Electronic Supplementary Material (ESI) for Analyst.

Supporting Information for

Resonant X-ray emission spectroscopy of platinum anticancer diastereomer complexes

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Contents

1. Preparation of the platinum complexes

The anticancer coordinates were prepared according to a previously published procedure by our group.[1]

2. NMR spectra

Purity of the final compounds was assessed by the means of qHNMR. Spectra are given below.

[1] Berger, G.; Leclercqz, H.; Derenne, A.; Gelbcke, M.; Goormaghtigh, E.; Nève, J.; Mathieu, V.; Dufrasne, F. *Bioorg. Med. Chem.* **2014**, *22*, 3527-3536.

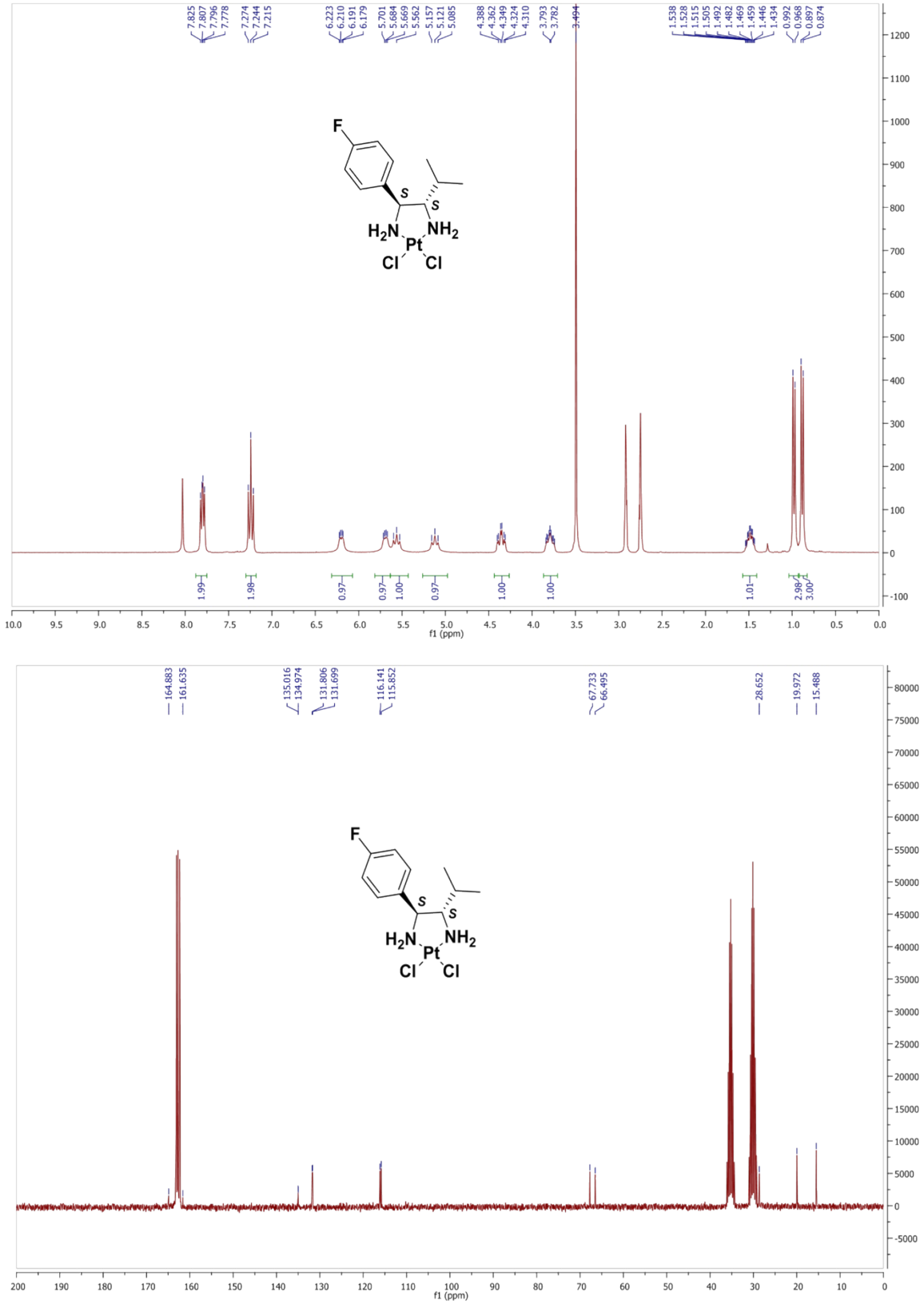


Figure S1. ^{1}H and ^{13}C NMR spectra of compound ***trans*-1**.

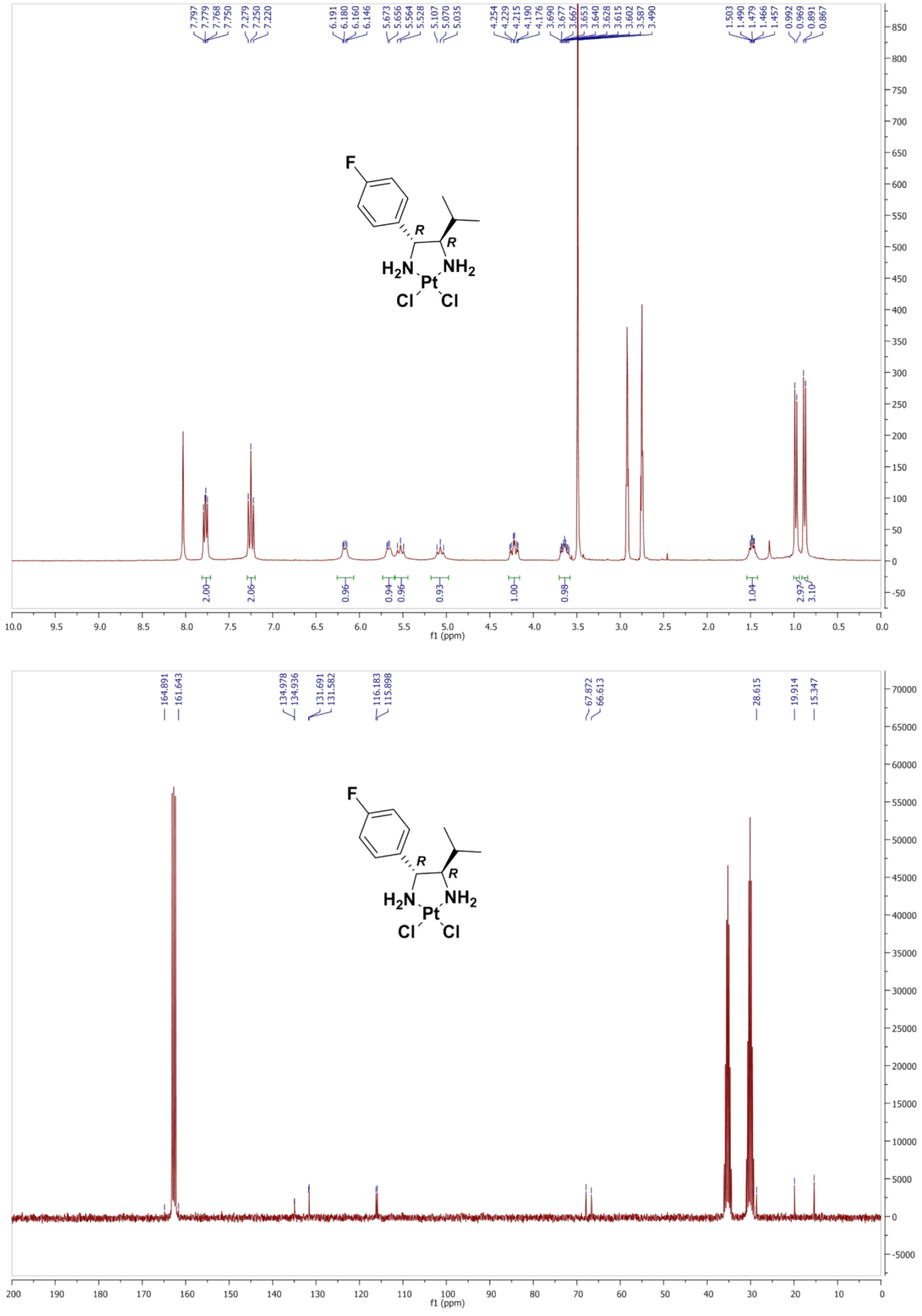


Figure S2. ^{1}H and ^{13}C NMR spectra of compound ***trans*-2**.

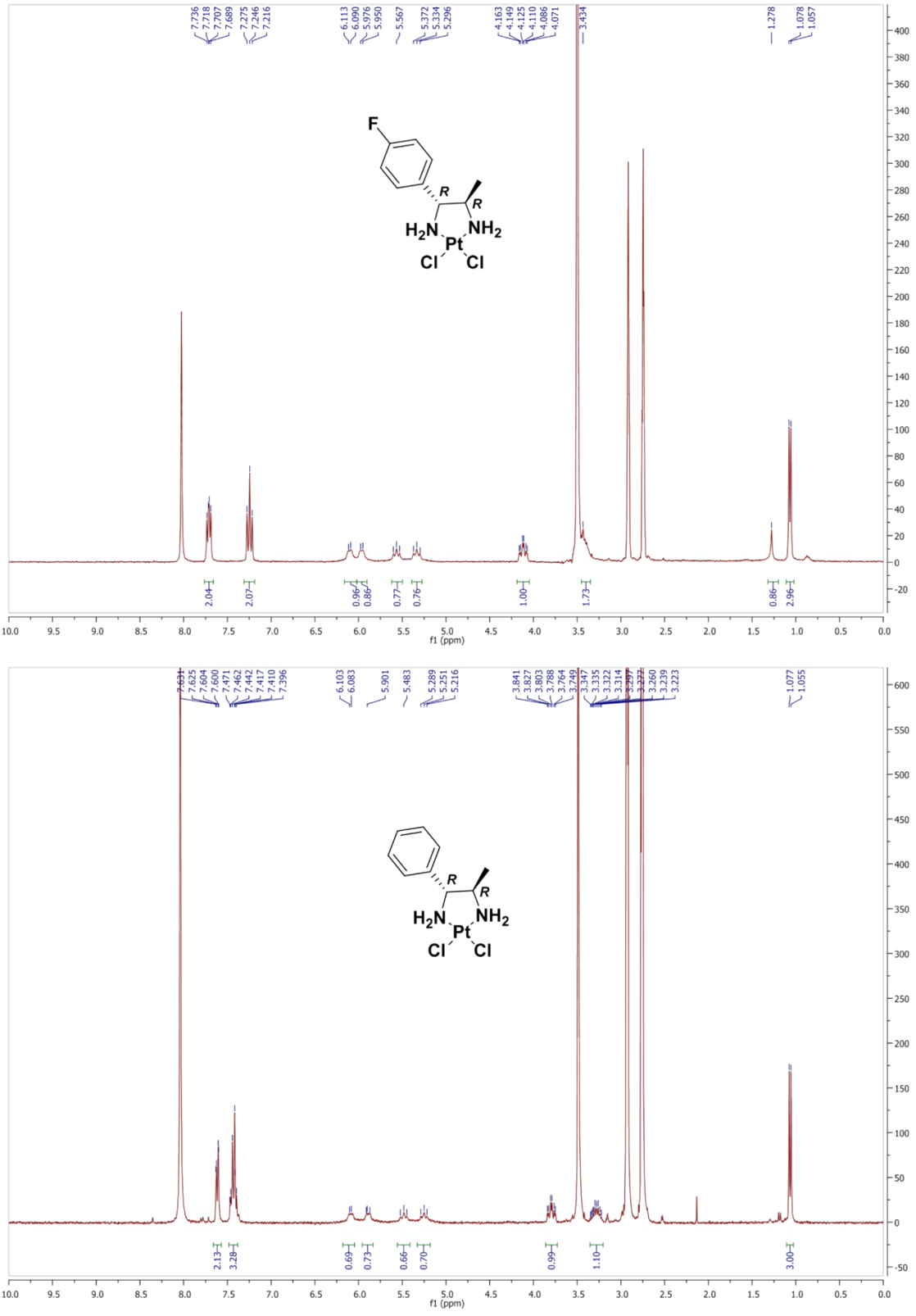


Figure S3. ^{1}H NMR spectra of compound ***trans*-3** and ***trans*-4**. No ^{13}C spectra due to low solubility in DMF-d_7

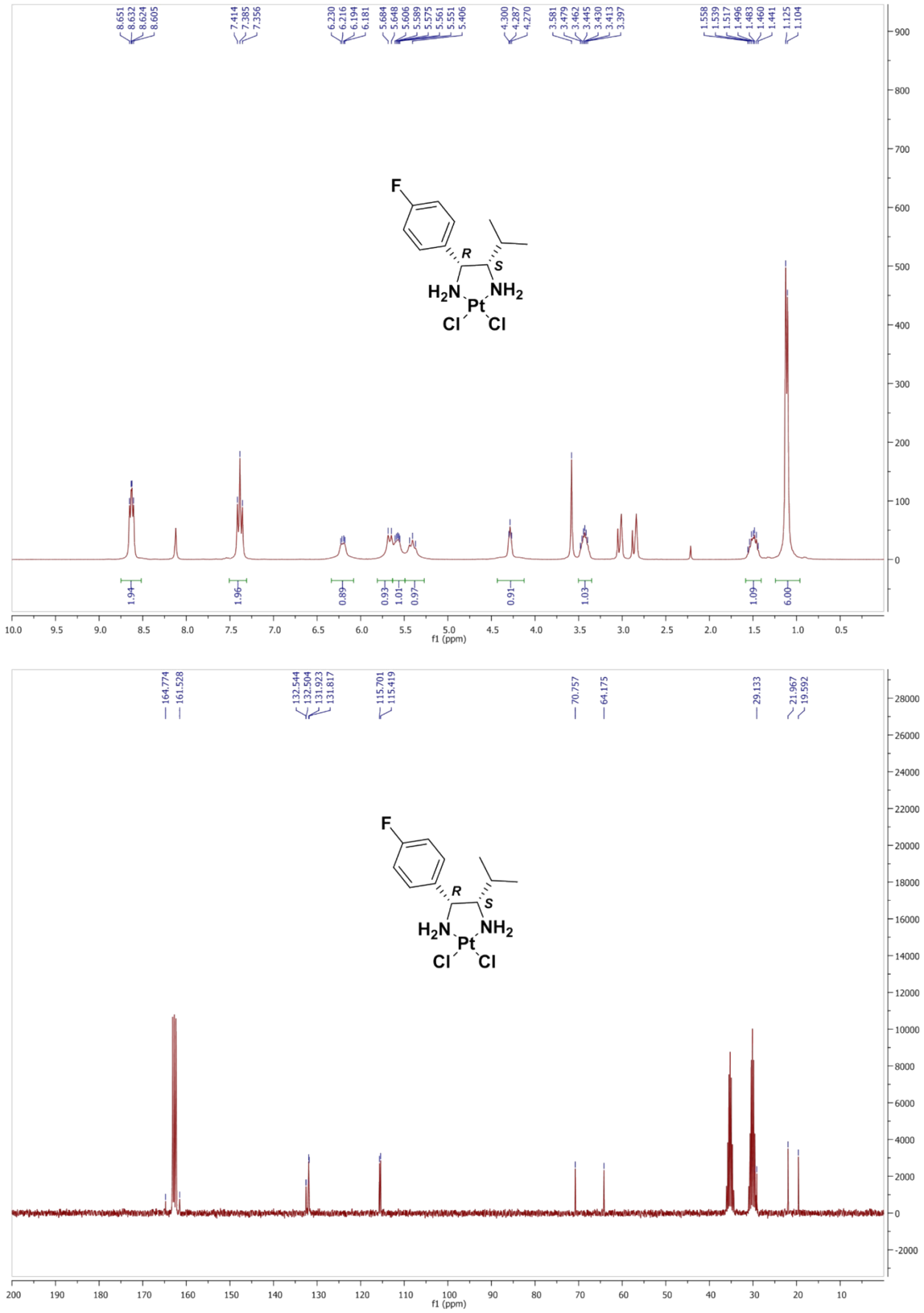


Figure S4. ^{1}H and ^{13}C NMR spectra of compound ***cis*-1**.

3. FEFF

The multi-objective genetic algorithm optimized the S02, FMS, SCF, EX1, and EX2 FEFF9.0 parameters, which are related to experimental resolution, Fermi level position and son on. For more information on physical meaning of parameters, the authors advise to readers to read support information of FEFF9.0 code, available elsewhere. [2]

4. DFT methods

All quantum chemical computations were performed using Gaussian09 revision D.01. Geometries were fully optimized using the ωB97x-D exchange-correlation functional[3] together with the balanced polarized triple-zeta basis set from Ahlrichs and co-workers, def2-TZVP.[4,5] The Stuttgart/Dresden effective core potential was used for the Pt atom.

Optimized geometries were verified by frequency calculations as minima (i.e. zero imaginary frequencies) and free energies were corrected to account for the zero-point energy.

Total DFT energy, root mean square (RMS) gradient norm at the end of the geometry optimization, number of imaginary frequencies, dipole moment and Cartesian coordinates are given for all the calculated structures.

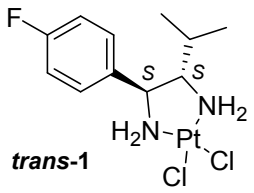
4.1. Gaussian full reference

Gaussian 09, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R.

[2] http://leonardo.phys.washington.edu/feff/Docs/feff9/feff90/feff90_users_guide.pdf
[3] Chai, J.-D.; Head-Gordon, M. *Phys. Chem. Chem. Phys.* **2008**, *10*, 6615-6620
[4] Weigend, F.; Ahlrichs, R. *Phys. Chem. Chem. Phys.* **2005**, *7*, 3297-3305.
[5] Weigend, F. *Phys. Chem. Chem. Phys.* **2006**, *8*, 1057-1065.

Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowskiand, D. J. Fox, Gaussian, Inc., Wallingford CT, 2010.

4.2. Geometries and optimization data

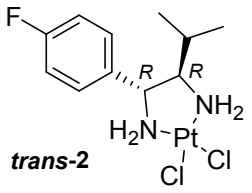


***trans*-1**

Level of theory: ωB97x-D/def2TZVP
Total Energy = -1678.80528460 au
RMS Gradient Norm = 0.00001032 au
Imaginary Frequencies = 0
Dipole Moment = 17.4850 Debye

Symbol	X	Y	Z
C	0.644628	1.296155	-0.35947
C	1.07217	0.055272	0.428562
H	0.704082	1.065481	-1.42547
H	0.923846	0.250195	1.490847
C	2.507544	-0.3442	0.202102
C	3.367011	-0.47803	1.285416
C	2.996134	-0.58373	-1.08009
C	4.693433	-0.83707	1.105241
H	2.999705	-0.30003	2.288672
C	4.316012	-0.94775	-1.28113
H	2.351036	-0.48369	-1.94534
C	5.14127	-1.06443	-0.17928
H	5.369913	-0.9397	1.942633
H	4.705771	-1.13342	-2.27249
C	1.506794	2.537677	-0.09783
C	1.60051	2.924404	1.376366
C	1.034664	3.714859	-0.94847
H	2.510278	2.267736	-0.43656
H	2.071743	2.146778	1.977967
H	2.203203	3.827122	1.478374
H	0.622175	3.144388	1.811343
H	0.916351	3.430112	-1.99595
H	0.081812	4.114105	-0.59186

H	1.76189	4.52538	-0.90002
N	0.120983	-1.0424	0.090441
H	0.197901	-1.78857	0.77529
N	-0.79982	1.513492	-0.07821
H	-1.21136	2.120493	-0.7799
Pt	-1.79347	-0.29185	-0.00567
H	0.361876	-1.45635	-0.80667
H	-0.92317	1.98157	0.815967
F	6.42378	-1.41182	-0.36706
Cl	-2.72186	-2.4357	0.095768
Cl	-3.87226	0.774663	-0.12371

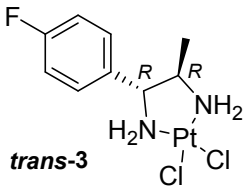


***trans*-2**

Level of theory: ωB97x-D/def2TZVP
Total Energy = -1678.80528450 au
RMS Gradient Norm = 0.00000906 au
Imaginary Frequencies = 0
Dipole Moment = 17.4851 Debye

Symbol	X	Y	Z
Pt	1.793466	-0.29183	-0.00553
N	0.799798	1.513483	-0.07802
N	-0.12098	-1.04236	0.090459
H	1.211347	2.120577	-0.77961
H	-0.1981	-1.78855	0.775247
H	0.923067	1.981464	0.81621
H	-0.36163	-1.45625	-0.80674
C	-0.6446	1.296132	-0.35949
C	-1.07222	0.055263	0.428511
H	-0.70382	1.065299	-1.42547
C	-2.50759	-0.34423	0.202082
C	-2.99623	-0.58377	-1.08007
C	-3.367	-0.47806	1.285429
C	-4.31611	-0.94778	-1.28105
H	-2.35116	-0.48372	-1.94535
C	-4.69343	-0.83709	1.105314
H	-2.99964	-0.30006	2.28866
C	-5.14131	-1.06444	-0.17918
H	-4.70592	-1.13345	-2.2724
H	-5.36987	-0.93972	1.942731
H	-0.92394	0.250205	1.490798
F	-6.42384	-1.41183	-0.3669

Cl	2.722011	-2.4356	0.095111
Cl	3.872315	0.774561	-0.12345
C	-1.50679	2.537662	-0.09819
C	-1.03446	3.714778	-0.9488
C	-1.60084	2.92448	1.375965
H	-2.51019	2.267692	-0.4371
H	-0.91601	3.42998	-1.99624
H	-1.76163	4.525345	-0.90049
H	-0.08165	4.113971	-0.59206
H	-2.07195	2.146776	1.977545
H	-0.62264	3.144769	1.811043
H	-2.20379	3.827033	1.477807

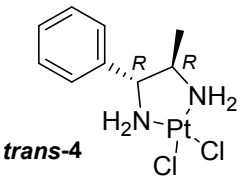


***trans*-3**

Level of theory: ωB97x-D/def2TZVP
Total Energy = -1599.94289864 au
RMS Gradient Norm = 0.00001904 au
Imaginary Frequencies = 0
Dipole Moment = 17.4427 Debye

Symbol	X	Y	Z
C	0.673269	1.610385	-0.31554
C	1.157578	0.384419	0.467692
H	0.775946	1.415806	-1.38626
H	0.999087	0.579638	1.531593
C	2.614985	0.060445	0.240573
C	3.495651	0.030926	1.321422
C	3.104783	-0.20375	-1.04202
C	4.845264	-0.25422	1.138065
H	3.129046	0.23468	2.321327
C	4.448103	-0.49487	-1.24605
H	2.445767	-0.18164	-1.90418
C	5.291532	-0.51224	-0.1463
H	5.537528	-0.27701	1.969903
H	4.839234	-0.69912	-2.23439
C	1.427197	2.879055	0.051864
H	2.479977	2.785922	-0.21957
N	0.261658	-0.7615	0.126987
H	0.365046	-1.49772	0.821562
N	-0.78908	1.744826	-0.06032
H	-1.21539	2.337583	-0.76838
Pt	-1.68667	-0.10853	-0.00083

H	0.534646	-1.17719	-0.7617
H	-0.94605	2.213574	0.830773
F	6.596203	-0.79012	-0.3366
Cl	-2.50764	-2.3159	0.08612
Cl	-3.83269	0.854174	-0.14719
H	1.011249	3.736678	-0.48044
H	1.365618	3.070042	1.127356

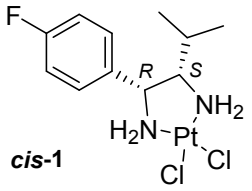


***trans*-4**

Level of theory: ωB97x-D/def2TZVP
Total Energy = -1500.72787987 au
RMS Gradient Norm = 0.00001244 au
Imaginary Frequencies = 0
Dipole Moment = 19.0592 Debye

Symbol	X	Y	Z
C	-1.00625	1.537008	0.324976
C	-1.45023	0.287656	-0.44477
H	-1.08531	1.342776	1.397828
H	-1.31592	0.482177	-1.51206
C	-2.88891	-0.09512	-0.18824
C	-3.79796	-0.13432	-1.24487
C	-3.32989	-0.40116	1.102615
C	-5.13057	-0.47078	-1.01808
H	-3.46445	0.102066	-2.2499
C	-4.65901	-0.74199	1.330201
H	-2.64333	-0.37045	1.9434
C	-5.56297	-0.77564	0.26967
H	-5.82877	-0.49445	-1.84665
H	-4.98934	-0.97572	2.335537
C	-1.81696	2.77192	-0.0359
H	-2.86121	2.63582	0.249944
N	-0.50137	-0.81633	-0.11013
H	-0.58258	-1.56035	-0.79926
N	0.445228	1.731298	0.046267
H	0.856165	2.350797	0.740412
Pt	1.4191	-0.08266	-0.00741
H	-0.74467	-1.2379	0.784505
H	0.567679	2.195509	-0.85271
H	-6.5999	-1.03561	0.447716
Cl	2.326501	-2.25558	-0.08923
Cl	3.524041	0.969262	0.11488

H	-1.43008	3.647666	0.488945
H	-1.77765	2.962364	-1.11252



***cis*-1**

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RMS Gradient Norm = 0.00001042 au
Imaginary Frequencies = 0
Dipole Moment = 18.2734 Debye

Symbol	X	Y	Z
C	0.559163	1.750366	-0.63298
C	0.998545	0.472543	-1.37453
H	-0.11274	2.270233	-1.32139
C	1.696934	2.722422	-0.25544
C	2.388969	2.405893	1.076659
C	1.176837	4.164053	-0.24575
H	2.442415	2.64337	-1.05375
H	2.708777	1.365175	1.159796
H	3.278215	3.031907	1.177566
H	1.73948	2.63776	1.927495
H	0.764726	4.446673	-1.21776
H	0.393109	4.296986	0.508223
H	1.983829	4.859299	-0.00222
N	-0.24084	-0.32801	-1.61925
H	-0.00339	-1.29581	-1.82516
N	-0.29693	1.358084	0.51961
H	-0.81769	2.161838	0.862026
Pt	-1.56973	-0.16145	-0.04522
H	-0.71205	0.026873	-2.44865
H	0.273239	1.038577	1.30071
Cl	-2.86036	-1.95731	-0.85092
Cl	-2.99024	0.24782	1.782265
H	1.390609	0.793151	-2.34189
C	2.076373	-0.34815	-0.69811
C	3.396998	-0.17245	-1.11918
C	1.817893	-1.24057	0.345811
C	4.446266	-0.8413	-0.50007
H	3.618052	0.502982	-1.93842
C	2.85337	-1.92697	0.972113

H	0.802628	-1.41669	0.685696
C	4.149513	-1.70594	0.540201
H	5.471131	-0.7028	-0.81968
H	2.658627	-2.62194	1.778817
F	5.157719	-2.36372	1.145307