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Supplementary Material

Intramolecular C(sp^2)-C (sp^2) bond formation between phenanthroline and ß-Diketone Thiosemicarbazones in Pt^{II} complexes: Crystal Structures and Computational Studies

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Contents

1.1 Materials and instruments

Benzoylacetone, 4-phenyl-3-thiosemicarbazide, 4-ethyl-3-thiosemicarbazide, triethylamine, phenanthroline and potassium tetrachloroplatinate(II) (Sigma-Aldrich) and solvents were reagent grade and used without further purification. [$PtCl_2$(phen)] and H_2L^R have been prepared as previously reported.[1, 2] The melting points were determined using a PF1500 FARMA-GEHAKA instrument. Elemental analyses (CHNS) were determined using a Perkin Elmer CHNS/O 2400 Series II equipment. FTIR spectra were measured as KBr pellets on a Shimadzu IR Prestige-21 spectrophotometer between 400 and 4000 cm^{-1}, with resolution of 4 cm^{-1}, on Bruker Alpha IR (PLATINUM-ATR). The ^{1}H NMR spectra were acquired using an Agilent 400/54 Premium Shielded 9.4 T spectrometer, operating at 399.8 MHz. The ^{1}H NMR spectra were internally referenced to TMS. The ^{195}Pt NMR spectra were acquired using a Bruker Avance III 600 MHz equipped with BBO probe with Z gradients spectrometer, operating at 128.98 MHz. The ^{195}Pt NMR spectra were internally referenced with K_2PtCl_4. Electrospray ionization mass spectrometry (ESI-MS) spectra were recorded on an Agilent 6130B single quadrupole detector instrument at 298 K with a scan range of m/z 50−2000 for positive ions. Samples were prepared in methanol or acetonitrile solutions. All chromatograms were obtained using an Agilent 1100 system with a DAD and a 100 µL loop. The HPLC column was an Agilent ZORBAX Eclipse Plus C18 250 × 4.6 mm column with a pore size of 5 µm. Mobile phases consisted of doubly deionized water 0.1% TFA and HPLC grade acetonitrile 0.1% TFA. Unfiltered volumes of <200 µ L were injected and analyzed at a detection wavelength of 254 nm. HPLC chromatograms were analyzed and integrated using DataAnalysis software. The following solvent gradient and 1 mL min – 1 flow rate was used: time (min)/% (B): 0 (min)/10%, 30 (min)/80%, 40 (min)/80%, 41 (min)/10%, 55 (min)/10%.

1.2 Synthesis of the complexes

1.2.1 Complexes of the type [Pt(phenL^R)] (R = Et or Ph). H_2L^R (0.1 mmol) was added to a suspension of [$PtCl_2$(phen)] (0.1 mmol) in MeCN (5 mL). After 10 min of stirring, approximately 0.3 mL of Et_3N were added. The mixtures were then kept under reflux for 8 hours. The dark red mixtures were kept in a refrigerator for 1 day in order to precipitate red solids which were filtered off, washed with a small

portion of *n*-hexane and dried under vacuum. Recrystallization from MeOH/CH_2Cl_2 (1:2) afforded single-crystals suitable for X-ray diffraction.

[Pt(phenL^{Et})]: Yield (27 mg, 43 %). mp: 250–252 ºC (from MeOH). Anal. calcd. for $C_{25}H_{21}N_5OPtS$: C, 47.3; H, 3.3; N, 11.0; S, 5.1%. Found: C, 46.5; H, 3.4; N, 10.7; S, 5.1 %. IR (Selected bands, ν_{max}/cm^{-1}): 3428 (NH), 1637 (C=O), 1564 (C=N), 1541 (C=C + C–C), 827 (CS). UV-Vis bands (λ_{max}) from CH_2Cl_2 solution [nm (log ε)]: 268 (3.74), 509 (3.02). ^{1}H NMR (400 MHz; $CDCl_3$; Me_4Si): 1.31 (t, J = 8 Hz, 3H, $–CH_2CH_3$), 2.46 (s, 3H, CH_3), 3.51 (q, J = 8 Hz, 2H, $–CH_2CH_3$), 4.67 (s, 1H, NH), 7.40-9.55 (m, 12H, Arom.). ^{1}H NMR (400 MHz; CD_2Cl_2): 1.29 (t, *J* = 8 Hz, 3H, $–CH_2CH_3$), 2.38 (s, 3H, CH_3), 3.47 (q, *J* = 8 Hz, 2H, $–CH_2CH_3$), 4.66 (s, 1H, NH), 7.39-9.26 (m, 12H, Arom.). ESI$^+$ MS (m/z, assignment): 634.1114 ([M+H]$^+$, 100%), calcd: 634.1109. HPLC (retention time): 26.8 min.

[Pt(phenL^{Ph})]: Yield (41 mg, 61 %). mp: 185–187 ºC (from MeOH). Anal. calcd for $C_{29}H_{21}N_5OPtS$: C, 51.0; H, 3.1; N, 10.3; S, 4.7 %. Found: C, 49.9; H, 3.4; N, 10.2; S, 4.8 %. IR (Selected bands, ν_{max}/cm^{-1}): 3384 (NH), 1655 (C=O), 1599 (C=N), 1551, 1556 (C=C + C–C), 820 (CS). UV-Vis bands (λ_{max}) from CH_2Cl_2 solution [nm (log ε)]: 250 (3.48), 506 (2.76). ^{1}H NMR (400 MHz, $CDCl_3$; Me_4Si): 2.50 (s, 3H, CH_3), 5.74 (s, 1H, NH), 6.60-8.37 (m, 17H, Ph). ESI+ MS (m/z, assignment): 682.1111 ([M+H]$^+$, 100%), calcd: 682.1109.

1.2.2 Synthesis of the intermediate ***I1^{Et}.*** The intermediate I1^{Et} was prepared by a similar procedure to that of the complex [Pt(phenL^{Et})] (**1**). H_2L^{Et} (0.1 mmol) was added to a suspension of [$PtCl_2$(phen)] (0.1 mmol) in HPLC grade MeCN (3 mL). After 10 min of stirring, 0.1 mL of Et_3N was added. The mixture was then kept under reflux for 2 hours. After cooling to room temperature, the yellow precipitate formed was filtered off washed with a small portion of *n*-hexane and dried under vacuum.

[Pt(phen)(HL^{Et})] (**I1^{Et}**): Color: yellow. Yield (35 mg, 55.0%). Anal. calcd for $C_{25}H_{24}N_5OPtS$: C, 47.1; H, 3.8; N, 11.0; S, 5.0. Found: C, 46.7; H, 3.5; N, 10.6; S, 5.2 %. IR (Selected bands, ν_{max}/cm^{-1}): 3329 (NH), 1585 (C=N), 1543, 1502 (C=C + C–C), 820 (CS). UV-Vis bands (λ_{max}) from CH_2Cl_2 solution [nm (log ε)]: 270 nm (3.37), 402 nm (2.89). ^{1}H NMR (400 MHz; CD_2Cl_2): 1.20 (t, *J* = 8 Hz, 3H,

–CH_2CH_3), 2.34 (s, 3H, CH_3), 3.36 (q, J = 8 Hz, 2H, –CH_2CH_3), 4.52 (s, 1H, NH), 5.64 (s, 1H, CH), 7.04 (t, *J* = 7.6 Hz, 2H, Ph), 7.12-7.17 (m, 3H, Ph), 7.64 (d, *J* = 4.6 Hz, 1H, Phen), 7.66 (d, *J* = 4.6 Hz, 1H, Phen), 7.92 (s, 2H, Phen), 8.38 (d, J = 6.0 Hz, 2H, Phen), 9.53 (s, 1H, Phen). ESI^+ MS (m/z, assignment): 637.1345 ($[M+H]^+$, 100%), calcd: 637.1349. HPLC (retention time): 21.5 min

1.3 X-ray Crystallography

The data collection was performed at room temperature (296 K) using Mo-Kα radiation (λ = 0.71073 Å) on a BRUKER APEX II Duo diffractometer. Standard procedures were applied for data reduction and absorption correction. The structure was solved with SHELXS97 using direct methods and refined by full-matrix least-square methods against F^2 (SHELXL2014).[3] All non-hydrogen atoms were refined with anisotropic displacement parameters with SHELXL2014.[3] The hydrogen atoms were calculated at idealized positions using the riding model option of SHELXL2014.[3] More details on data collections and structure refinement are reported in Table S1. Selected bond lengths and angles are given in Tables S2.

Table S1 - X-ray Structure Data Collection and Refinement Parameters for **1** and **2**.

	1	**2**
Formula	$C_{25}H_{21}N_5OPtS$	$C_{29}H_{21}N_5OPtS$
Fw	634.62	682.66
Crystalline system	Monoclinic	Triclinic
Space Group	$P2_1/c$	$P\bar{1}$
a (Å)	7.3572(3)	12.7380(4)
b (Å)	12.3495(5)	14.3284(5)
c (Å)	24.1793(9)	14.5859(5)
α (°)	90	69.471(2)
β (°)	92.552(2)	85.039(2)
γ (°)	90	77.604(2)
V (Å^3)	2194.70(15)	2434.79(15)
Z	4	4
μ (mm^{-1})	6.518	5.883
Crystal size	0.430 x 0.190 x 0.100	0.260 x 0.100 x 0.070
θ range for data collection (°)	2.359 to 25.112	1.491 to 25.038
Index range	-8<=h<=8, -14<=k<=14, -28<=l<=28	-15<=h<=15, -17<=k<=17, -17<=l<=17
reflections collected	13553	28508
reflections unique / R_{int}	3890 / 0.0355	8551 / 0.0321
data/restraints/param.	3890 / 0 / 300	8551 / 1 / 663
absorption correction	Multi-scan	Multi-scan
max/min transmission	0.5618 and 0.1660	0.7452 / 0.6661
Final R indices [I>2sigma(I)]	R_1 = 0.0293, wR_2 = 0.0768	R_1 = 0.0296, wR_2 = 0.0553
R indices (all data)	R_1 = 0.0474, wR_2 = 0.0899	R_1 = 0.0489, wR_2 = 0.0614
GOF on F^2, S	1.019	1.023
Largest diff. peak and hole (e.Å^{-3})	1.141 and -0.799	0.745 and -0.412
Deposit number	CCDC-1979092	CCDC-1979093

Table S2 – Selected bond lengths (Å) and angles (°) in **1** and **2**.

	1	**2***	
Bond lengths (Å)			
Pt-S(1)	2.2593(14)	2.2572(15)	2.2536(15)
Pt-N(1)	1.954(4)	1.964(3)	1.968(3)
Pt-N(4)	1.997(4)	1.989(4)	1.988(4)
Pt-N(5)	2.027(5)	2.016(4)	2.024(4)
S(1)-C(1)	1.752(5)	1.740(5)	1.743(5)
O(1)-C(5)	1.219(5)	1.222(6)	1.201(6)
N(1)-C(2)	1.333(7)	1.334(6)	1.349(6)
Bond Angles (º)			
N(4)-Pt-S(1)	179.42(11)	178.89(11)	178.59(12)
N(1)-Pt-N(5)	175.14(15)	175.85(18)	175.90(17)
N(1)-Pt-N(4)	93.62(17)	94.35(15)	94.25(16)
S(1)-Pt-N(5)	98.98(12)	98.97(14)	98.78(13)
S(1)-Pt-N(1)	85.83(13)	85.17(12)	85.24(13)
N(5)-Pt-N(4)	81.56(17)	81.51(17)	81.75(16)
C(1)-S(1)-Pt	94.51(18)	95.18(19)	95.15(19)
C(4)-C(5)-O(1)	120.7(5)	120.6(5)	120.8(5)

* *Values for two crystallographically independent molecules.*

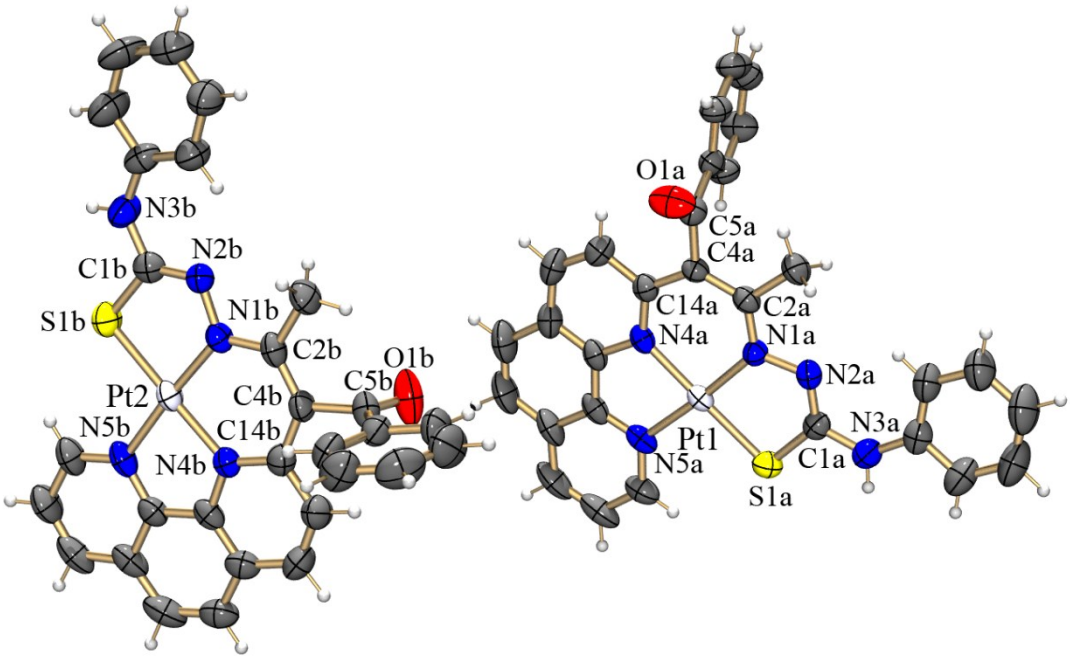


Figure S1. ORTEP view of [Pt(phenL^{Ph})] (**2**) with the thermal ellipsoids at the 50% probability level, including the atoms numbering scheme.

1.4 DFT Calculations

Geometry optimization and analysis of the vibrational frequencies were performed for all structures, apart from the structure of the transition state, which was only done the analysis of the vibrational frequencies. The calculations were done using the Density Functional Theory hybrid functional m06 combined with TZP (Triple zeta valence quality plus polarization) atomic basis set.[4-6] In all calculations the compounds were considered solvated in acetonitrile, using the Polarizable Continuum Model IEFPCM[7] (see the parameters at the end of this document).

The "Transition State Search" was performed (software Gaussian 16, Revision A.03) using the *Synchronous Transit-guided Quasi-Newton* method[8,9] through the keyword QST3.

The vibrational spectra calculated for these compounds, did not present imaginary frequencies (except in the case of the transition state that presented only one of such frequencies) indicating that the stationary point found in the optimizations corresponds to the global minima of energy, apart from the structure of the transition state, for not being a global minimum structure. From the analysis of the vibrational frequencies, it was possible to estimate the thermal correction to Gibbs free energy (G_T) of all species (**Table S3**), including the transition state.

In order to test the reliability of the transition state, a scan analysis was done from this state until the formation of the product, considering the relaxation of the resulting structures in each stage.

Except the "Transition State Search" all calculations were performed using the software Gaussian G09 revision E.01.[10]

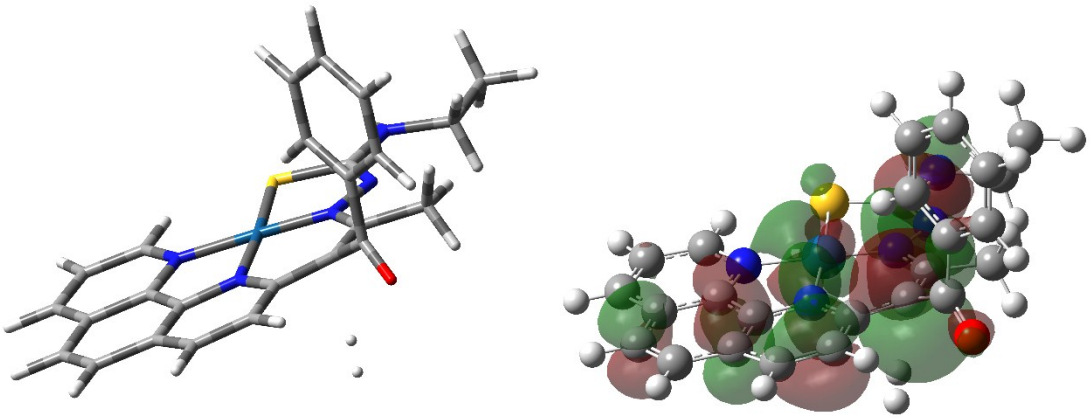


Figure S2. Structure (left) and HOMO (right) of TS^{Et}. The HOMO diagram (right picture) shows a nodal plane between the hydrogen molecule and the complex molecule.

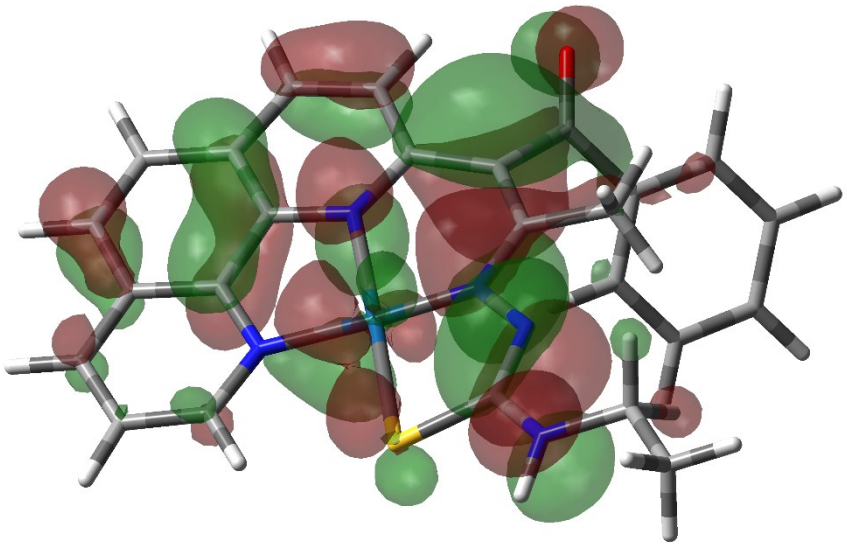
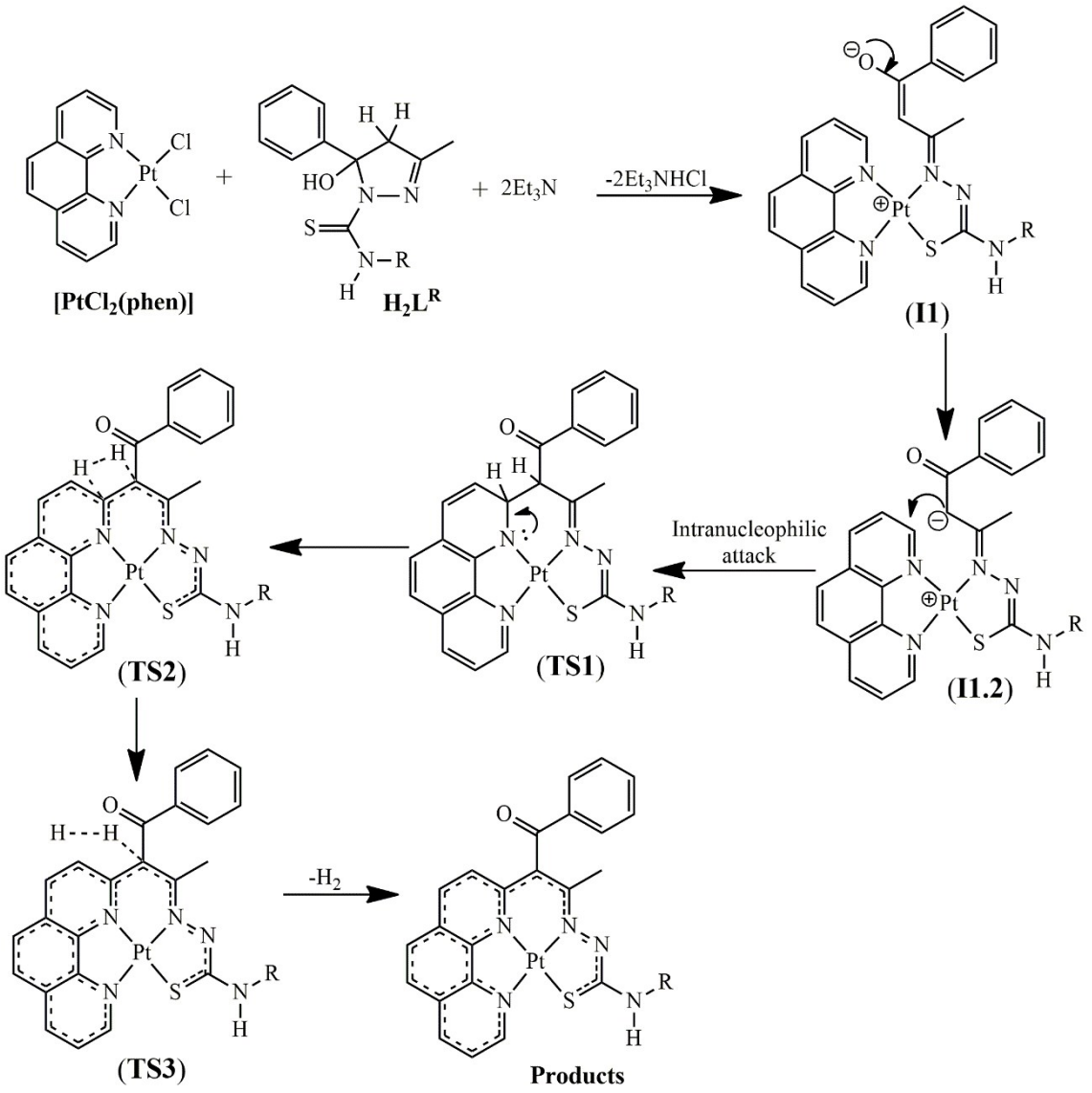


Figure S3. HOMO of the complex **1** showing a high distribution of π electron density.



Scheme S1. Proposed reaction pathway for the formation of the [Pt(phenL^{R})] complexes.

FTIR DATA

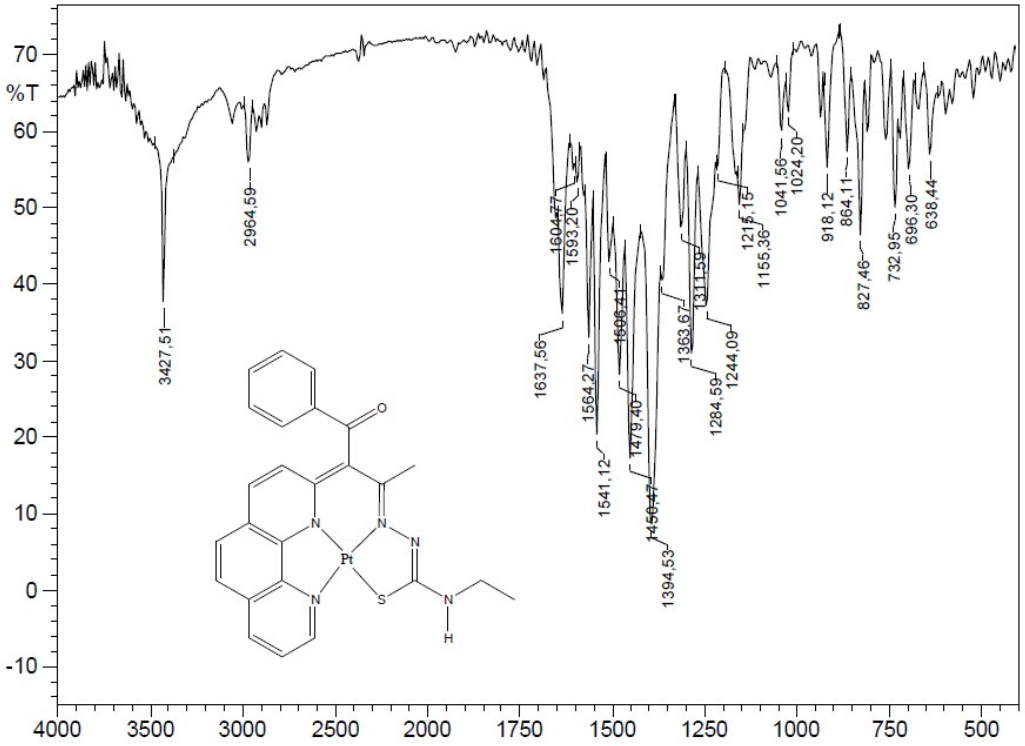


Figure S4. FTIR spectrum of the complex **1** from KBr pellets (cm^{-1}).

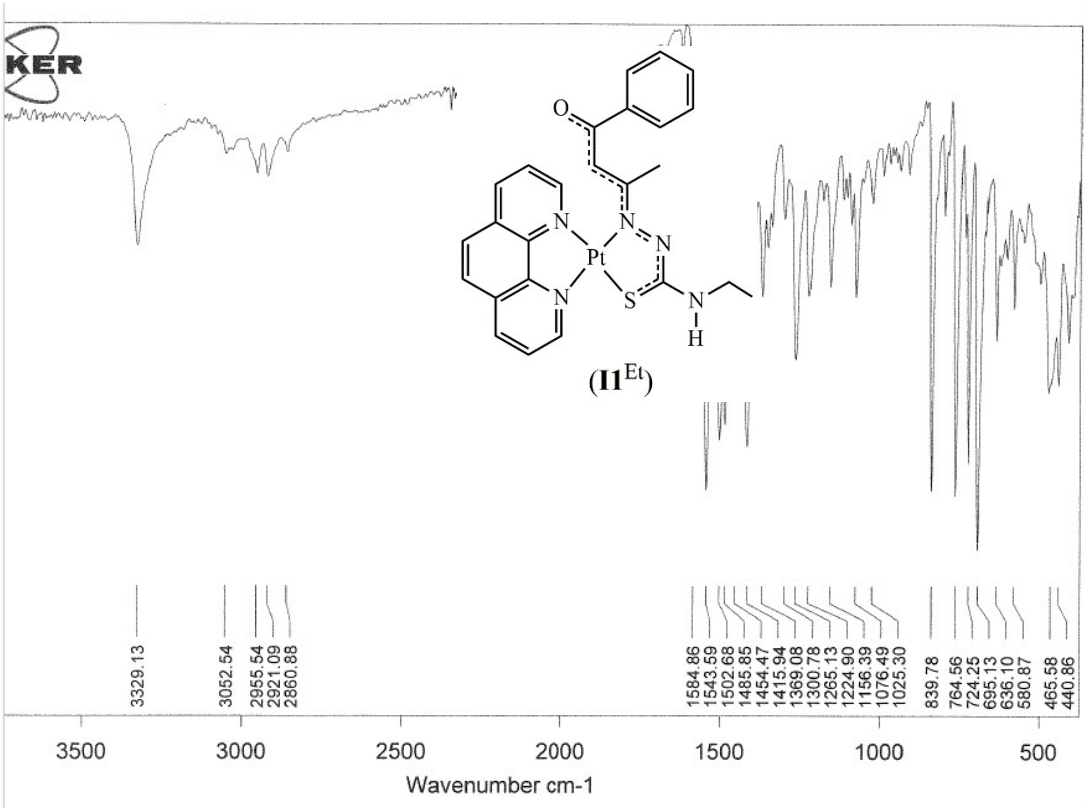


Figure S5. FTIR spectrum of the intermediate **I1^{Et}**.

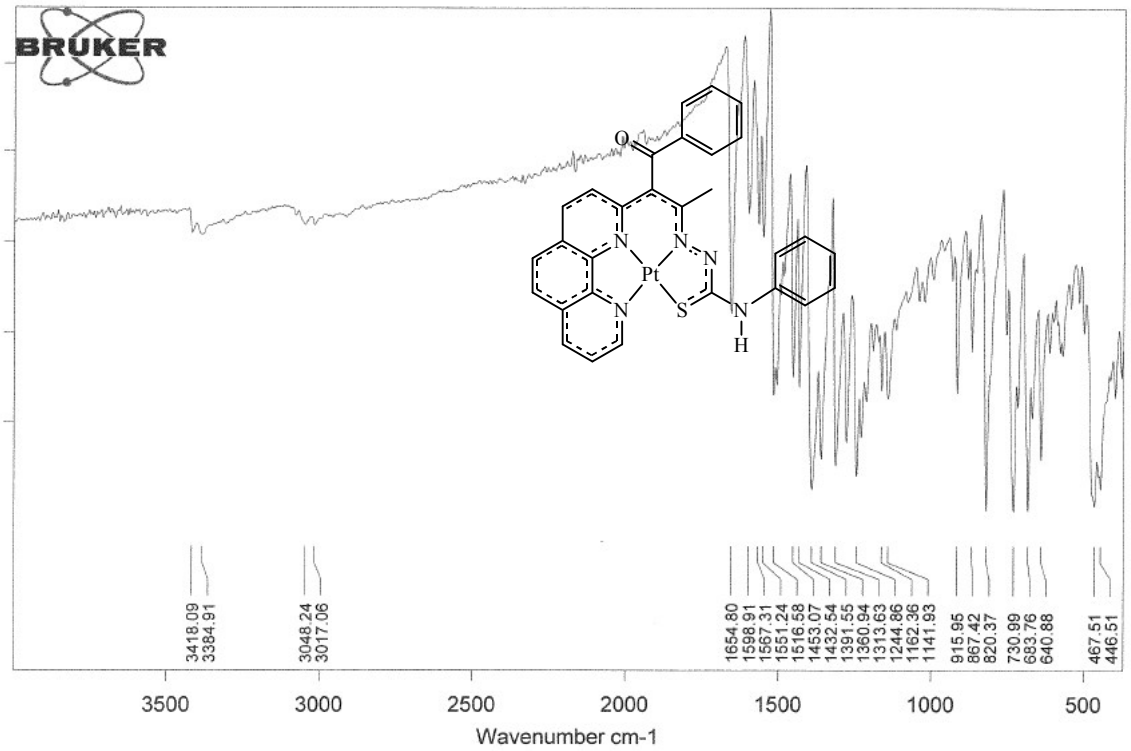


Figure S6. FTIR spectrum of the complex **2.**

NMR DATA

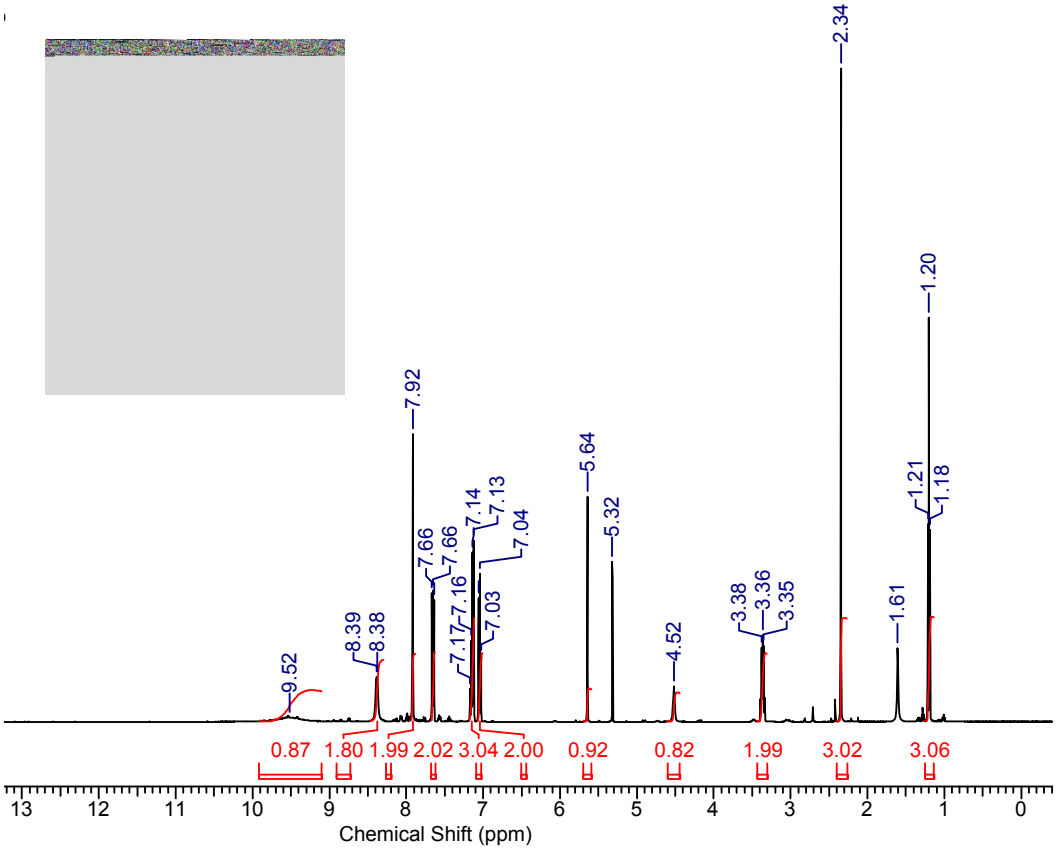


Figure S7. ^{1}H NMR spectrum from a fresh CD_2Cl_2 solution of the intermediate **I1^{Et}**.

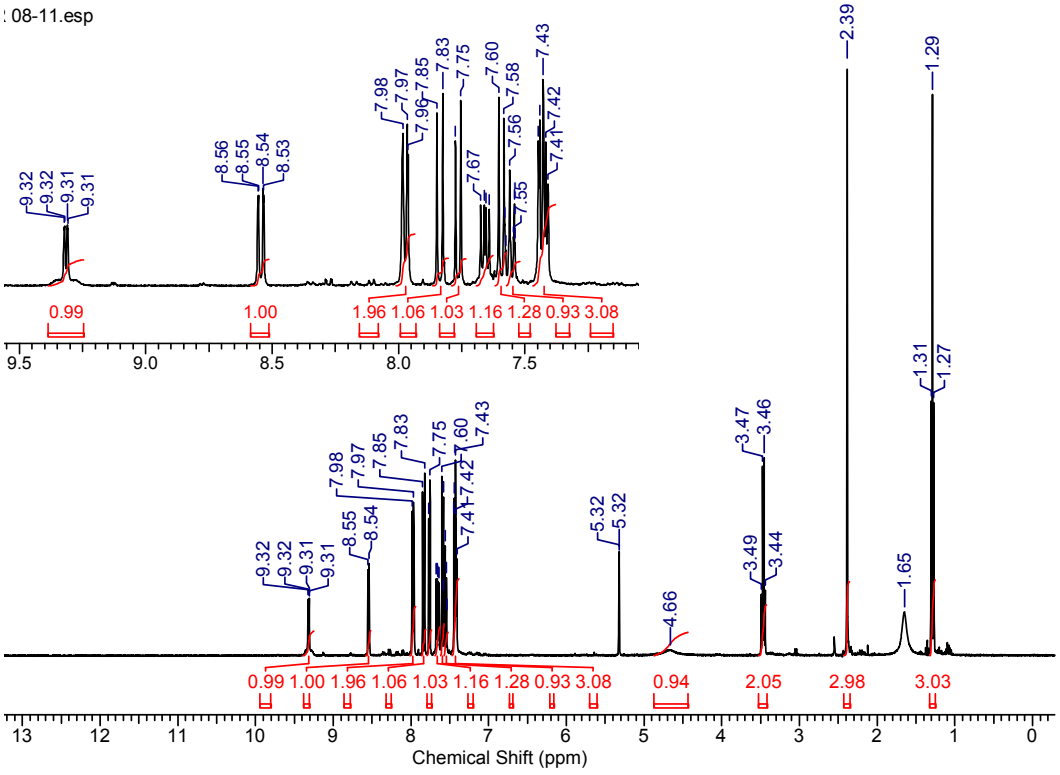


Figure S8. ^{1}H NMR spectrum of the intermediate **I1^{Et}** after 4 days in CD_2Cl_2 solution.

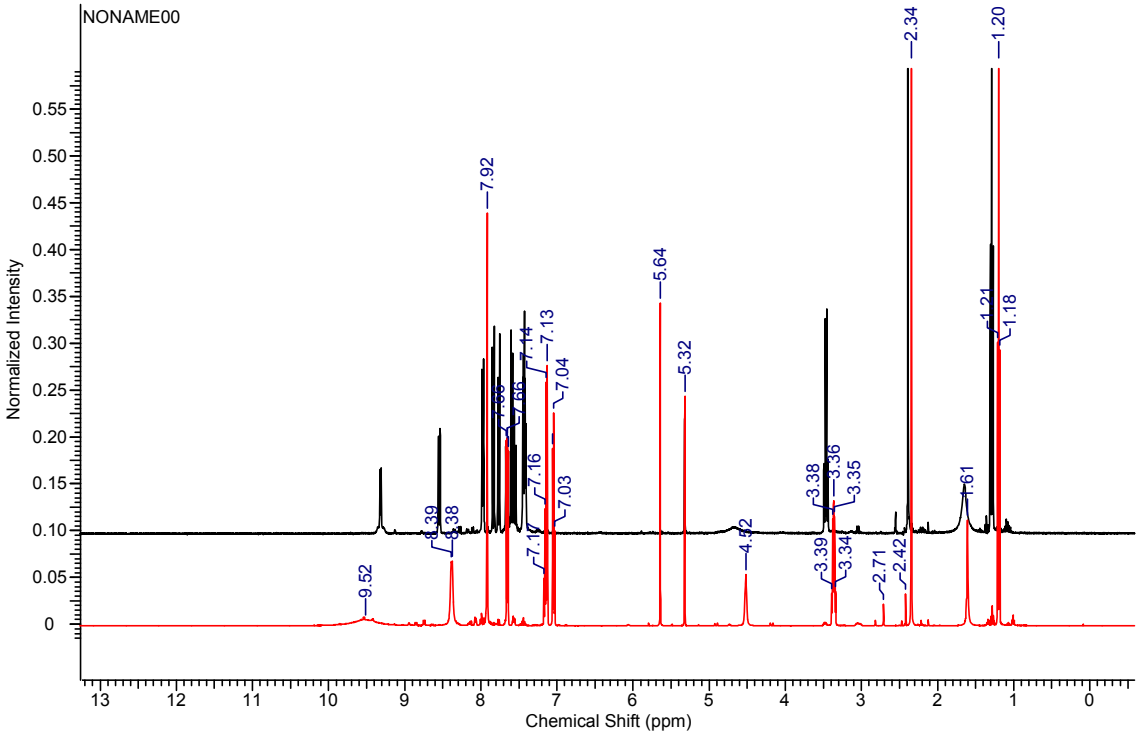


Figure S9. Superposition of the ^{1}H NMR spectra of the intermediate **I1^{Et}:** from a fresh CD_2Cl_2 solution (red line) and after 4 days in CD_2Cl_2 solution (black line).

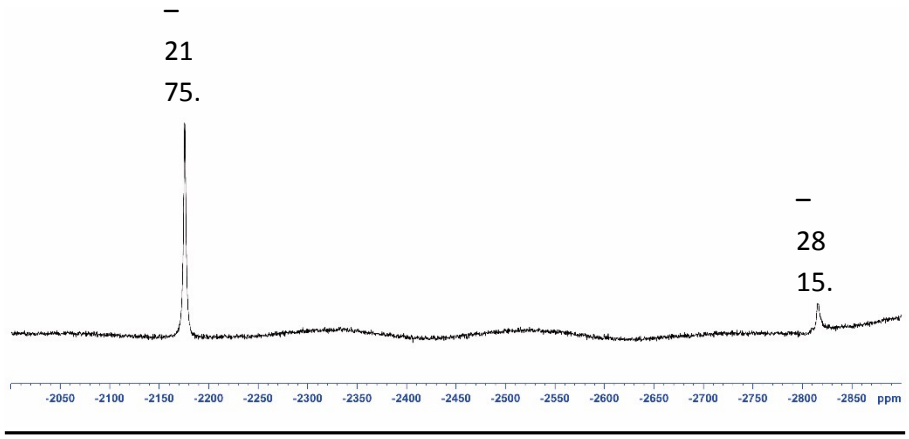


Figure S10. ^{195}Pt NMR spectrum of the intermediate **I1^{Et}** from a fresh CD_2Cl_2 solution.

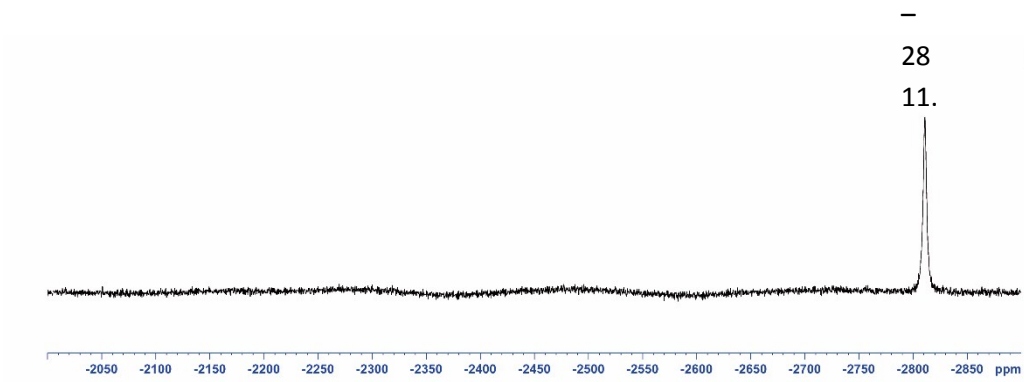


Figure S11. ^{195}Pt NMR spectrum of the intermediate **I1^{Et}** after two weeks in CD_2Cl_2 solution.

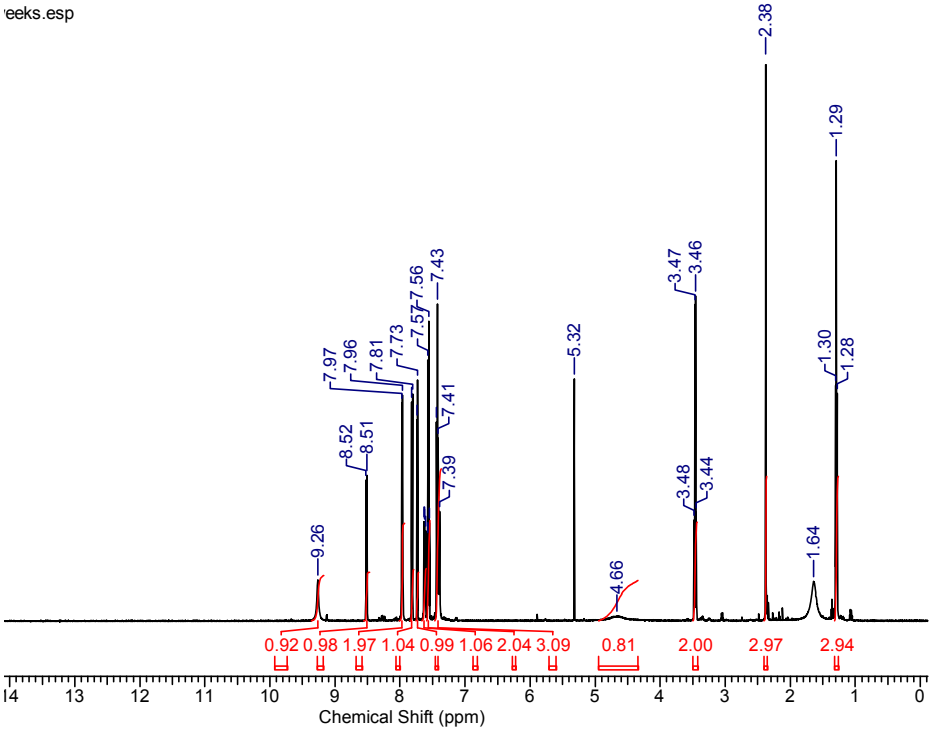


Figure S12. ^{1}H NMR spectrum of the intermediate **I1^{Et}** after two weeks in CD_2Cl_2 solution.

HRMS DATA

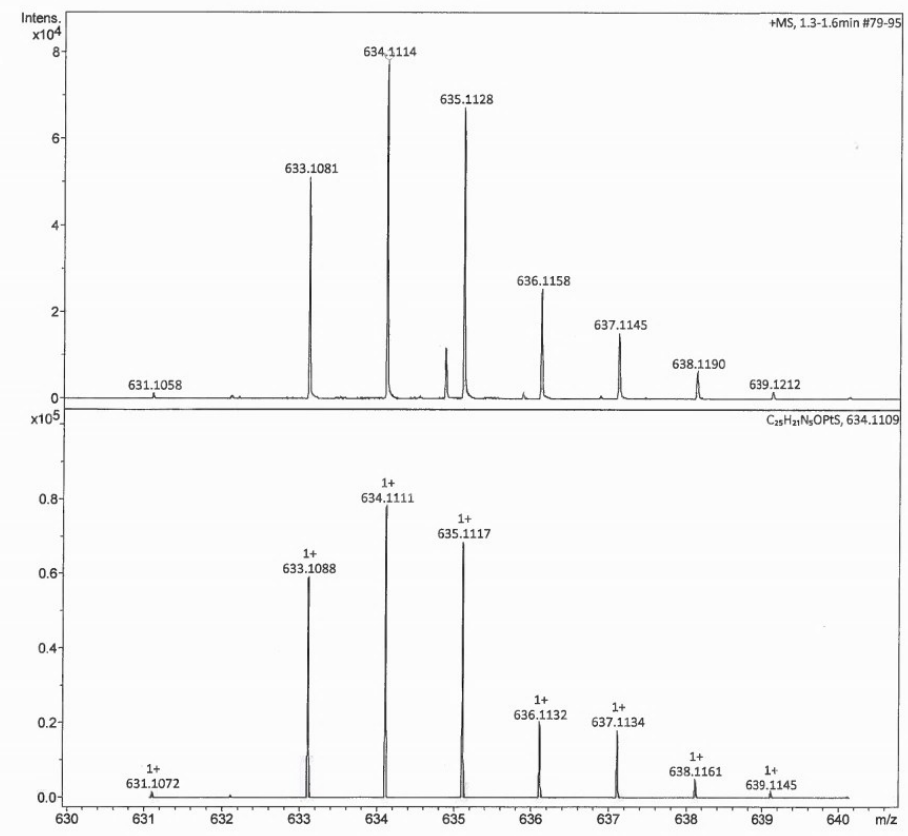


Figure S13. ESI(+) MS spectrum of the complex **1** from a 9:1 MeOH/MeCN solution.

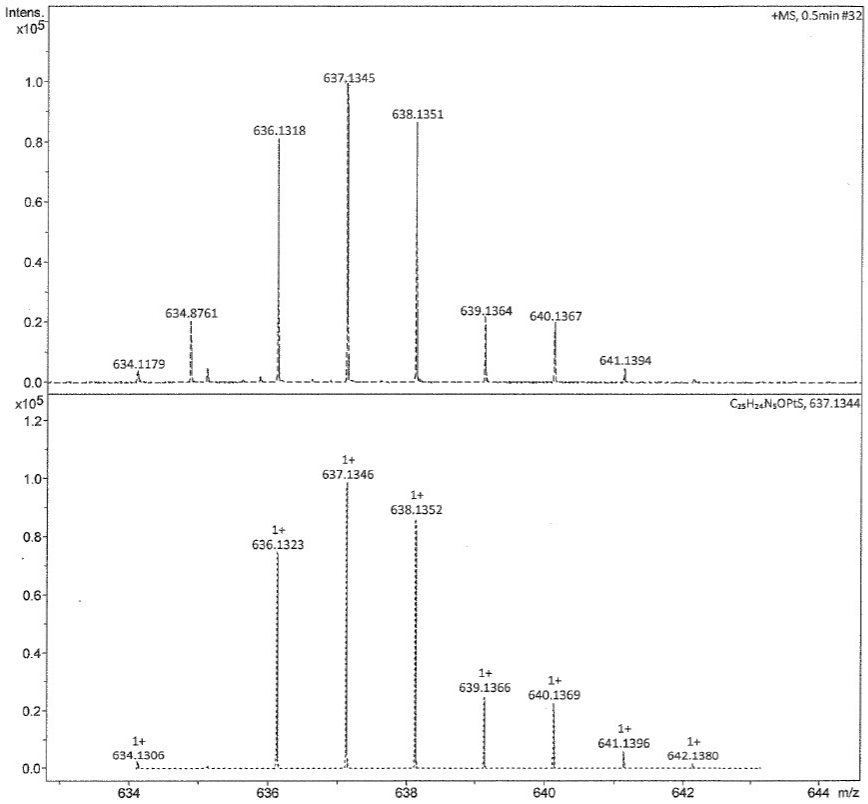


Figure S14. ESI(+) MS spectrum of the intermediate **I1^{Et}** from a 9:1 MeOH/MeCN solution.

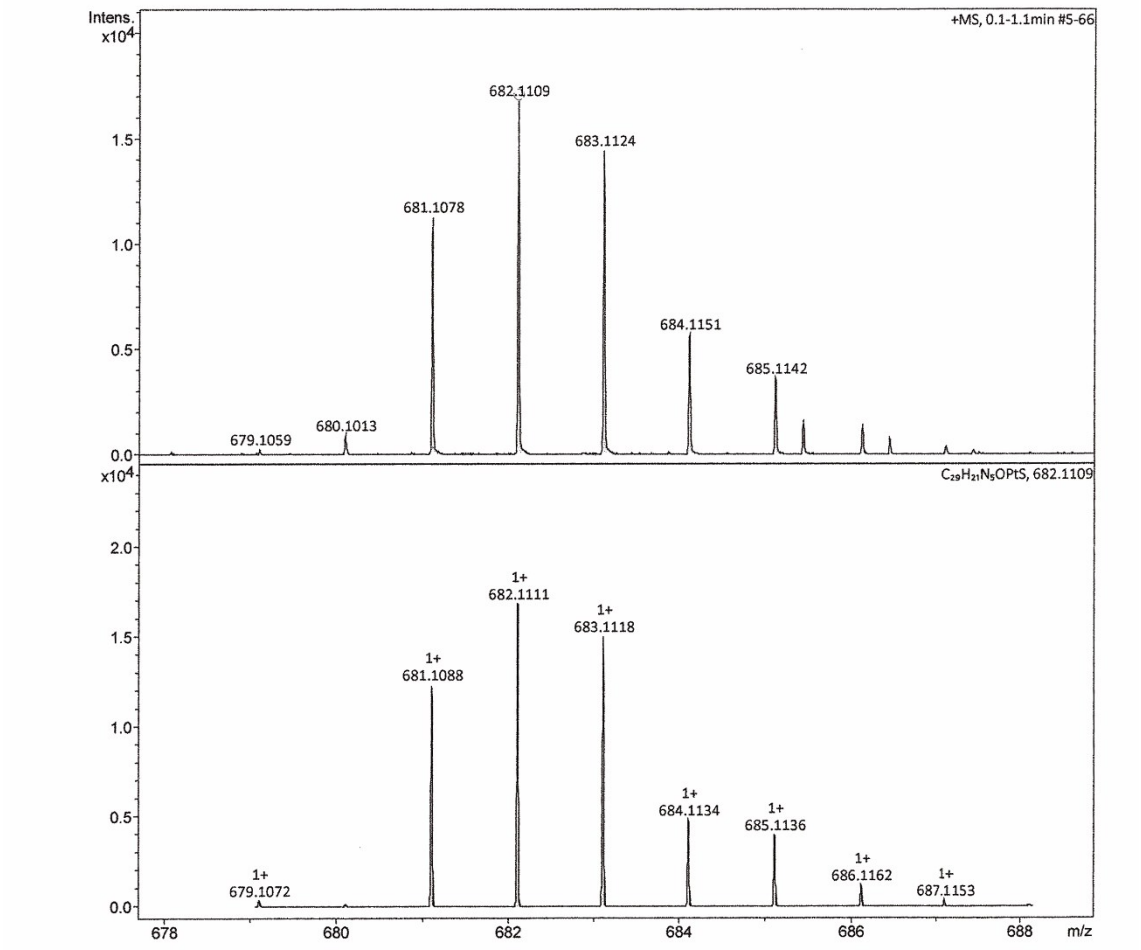
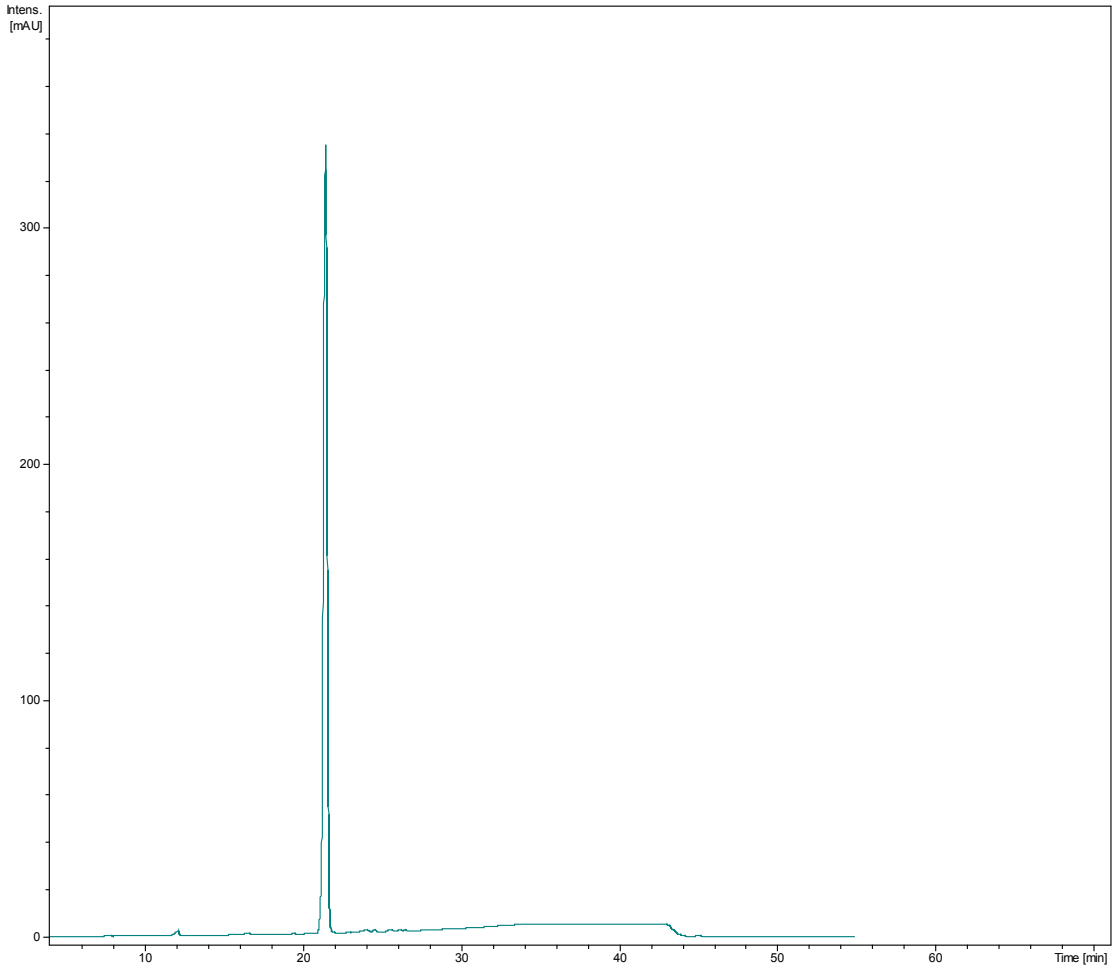


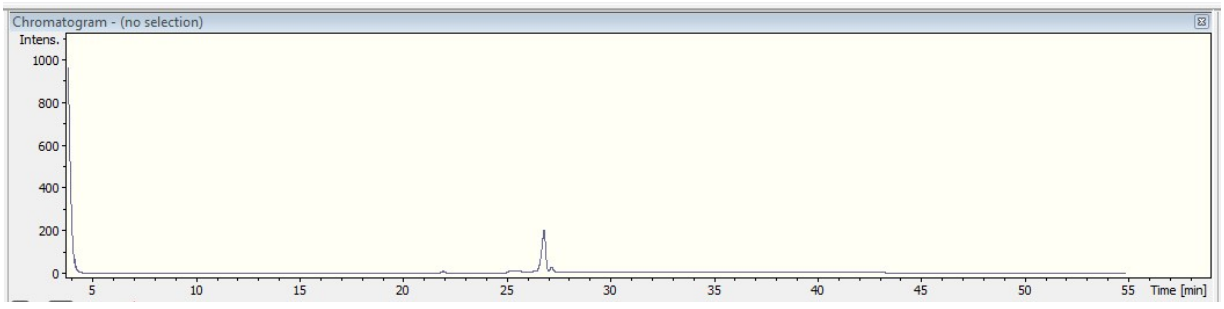
Figure S15. ESI(+) MS spectrum of the complex **2** from a 9:1 MeOH/MeCN solution.

HPLC DATA



Retention time: 21.5 min

Figure S16. HPLC of the intermediate **I1^{Et}** from Acetone/MeOH (1:9) solution.



Retention time: 26.8 min

Figure S17. HPLC of the complex **1** from Acetone/MeOH (1:9) solution.

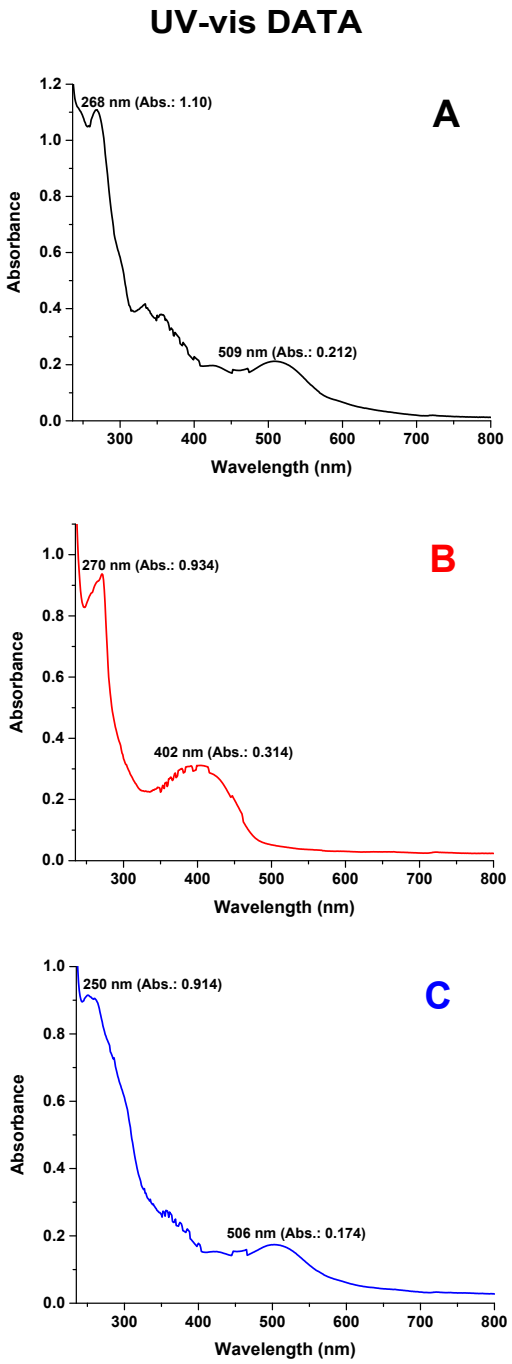


Figure S18. UV-Vis spectra of (**A**) [Pt(phenL^{Et})] (20 μM), (**B**) Intermediate **I1^{Et}** (40 μM) and (**C**) [Pt(phenL^{Ph})] (30 μM) in dichloromethane.

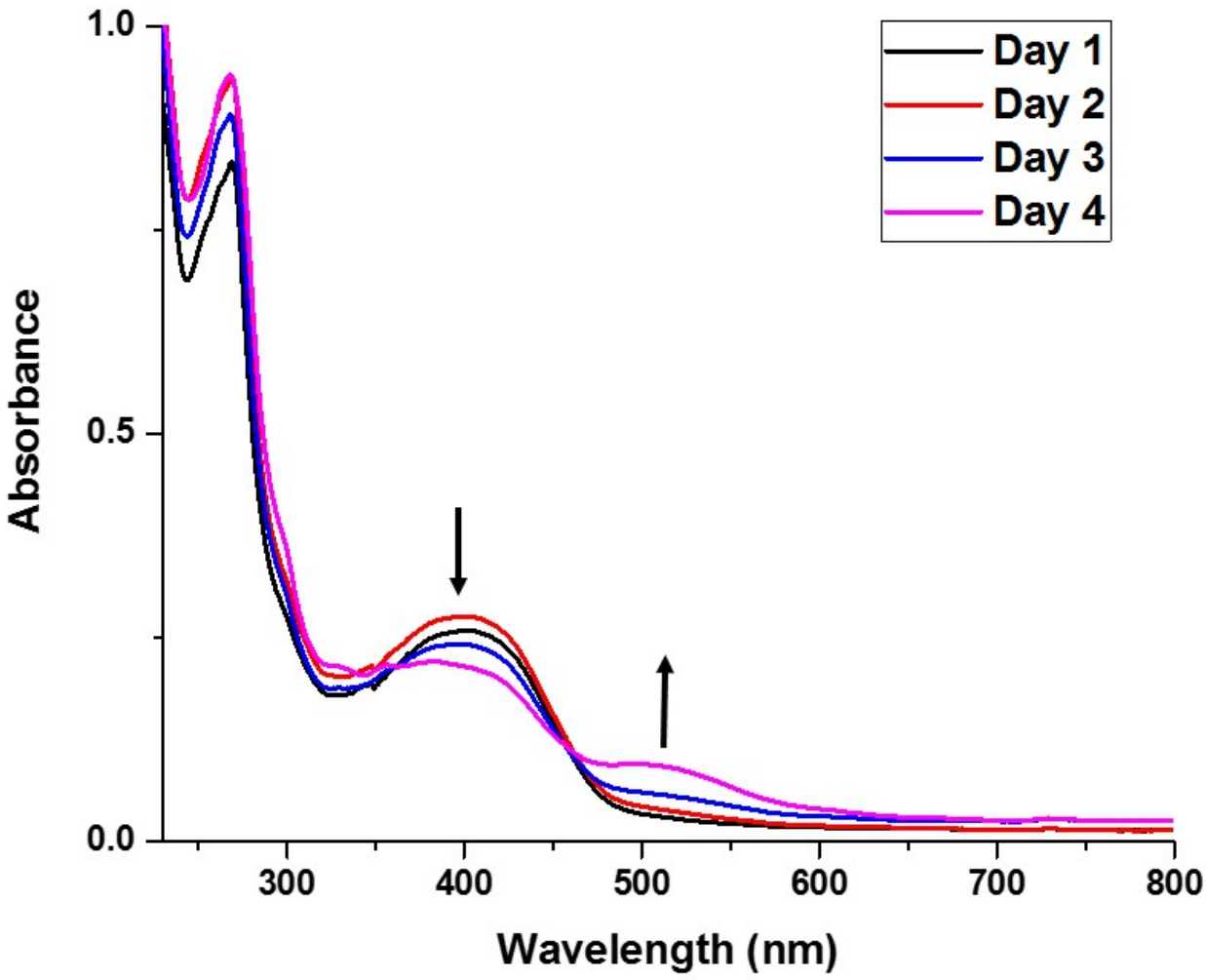


Figure S19. UV-Vis spectra of Intermediate **I1**^{Et} from acetonitrile solution (20 μM) monitored during four days.

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Optimized parameters for the TS, Reagents and Products.

"Optimization completed.

-- Stationary point found.

! Optimized Parameters !

! (Angstroms and Degrees) !

Name	Definition	TS	Reactant	Product	Derivative Info.
R1	R(1,3)	1.0843	1.0943	1.0931	-DE/DX = 0.0
R2	R(2,4)	1.0842	1.0946	1.0936	-DE/DX = 0.0
R3	R(3,4)	1.387	1.423	1.4235	-DE/DX = 0.0
R4	R(3,7)	1.3828	1.4194	1.4197	-DE/DX = 0.0
R5	R(4,13)	1.3881	1.4237	1.4255	-DE/DX = 0.0
R6	R(5,7)	1.0854	1.0948	1.0946	-DE/DX = 0.0
R7	R(6,20)	1.0926	1.1049	1.1042	-DE/DX = 0.0
R8	R(7,32)	1.3972	1.4257	1.4269	-DE/DX = 0.0
R9	R(8,10)	1.0816	1.0909	1.0899	-DE/DX = 0.0
R10	R(9,12)	1.0841	1.0939	1.0931	-DE/DX = 0.0
R11	R(10,12)	1.3656	1.4114	1.4082	-DE/DX = 0.0
R12	R(10,16)	1.387	1.4239	1.4279	-DE/DX = 0.0
R13	R(11,28)	1.0954	1.1067	1.1061	-DE/DX = 0.0
R14	R(12,19)	1.3962	1.4315	1.435	-DE/DX = 0.0
R15	R(13,18)	1.0844	1.0942	1.0931	-DE/DX = 0.0
R16	R(13,37)	1.3821	1.419	1.4178	-DE/DX = 0.0
R17	R(14,16)	1.0807	1.0921	1.0917	-DE/DX = 0.0
R18	R(15,23)	1.0077	1.0165	1.0186	-DE/DX = 0.0
R19	R(16,24)	1.326	1.3631	1.3559	-DE/DX = 0.0
R20	R(17,21)	1.0841	1.0942	1.0931	-DE/DX = 0.0

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! R21   R(19,21)       1.4196   1.4587   1.453  -DE/DX =    0.0       !
! R22   R(19,26)       1.4117   1.4348   1.4357 -DE/DX =    0.0       !
! R23   R(20,25)       1.0905   1.1022   1.1016 -DE/DX =    0.0       !
! R24   R(20,28)       1.5067   1.5421   1.5415 -DE/DX =    0.0       !
! R25   R(20,34)       1.0936   1.1055   1.1045 -DE/DX =    0.0       !
! R26   R(21,31)       1.3562   1.3907   1.3963 -DE/DX =    0.0       !
! R27   R(22,29)       1.7419   1.8424   1.8356 -DE/DX =    0.0       !
! R28   R(22,33)       2.4108   3.2766   2.3868 -DE/DX =    0.0       !
! R29   R(23,28)       1.4453   1.4727   1.4775 -DE/DX =    0.0       !
! R30   R(23,29)       1.3598   1.3836   1.3765 -DE/DX =    0.0       !
! R31   R(24,26)       1.3719   1.3918   1.3931 -DE/DX =    0.0       !
! R32   R(24,33)       1.8573   2.0617   2.0634 -DE/DX =    0.0       !
! R33   R(26,35)       1.4079   1.4389   1.4385 -DE/DX =    0.0       !
! R34   R(27,43)       1.0862   1.1037   1.1031 -DE/DX =    0.0       !
! R35   R(28,44)       1.0998   1.1075   1.1068 -DE/DX =    0.0       !
! R36   R(29,52)       1.2841   1.3181   1.3298 -DE/DX =    0.0       !
! R37   R(30,31)       1.0854   1.0943   1.0937 -DE/DX =    0.0       !
! R38   R(31,36)       1.414    1.4576   1.4519 -DE/DX =    0.0       !
! R39   R(32,37)       1.3903   1.4255   1.4274 -DE/DX =    0.0       !
! R40   R(32,48)       1.4934   1.5143   1.5079 -DE/DX =    0.0       !
! R41   R(33,38)       2.0327   2.0535   2.0375 -DE/DX =    0.0       !
! R42   R(33,53)       1.6673   3.9743   2.0119 -DE/DX =    0.0       !
! R43   R(35,36)       1.3894   1.4344   1.4229 -DE/DX =    0.0       !
! R44   R(35,38)       1.3371   1.3902   1.3935 -DE/DX =    0.0       !
! R45   R(36,40)       1.4193   1.4323   1.4458 -DE/DX =    0.0       !
! R46   R(37,49)       1.0846   1.094    1.0937 -DE/DX =    0.0       !
! R47   R(38,55)       1.324    1.356    1.3834 -DE/DX =    0.0       !
! R48   R(39,40)       1.0853   1.0938   1.0932 -DE/DX =    0.0       !
! R49   R(40,42)       1.3594   1.4071   1.3909 -DE/DX =    0.0       !
! R50   R(41,43)       1.4957   1.5265   1.5298 -DE/DX =    0.0       !
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! R51   R(41,45)        1.4062   1.4114   1.4491 -DE/DX =    0.0       !
! R52   R(41,53)        1.3285   1.3896   1.3622 -DE/DX =    0.0       !
! R53   R(41,54)        2.4921   2.1372   3.7197 -DE/DX =    0.0       !
! R54   R(42,46)        1.0828   1.0897   1.0889 -DE/DX =    0.0       !
! R55   R(42,55)        1.4264   1.4278   1.4648 -DE/DX =    0.0       !
! R56   R(43,47)        1.0861   1.0996   1.0986 -DE/DX =    0.0       !
! R57   R(43,50)        1.0764   1.1012   1.1017 -DE/DX =    0.0       !
! R58   R(45,48)        1.4874   1.4659   1.5096 -DE/DX =    0.0       !
! R59   R(45,54)        2.4095   1.0968   3.66   -DE/DX =    0.0       !
! R60   R(45,55)        1.3956   4.4596   1.45   -DE/DX =    0.0       !
! R61   R(48,51)        1.2135   1.2873   1.2742 -DE/DX =    0.0       !
! R62   R(50,54)        3.9017   4.2341   3.6621 -DE/DX =    0.0       !
! R63   R(52,53)        1.3847   1.425    1.4236 -DE/DX =    0.0       !
! R64   R(54,56)        0.7499   3.082    0.93   -DE/DX =    0.0       !
! R65   R(55,56)        3.2122   1.0903   4.9371 -DE/DX =    0.0       !
! A1    A(1,3,4)       119.9631  120.0355  120.0272 -DE/DX =    0.0       !
! A2    A(1,3,7)       120.016   119.9457  119.9306 -DE/DX =    0.0       !
! A3    A(4,3,7)       120.0205  120.0178  120.0421 -DE/DX =    0.0       !
! A4    A(2,4,3)       119.9295  119.9709  119.9037 -DE/DX =    0.0       !
! A5    A(2,4,13)      119.7856  119.9688  119.8754 -DE/DX =    0.0       !
! A6    A(3,4,13)      120.2848  120.0576  120.2209 -DE/DX =    0.0       !
! A7    A(3,7,5)       121.8809  120.7939  120.2466 -DE/DX =    0.0       !
! A8    A(3,7,32)      119.8279  120.0542  119.7919 -DE/DX =    0.0       !
! A9    A(5,7,32)      118.286   119.1365  119.9424 -DE/DX =    0.0       !
! A10   A(8,10,12)     121.7887  121.1368  121.1943 -DE/DX =    0.0       !
! A11   A(8,10,16)     118.1837  118.7753  118.9726 -DE/DX =    0.0       !
! A12   A(12,10,16)    120.0275  120.0878  119.833  -DE/DX =    0.0       !
! A13   A(9,12,10)     121.663   121.1045  120.9058 -DE/DX =    0.0       !
! A14   A(9,12,19)     120.4715  119.8167  119.5284 -DE/DX =    0.0       !
! A15   A(10,12,19)    117.8653  119.0771  119.5658 -DE/DX =    0.0       !
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! A16   A(4,13,18)     119.9777  120.0305  120.0581 -DE/DX =    0.0       !
! A17   A(4,13,37)     119.9191  119.9305  119.8457 -DE/DX =    0.0       !
! A18   A(18,13,37)    120.1032  120.037   120.0962 -DE/DX =    0.0       !
! A19   A(10,16,14)    118.3255  121.4845  121.3179 -DE/DX =    0.0       !
! A20   A(10,16,24)    125.5838  122.0482  121.7859 -DE/DX =    0.0       !
! A21   A(14,16,24)    116.0901  116.4674  116.8962 -DE/DX =    0.0       !
! A22   A(12,19,21)    122.2508  123.9954  124.16   -DE/DX =    0.0       !
! A23   A(12,19,26)    117.9664  117.4057  117.0915 -DE/DX =    0.0       !
! A24   A(21,19,26)    119.7811  118.5958  118.7484 -DE/DX =    0.0       !
! A25   A(6,20,25)     108.1642  108.1006  108.2221 -DE/DX =    0.0       !
! A26   A(6,20,28)     111.0324  110.7809  110.8128 -DE/DX =    0.0       !
! A27   A(6,20,34)     107.9741  108.4916  108.5051 -DE/DX =    0.0       !
! A28   A(25,20,28)    110.7556  110.5933  110.222  -DE/DX =    0.0       !
! A29   A(25,20,34)    107.7091  107.9155  108.1047 -DE/DX =    0.0       !
! A30   A(28,20,34)    111.072   110.8555  110.8831 -DE/DX =    0.0       !
! A31   A(17,21,19)    118.0249  118.3039  118.7331 -DE/DX =    0.0       !
! A32   A(17,21,31)    120.4504  120.821   121.0863 -DE/DX =    0.0       !
! A33   A(19,21,31)    121.5243  120.8718  120.1803 -DE/DX =    0.0       !
! A34   A(29,22,33)     87.1496  126.0261   93.2962 -DE/DX =    0.0       !
! A35   A(15,23,28)    117.7969  119.944   119.0918 -DE/DX =    0.0       !
! A36   A(15,23,29)    116.3906  118.5847  118.5019 -DE/DX =    0.0       !
! A37   A(28,23,29)    121.5703  121.342   122.3998 -DE/DX =    0.0       !
! A38   A(16,24,26)    114.1315  118.2771  119.0359 -DE/DX =    0.0       !
! A39   A(16,24,33)    133.3394  128.9758  128.7728 -DE/DX =    0.0       !
! A40   A(26,24,33)    112.5244  112.74    112.1911 -DE/DX =    0.0       !
! A41   A(19,26,24)    124.424   123.0924  122.6857 -DE/DX =    0.0       !
! A42   A(19,26,35)    116.9315  120.4751  120.9278 -DE/DX =    0.0       !
! A43   A(24,26,35)    118.6438  116.4096  116.3858 -DE/DX =    0.0       !
! A44   A(11,28,20)    110.8791  111.2721  111.1658 -DE/DX =    0.0       !
! A45   A(11,28,23)    108.4306  108.8351  108.9361 -DE/DX =    0.0       !
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! A46 A(11,28,44) 105.8074 106.4224 106.7578 -DE/DX = 0.0 !

! A47 A(20,28,23) 110.341 109.4878 109.4608 -DE/DX = 0.0 !

! A48 A(20,28,44) 110.7228 111.2783 111.0593 -DE/DX = 0.0 !

! A49 A(23,28,44) 110.5487 109.4695 109.3976 -DE/DX = 0.0 !

! A50 A(22,29,23) 117.5049 116.3506 116.4702 -DE/DX = 0.0 !

! A51 A(22,29,52) 124.0403 123.1025 124.2861 -DE/DX = 0.0 !

! A52 A(23,29,52) 118.4484 120.5252 119.2426 -DE/DX = 0.0 !

! A53 A(21,31,30) 120.8344 120.6796 120.5756 -DE/DX = 0.0 !

! A54 A(21,31,36) 120.2843 121.0494 121.1504 -DE/DX = 0.0 !

! A55 A(30,31,36) 118.8799 118.2698 118.274 -DE/DX = 0.0 !

! A56 A(7,32,37) 119.8435 119.7717 120.0737 -DE/DX = 0.0 !

! A57 A(7,32,48) 119.7423 120.9216 120.7542 -DE/DX = 0.0 !

! A58 A(37,32,48) 120.3918 119.1562 119.1056 -DE/DX = 0.0 !

! A59 A(22,33,24) 91.1665 129.2582 98.6557 -DE/DX = 0.0 !

! A60 L(22,33,38,53,-1) 184.7047 148.8457 179.524 -DE/DX = 0.0 !

! A61 L(22,33,38,53,-2) 180.0828 180.4564 179.6618 -DE/DX = 0.0 !

! A62 A(22,33,53) 88.0816 46.4328 85.2319 -DE/DX = 0.0 !

! A63 A(24,33,38) 84.1287 81.2721 81.8252 -DE/DX = 0.0 !

! A64 L(24,33,53,38,-1) 180.7518 183.685 176.1174 -DE/DX = 0.0 !

! A65 L(24,33,53,38,-2) 178.0686 191.0561 179.1355 -DE/DX = 0.0 !

! A66 A(38,33,53) 96.6231 102.4129 94.2921 -DE/DX = 0.0 !

! A67 A(26,35,36) 123.2804 120.3293 119.537 -DE/DX = 0.0 !

! A68 A(26,35,38) 113.9971 116.5711 116.7928 -DE/DX = 0.0 !

! A69 A(36,35,38) 122.6944 123.0892 123.67 -DE/DX = 0.0 !

! A70 A(31,36,35) 118.1733 118.6244 119.4519 -DE/DX = 0.0 !

! A71 A(31,36,40) 126.1467 124.0468 124.5463 -DE/DX = 0.0 !

! A72 A(35,36,40) 115.6762 117.3282 115.9992 -DE/DX = 0.0 !

! A73 A(13,37,32) 120.1015 120.1412 120.019 -DE/DX = 0.0 !

! A74 A(13,37,49) 121.0743 121.5588 121.0949 -DE/DX = 0.0 !

! A75 A(32,37,49) 118.8236 118.2973 118.886 -DE/DX = 0.0 !

! A76 A(33,38,35)   110.6817 112.9842 112.7896 -DE/DX =   0.0   !

! A77 A(33,38,55)   126.4449 128.4743 126.062 -DE/DX =   0.0   !

! A78 A(35,38,55)   122.8734 118.1549 121.1204 -DE/DX =   0.0   !

! A79 A(36,40,39)   119.1774 119.753   119.6035 -DE/DX =   0.0   !

! A80 A(36,40,42)   120.5745 119.1303 120.089 -DE/DX =   0.0   !

! A81 A(39,40,42)   120.248   121.1163 120.3073 -DE/DX =   0.0   !

! A82 A(43,41,45)   113.0375 124.8599 118.9585 -DE/DX =   0.0   !

! A83 A(43,41,53)   119.2401 116.4649 116.0737 -DE/DX =   0.0   !

! A84 A(43,41,54)   112.2373 152.2496   86.9734 -DE/DX =   0.0   !

! A85 A(45,41,53)   127.7165 118.6181 124.88   -DE/DX =   0.0   !

! A86 A(53,41,54)   90.4685   91.2605 104.0364 -DE/DX =   0.0   !

! A87 A(40,42,46)   119.9398 121.6416 119.1063 -DE/DX =   0.0   !

! A88 A(40,42,55)   120.5754 119.8171 122.2471 -DE/DX =   0.0   !

! A89 A(46,42,55)   119.4833 118.4824 118.6393 -DE/DX =   0.0   !

! A90 A(27,43,41)   111.0075 110.3488 111.3653 -DE/DX =   0.0   !

! A91 A(27,43,47)   107.649   108.8035 109.1858 -DE/DX =   0.0   !

! A92 A(27,43,50)   106.822   106.4339 106.4561 -DE/DX =   0.0   !

! A93 A(41,43,47)   110.0236 110.9683 112.0957 -DE/DX =   0.0   !

! A94 A(41,43,50)   114.0221 109.8285 108.9778 -DE/DX =   0.0   !

! A95 A(47,43,50)   107.0312 110.3528 108.5645 -DE/DX =   0.0   !

! A96 A(41,45,48)   116.9692 129.5804 115.6949 -DE/DX =   0.0   !

! A97 A(41,45,54)   76.5817 116.3115   81.0   -DE/DX =   0.0   !

! A98 A(41,45,55)   127.4195 104.2491 128.4213 -DE/DX =   0.0   !

! A99 A(48,45,54)   131.7652 112.7202   95.1725 -DE/DX =   0.0   !

! A100 A(48,45,55)   113.3593 102.5984 115.808 -DE/DX =   0.0   !

! A101 A(54,45,55)   81.4534   43.9267   97.0506 -DE/DX =   0.0   !

! A102 A(32,48,45)   113.2457 122.5478 118.4186 -DE/DX =   0.0   !

! A103 A(32,48,51)   121.5096 118.3874 119.1986 -DE/DX =   0.0   !

! A104 A(45,48,51)   125.0407 118.9699 122.2869 -DE/DX =   0.0   !

! A105 A(43,50,54)   52.5019   46.0796   96.7638 -DE/DX =   0.0   !

! A106 A(29,52,53) 116.5017 114.647 115.7227 -DE/DX = 0.0 !

! A107 A(33,53,41) 125.5029 127.6549 124.5836 -DE/DX = 0.0 !

! A108 A(33,53,52) 124.0918 119.1699 121.3909 -DE/DX = 0.0 !

! A109 A(41,53,52) 110.3818 113.1752 113.9555 -DE/DX = 0.0 !

! A110 A(41,54,50) 30.665 10.1984 33.9591 -DE/DX = 0.0 !

! A111 L(41,54,56,50,-1) 161.1997 101.7887 169.4507 -DE/DX = 0.0 !

! A112 L(41,54,56,50,-2) 188.1518 219.0811 191.4438 -DE/DX = 0.0 !

! A113 A(45,54,50) 59.0114 34.4301 53.9889 -DE/DX = 0.0 !

! A114 L(45,54,56,50,-1) 189.5461 126.0203 189.4804 -DE/DX = 0.0 !

! A115 L(45,54,56,50,-2) 162.1716 125.7355 175.911 -DE/DX = 0.0 !

! A116 A(50,54,56) 130.5347 91.5902 135.4916 -DE/DX = 0.0 !

! A117 A(38,55,42) 117.5748 122.3074 116.8619 -DE/DX = 0.0 !

! A118 A(38,55,45) 116.0256 103.1988 121.5638 -DE/DX = 0.0 !

! A119 A(38,55,56) 83.1777 116.3849 100.3748 -DE/DX = 0.0 !

! A120 A(42,55,45) 126.3863 122.5093 121.548 -DE/DX = 0.0 !

! A121 A(42,55,56) 113.1552 121.2641 104.4329 -DE/DX = 0.0 !

! A122 A(54,56,55) 31.0753 119.9743 23.2264 -DE/DX = 0.0 !

! D1 D(1,3,4,2) 0.0022 -0.7039 -0.4271 -DE/DX = 0.0 !

! D2 D(1,3,4,13) 179.9257 178.688 179.4995 -DE/DX = 0.0 !

! D3 D(7,3,4,2) 179.8019 179.6811 179.589 -DE/DX = 0.0 !

! D4 D(7,3,4,13) -0.2746 -0.927 -0.4843 -DE/DX = 0.0 !

! D5 D(1,3,7,5) 1.1308 -0.7704 -0.7229 -DE/DX = 0.0 !

! D6 D(1,3,7,32) -179.7074 -179.3297 -179.1346 -DE/DX = 0.0 !

! D7 D(4,3,7,5) -178.6688 178.845 179.261 -DE/DX = 0.0 !

! D8 D(4,3,7,32) 0.4931 0.2857 0.8492 -DE/DX = 0.0 !

! D9 D(2,4,13,18) -0.2637 0.0401 -0.3121 -DE/DX = 0.0 !

! D10 D(2,4,13,37) 179.7187 179.5284 179.6454 -DE/DX = 0.0 !

! D11 D(3,4,13,18) 179.8128 -179.3518 179.7613 -DE/DX = 0.0 !

! D12 D(3,4,13,37) -0.2049 0.1364 -0.2813 -DE/DX = 0.0 !

! D13 D(3,7,32,37) -0.2366 1.1387 -0.4553 -DE/DX = 0.0 !

```
! D14   D(3,7,32,48)    178.0528  176.6418  176.5539 -DE/DX =    0.0       !
! D15   D(5,7,32,37)    178.9551 -177.4444 -178.8719 -DE/DX =    0.0       !
! D16   D(5,7,32,48)     -2.7555   -1.9413   -1.8627 -DE/DX =    0.0       !
! D17   D(8,10,12,9)      0.0258   -0.1162   -0.0603 -DE/DX =    0.0       !
! D18   D(8,10,12,19)   -179.7832  179.4118  179.9133 -DE/DX =    0.0       !
! D19   D(16,10,12,9)    179.8946  179.9806  179.868  -DE/DX =    0.0       !
! D20   D(16,10,12,19)     0.0855   -0.4914   -0.1583 -DE/DX =    0.0       !
! D21   D(8,10,16,14)     -0.1254   -0.4169    0.0201 -DE/DX =    0.0       !
! D22   D(8,10,16,24)   -179.82    179.5704 -179.954  -DE/DX =    0.0       !
! D23   D(12,10,16,14)  -179.9989  179.4886 -179.9098 -DE/DX =    0.0       !
! D24   D(12,10,16,24)     0.3065   -0.5241    0.1161 -DE/DX =    0.0       !
! D25   D(9,12,19,21)     -0.5884    1.0144   -0.2888 -DE/DX =    0.0       !
! D26   D(9,12,19,26)    179.8846 -179.6415  179.8368 -DE/DX =    0.0       !
! D27   D(10,12,19,21)   179.223  -178.5198  179.7372 -DE/DX =    0.0       !
! D28   D(10,12,19,26)    -0.304     0.8243   -0.1372 -DE/DX =    0.0       !
! D29   D(4,13,37,32)      0.4615    1.2945    0.6751 -DE/DX =    0.0       !
! D30   D(4,13,37,49)   -179.8191 -178.0921 -179.4687 -DE/DX =    0.0       !
! D31   D(18,13,37,32)  -179.5562 -179.2173 -179.3675 -DE/DX =    0.0       !
! D32   D(18,13,37,49)     0.1632    1.3961    0.4887 -DE/DX =    0.0       !
! D33   D(10,16,24,26)    -0.4154    1.1357    0.2363 -DE/DX =    0.0       !
! D34   D(10,16,24,33)   178.714  -179.915  -179.9431 -DE/DX =    0.0       !
! D35   D(14,16,24,26)   179.8839 -178.8764 -179.7389 -DE/DX =    0.0       !
! D36   D(14,16,24,33)    -0.9867    0.0728    0.0817 -DE/DX =    0.0       !
! D37   D(12,19,21,17)     0.7661   -1.7455    0.1363 -DE/DX =    0.0       !
! D38   D(12,19,21,31)  -179.0041  177.5974 -179.6604 -DE/DX =    0.0       !
! D39   D(26,19,21,17)  -179.7153  178.9177 -179.9913 -DE/DX =    0.0       !
! D40   D(26,19,21,31)     0.5145   -1.7394    0.2121 -DE/DX =    0.0       !
! D41   D(12,19,26,24)     0.1874   -0.2104    0.5046 -DE/DX =    0.0       !
! D42   D(12,19,26,35)   179.8632 -178.4084 -179.7999 -DE/DX =    0.0       !
! D43   D(21,19,26,24)  -179.3517  179.1702 -179.3768 -DE/DX =    0.0       !
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! D44   D(21,19,26,35)    0.3242    0.9723    0.3186 -DE/DX =    0.0       !
! D45   D(6,20,28,11)    -60.4087  -60.3534  -59.745  -DE/DX =    0.0       !
! D46   D(6,20,28,23)     59.743    59.9963   60.6452 -DE/DX =    0.0       !
! D47   D(6,20,28,44)    -177.5396 -178.8563 -178.4565 -DE/DX =    0.0       !
! D48   D(25,20,28,11)    59.7831   59.4864   60.0256 -DE/DX =    0.0       !
! D49   D(25,20,28,23)    179.9347  179.8361 -179.5842 -DE/DX =    0.0       !
! D50   D(25,20,28,44)    -57.3479  -59.0165  -58.686  -DE/DX =    0.0       !
! D51   D(34,20,28,11)    179.4284  179.143   179.6948 -DE/DX =    0.0       !
! D52   D(34,20,28,23)    -60.4199  -60.5074  -59.9151 -DE/DX =    0.0       !
! D53   D(34,20,28,44)     62.2974   60.6401   60.9832 -DE/DX =    0.0       !
! D54   D(17,21,31,30)     -0.3574    0.1131   -0.1484 -DE/DX =    0.0       !
! D55   D(17,21,31,36)    -179.9226  179.7147  179.8826 -DE/DX =    0.0       !
! D56   D(19,21,31,30)    179.4073 -179.2133  179.6434 -DE/DX =    0.0       !
! D57   D(19,21,31,36)     -0.1579    0.3884   -0.3256 -DE/DX =    0.0       !
! D58   D(33,22,29,23)    -178.8564  151.3349  179.8924 -DE/DX =    0.0       !
! D59   D(33,22,29,52)     0.2109  -30.3541   -0.4949 -DE/DX =    0.0       !
! D60   D(29,22,33,24)    -176.4925 -169.6557 -177.7181 -DE/DX =    0.0       !
! D61   D(29,22,33,53)     1.5869   24.5506    1.4396 -DE/DX =    0.0       !
! D62   D(29,22,38,35)    -175.1692 -171.9022 -178.848  -DE/DX =    0.0       !
! D63   D(29,22,38,55)     4.9789    6.2735    3.2735 -DE/DX =    0.0       !
! D64   D(15,23,28,11)    147.0965  128.2566  125.8564 -DE/DX =    0.0       !
! D65   D(15,23,28,20)     25.4824    6.4314    4.1153 -DE/DX =    0.0       !
! D66   D(15,23,28,44)    -97.3368 -115.8041 -117.7861 -DE/DX =    0.0       !
! D67   D(29,23,28,11)    -56.8821  -55.935   -55.0846 -DE/DX =    0.0       !
! D68   D(29,23,28,20)    -178.4962 -177.7602 -176.8257 -DE/DX =    0.0       !
! D69   D(29,23,28,44)     58.6846   60.0043   61.2729 -DE/DX =    0.0       !
! D70   D(15,23,29,22)    -15.8293   -8.9887   -1.4752 -DE/DX =    0.0       !
! D71   D(15,23,29,52)    165.0496  172.6538  178.8915 -DE/DX =    0.0       !
! D72   D(28,23,29,22)    -172.1684  175.1475  179.4605 -DE/DX =    0.0       !
! D73   D(28,23,29,52)     8.7106   -3.21    -0.1728 -DE/DX =    0.0       !
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! D74 D(16,24,26,19)   0.1631 -0.7681 -0.558 -DE/DX =   0.0   !

! D75 D(16,24,26,35) -179.5076 177.4979 179.7337 -DE/DX =   0.0   !

! D76 D(33,24,26,19) -179.1514 -179.8824 179.5931 -DE/DX =   0.0   !

! D77 D(33,24,26,35)   1.1779 -1.6164 -0.1153 -DE/DX =   0.0   !

! D78 D(16,24,33,22) -0.3979   8.821   1.1582 -DE/DX =   0.0   !

! D79 D(16,24,33,38) 179.5264 -178.1181 -179.1754 -DE/DX =   0.0   !

! D80 D(26,24,33,22) 178.742 -172.1823 -179.0112 -DE/DX =   0.0   !

! D81 D(26,24,33,38) -1.3337   0.8785   0.6552 -DE/DX =   0.0   !

! D82 D(16,24,53,41) 179.6342 142.9151 -177.5523 -DE/DX =   0.0   !

! D83 D(16,24,53,52) -3.6797 -32.0095 -1.3753 -DE/DX =   0.0   !

! D84 D(26,24,53,41) -2.4606 -29.4181   1.7232 -DE/DX =   0.0   !

! D85 D(26,24,53,52) 174.2254 155.6573 177.9003 -DE/DX =   0.0   !

! D86 D(19,26,35,36) -1.5851   1.1349 -0.7344 -DE/DX =   0.0   !

! D87 D(19,26,35,38) -179.7039 179.9989 179.4466 -DE/DX =   0.0   !

! D88 D(24,26,35,36) 178.1102 -177.1795 178.9795 -DE/DX =   0.0   !

! D89 D(24,26,35,38) -0.0087   1.6845 -0.8395 -DE/DX =   0.0   !

! D90 D(22,29,52,53) -2.5208 -1.5168 -1.3508 -DE/DX =   0.0   !

! D91 D(23,29,52,53) 176.5384 176.7262 178.2519 -DE/DX =   0.0   !

! D92 D(21,31,36,35) -1.0312   1.721   -0.0929 -DE/DX =   0.0   !

! D93 D(21,31,36,40) 178.2239 -177.9697 179.2985 -DE/DX =   0.0   !

! D94 D(30,31,36,35) 179.3952 -178.6679 179.9374 -DE/DX =   0.0   !

! D95 D(30,31,36,40) -1.3496   1.6413 -0.6712 -DE/DX =   0.0   !

! D96 D(7,32,37,13)   -0.2418 -1.9311 -0.3089 -DE/DX =   0.0   !

! D97 D(7,32,37,49) -179.9674 177.4754 179.8318 -DE/DX =   0.0   !

! D98 D(48,32,37,13) -178.5199 -177.5138 -177.3672 -DE/DX =   0.0   !

! D99 D(48,32,37,49)   1.7544   1.8926   2.7734 -DE/DX =   0.0   !

! D100 D(7,32,48,45)   7.3802 30.4141 21.6707 -DE/DX =   0.0   !

! D101 D(7,32,48,51) -167.6793 -146.0044 -154.8509 -DE/DX =   0.0   !

! D102 D(37,32,48,45) -174.3399 -154.0555 -161.2915 -DE/DX =   0.0   !

! D103 D(37,32,48,51)   10.6006 29.526   22.1869 -DE/DX =   0.0   !

! D104 D(24,33,38,35) 1.3571 -0.0008 -1.0924 -DE/DX = 0.0 !

! D105 D(24,33,38,55) -178.6114 172.6392 -179.1743 -DE/DX = 0.0 !

! D106 D(53,33,38,35) -176.7115 168.9431 179.772 -DE/DX = 0.0 !

! D107 D(53,33,38,55) 3.32 -18.4169 1.6902 -DE/DX = 0.0 !

! D108 D(22,33,53,41) 178.4078 151.9029 -179.4561 -DE/DX = 0.0 !

! D109 D(22,33,53,52) -3.5254 -28.1118 -2.685 -DE/DX = 0.0 !

! D110 D(38,33,53,41) -1.675 -28.5535 0.8821 -DE/DX = 0.0 !

! D111 D(38,33,53,52) 176.3918 151.4318 177.6531 -DE/DX = 0.0 !

! D112 D(26,35,36,31) 1.9499 -2.4675 0.617 -DE/DX = 0.0 !

! D113 D(26,35,36,40) -177.3828 177.2441 -178.8252 -DE/DX = 0.0 !

! D114 D(38,35,36,31) 179.9077 178.7452 -179.5771 -DE/DX = 0.0 !

! D115 D(38,35,36,40) 0.5751 -1.5432 0.9806 -DE/DX = 0.0 !

! D116 D(26,35,38,33) -1.0505 -0.8749 1.3666 -DE/DX = 0.0 !

! D117 D(26,35,38,55) 178.9193 -174.3433 179.5554 -DE/DX = 0.0 !

! D118 D(36,35,38,33) -179.1818 177.9548 -178.4442 -DE/DX = 0.0 !

! D119 D(36,35,38,55) 0.788 4.4864 -0.2554 -DE/DX = 0.0 !

! D120 D(31,36,40,39) 0.1724 -1.9589 -0.2165 -DE/DX = 0.0 !

! D121 D(31,36,40,42) -179.9036 177.8116 179.9182 -DE/DX = 0.0 !

! D122 D(35,36,40,39) 179.4439 178.3466 179.1939 -DE/DX = 0.0 !

! D123 D(35,36,40,42) -0.6321 -1.8829 -0.6714 -DE/DX = 0.0 !

! D124 D(33,38,55,42) 177.9875 -176.3341 177.1854 -DE/DX = 0.0 !

! D125 D(33,38,55,45) -0.7746 40.399 -0.9763 -DE/DX = 0.0 !

! D126 D(33,38,55,56) -69.4122 6.0426 -70.6812 -DE/DX = 0.0 !

! D127 D(35,38,55,42) -1.9774 -4.0211 -0.7489 -DE/DX = 0.0 !

! D128 D(35,38,55,45) 179.2605 -147.288 -178.9105 -DE/DX = 0.0 !

! D129 D(35,38,55,56) 110.6229 178.3556 111.3846 -DE/DX = 0.0 !

! D130 D(36,40,42,46) 179.8726 179.4968 -179.3172 -DE/DX = 0.0 !

! D131 D(36,40,42,55) -0.5595 2.3331 -0.3092 -DE/DX = 0.0 !

! D132 D(39,40,42,46) -0.2041 -0.7359 0.8183 -DE/DX = 0.0 !

! D133 D(39,40,42,55) 179.3638 -177.8996 179.8264 -DE/DX = 0.0 !

! D134 D(45,41,43,27) -63.9636 -106.8663 -114.3002 -DE/DX = 0.0 !

! D135 D(45,41,43,47) 55.0892 13.8168 8.3611 -DE/DX = 0.0 !

! D136 D(45,41,43,50) 175.3358 136.1015 128.5576 -DE/DX = 0.0 !

! D137 D(53,41,43,27) 115.2221 75.9288 68.9407 -DE/DX = 0.0 !

! D138 D(53,41,43,47) -125.725 -163.388 -168.398 -DE/DX = 0.0 !

! D139 D(53,41,43,50) -5.4784 -41.1033 -48.2015 -DE/DX = 0.0 !

! D140 D(54,41,43,27) -140.9503 -106.6923 173.0944 -DE/DX = 0.0 !

! D141 D(54,41,43,47) -21.8975 13.9909 -64.2444 -DE/DX = 0.0 !

! D142 D(54,41,43,50) 98.3491 136.2756 55.9521 -DE/DX = 0.0 !

! D143 D(43,41,45,48) 23.8365 -14.7494 12.7562 -DE/DX = 0.0 !

! D144 D(43,41,45,54) -106.4741 179.8238 -78.6813 -DE/DX = 0.0 !

! D145 D(43,41,45,55) -174.4557 -134.8766 -170.572 -DE/DX = 0.0 !

! D146 D(53,41,45,48) -155.2653 162.4001 -170.7927 -DE/DX = 0.0 !

! D147 D(53,41,45,54) 74.4241 -3.0267 97.7698 -DE/DX = 0.0 !

! D148 D(53,41,45,55) 6.4425 42.2729 5.8791 -DE/DX = 0.0 !

! D149 D(43,41,53,33) 178.6035 161.1911 172.2192 -DE/DX = 0.0 !

! D150 D(43,41,53,52) 0.3113 -18.795 -4.7649 -DE/DX = 0.0 !

! D151 D(45,41,53,33) -2.3437 -16.1963 -4.3239 -DE/DX = 0.0 !

! D152 D(45,41,53,52) 179.3641 163.8177 178.692 -DE/DX = 0.0 !

! D153 D(54,41,53,33) 62.6081 -17.5885 78.6794 -DE/DX = 0.0 !

! D154 D(54,41,53,52) -115.6841 162.4254 -98.3047 -DE/DX = 0.0 !

! D155 D(43,41,54,50) -29.2628 -72.7598 -24.9598 -DE/DX = 0.0 !

! D156 D(53,41,54,50) 92.8158 104.8934 91.1739 -DE/DX = 0.0 !

! D157 D(40,42,55,38) 1.858 0.6863 1.0365 -DE/DX = 0.0 !

! D158 D(40,42,55,45) -179.5237 137.0177 179.1985 -DE/DX = 0.0 !

! D159 D(40,42,55,56) -92.592 178.1954 -108.7674 -DE/DX = 0.0 !

! D160 D(46,42,55,38) -178.5721 -176.5667 -179.951 -DE/DX = 0.0 !

! D161 D(46,42,55,45) 0.0461 -40.2352 -1.789 -DE/DX = 0.0 !

! D162 D(46,42,55,56) 86.9779 0.9424 70.2451 -DE/DX = 0.0 !

! D163 D(27,43,50,54) -170.5113 -132.4893 -178.0303 -DE/DX = 0.0 !

! D164 D(41,43,50,54) -47.5018 -13.0334 -57.8125 -DE/DX = 0.0 !

! D165 D(47,43,50,54) 74.4088 109.616 64.5386 -DE/DX = 0.0 !

! D166 D(41,45,48,32) 70.338 44.6227 58.7641 -DE/DX = 0.0 !

! D167 D(41,45,48,51) -114.8071 -138.9788 -124.8278 -DE/DX = 0.0 !

! D168 D(54,45,48,32) 166.3838 -149.5309 141.2509 -DE/DX = 0.0 !

! D169 D(54,45,48,51) -18.7613 26.8676 -42.341 -DE/DX = 0.0 !

! D170 D(55,45,48,32) -93.9068 165.4199 -118.3398 -DE/DX = 0.0 !

! D171 D(55,45,48,51) 80.9481 -18.1817 58.0683 -DE/DX = 0.0 !

! D172 D(48,45,54,50) -90.313 -150.4912 -92.364 -DE/DX = 0.0 !

! D173 D(55,45,54,50) 155.8995 -65.8767 150.7856 -DE/DX = 0.0 !

! D174 D(41,45,55,38) -4.2116 -78.4845 -2.8992 -DE/DX = 0.0 !

! D175 D(41,45,55,42) 177.1514 138.3444 179.0252 -DE/DX = 0.0 !

! D176 D(48,45,55,38) 158.0479 144.5988 173.7693 -DE/DX = 0.0 !

! D177 D(48,45,55,42) -20.5891 1.4278 -4.3062 -DE/DX = 0.0 !

! D178 D(54,45,55,38) -69.9785 34.8167 -86.9822 -DE/DX = 0.0 !

! D179 D(54,45,55,42) 111.3845 -108.3543 94.9423 -DE/DX = 0.0 !

! D180 D(43,50,54,41) 52.4173 58.8531 36.1012 -DE/DX = 0.0 !

! D181 D(43,50,54,45) 26.437 -34.4925 20.5685 -DE/DX = 0.0 !

! D182 D(43,50,54,56) -135.7346 -160.228 -155.3426 -DE/DX = 0.0 !

! D183 D(29,52,53,33) 4.5503 24.7945 3.0254 -DE/DX = 0.0 !

! D184 D(29,52,53,41) -177.1285 -155.2182 -179.8833 -DE/DX = 0.0 !

! D185 D(38,55,56,54) 94.0931 66.8798 105.4349 -DE/DX = 0.0 !

! D186 D(42,55,56,54) -148.7848 -110.7701 -133.1362 -DE/DX = 0.0 !

Largest change from initial coordinates is atom 25 2.022 Angstoms.

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