(5)	C(12)-C(14)-H(14B)	109.9
C(5)-C(10)-H(10A)	109.7	C(4)-C(14)-H(14B)	109.9
C(8)-C(10)-H(10A)	109.7	H(14A)-C(14)-H(14B)	108.3
C(5)-C(10)-H(10B)	109.7		
C(8)-C(10)-H(10B)	109.7		

Table S10 Anisotropic displacement parameters *(Å^2 × 10^3)* for (*S*,*S*)-**1**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Pt(1)	25(1)	27(1)	14(1)	0(1)	-1(1)	17(1)
Cl(1)	42(1)	50(1)	16(1)	3(1)	4(1)	35(1)
Cl(2)	36(1)	31(1)	17(1)	3(1)	1(1)	23(1)
N(1)	30(3)	31(3)	15(2)	5(2)	7(2)	19(2)
N(2)	35(3)	38(3)	15(2)	0(2)	-1(2)	23(2)

C(1)	33(3)	29(3)	13(2)	0(2)	-2(2)	20(3)
C(2)	30(3)	33(3)	20(3)	4(2)	3(2)	22(3)
C(3)	42(3)	39(3)	25(3)	6(3)	11(3)	30(3)
C(4)	49(4)	36(4)	28(3)	7(3)	13(3)	33(3)
C(5)	34(3)	28(3)	29(3)	5(3)	2(3)	21(3)
C(6)	31(3)	28(3)	17(3)	4(2)	1(2)	16(2)
C(7)	33(3)	26(3)	37(3)	-2(2)	-13(3)	17(3)
C(8)	17(3)	28(4)	91(6)	8(4)	-4(3)	11(3)
C(9)	43(4)	49(4)	56(5)	32(4)	21(3)	39(4)
C(10)	33(3)	35(3)	56(4)	8(3)	-6(3)	22(3)
C(11)	47(4)	29(3)	19(3)	-2(2)	-7(3)	21(3)
C(12)	42(3)	22(3)	26(3)	-6(2)	-19(3)	10(2)
C(13)	37(3)	28(3)	27(3)	4(3)	0(3)	16(3)
C(14)	71(5)	30(3)	28(3)	-2(3)	0(3)	32(3)

Table S11 Hydrogen coordinates *(× 10^4)* and isotropic displacement parameters *(Å^2 × 10^3)* for (*S*,*S*)-**1**.

Atom	x	y	z	U(eq)
H(1A)	4550(30)	3910(30)	820(20)	28
H(1B)	4983(18)	4273(18)	1520(50)	28
H(2A)	4220(30)	3630(30)	4290(20)	33
H(2B)	3762(15)	3250(20)	3640(50)	33
H(3)	5100	3192	714	38
H(4)	5360	2536	1766	39
H(5)	5017	2283	3626	34
H(6)	4568	2817	4517	30
H(7A)	5333	4323	3248	37
H(7AB)	5306	3969	4365	37
H(8)	6209	4180	3348	55
H(9A)	5818	4139	1528	51
H(9AB)	6075	3664	1607	51
H(10A)	6033	3137	3408	47
H(10B)	5713	3249	4460	47
H(11A)	3621	2831	1890	37
H(11B)	3942	2745	814	37
H(12)	3483	1817	1868	40

H(13A)	3577	2292	3651	37
H(13B)	3867	1843	3717	37
H(14A)	4387	2026	883	47
H(14B)	4356	1677	2011	47

Table S12 Hydrogen bonds for (*S*,*S*)-**1** *(Å and °)*.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1A)...Cl(2)#1	0.90(2)	2.41(3)	3.268(5)	159(5)
N(1)-H(1B)...Cl(2)#2	0.89(3)	2.54(3)	3.418(5)	171(5)
N(2)-H(2A)...Cl(1)#3	0.87(2)	2.48(3)	3.318(5)	160(6)

Symmetry transformations used to generate equivalent atoms:

#1 y,x,-z #2 -x+1,-y+1,z #3 y,x,-z+1

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