Supplementary Information

Controlling Pt nanoparticle formation through Se•••Pt interactions on electrode surface

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Materials and Methods

Chemicals and reagents: All chemicals except EDOS[1] were purchased from Aldrich. Reagent grade sodium dodecyl sulfate (SDS, $C_{12}H_{25}NaOSO_3$) was used as the surface-active agent. Toray™ carbon paper foils (thickness: 0.2 mm, purchased from Alfa Aesar) were used as the substrate for electrodepositon of PEDOT, PEDOS and Pt. All solutions were prepared in doubly distilled water. A glass cell of about 50 ml capacity with suitable ground–glass joints through which to introduce a working electrode, Pt foil auxiliary electrodes, and a saturated calomel reference electrode (SCE) was used for the electrochemical deposition and characterization of PEDOT/C, PEDOS/C, Pt/C, Pt-PEDOT/C, and Pt-PEDOS/C electrodes. All potential values are reported against SCE.

Electrode assembly: A 7 mm × 3 cm foil was sectioned out of a carbon sheet. A 1.4 cm^2 area at one end was exposed to the electrolyte and the rest of the length of the foil was used to make electrical contact through a Cu wire. An electrolyte of 0.1 M $NaNO_3$ + 0.01 M EDOT or EDOS + 0.01 M SDS was used for PEDOT or PEDOS deposition. The electrodeposition was carried out at a constant potential of 0.9 V. A charge of 0.03 C was used for preparation of both PEDOS/C and PEDOT/C. After the electrochemical deposition of PEDOT/PEDOS, the electrode was separated from the cell and washed repeatedly in 0.1 M $NaNO_3$ solution under stirring for about 5 min. Pt particles were potentiostatically deposited at 0.10 V in an aqueous electrolyte consisting of 0.001 M H_2PtCl_6 and 0.1 M H_2SO_4. Current was monitored for the intended duration of deposition. The geometric area of the carbon substrate exposed to electrolyte was used to calculate the current density.

Instruments: Potentiostatic deposition of PEDOS/PEDOT and Pt as well as cyclic voltammetry experiments were carried out using a Bio-Logic SAS (model VSP) Potentiostat/Galvanostat. Scanning electron microscopy (SEM) images were recorded using a Leo Ultra 55 FEG SEM with

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an operating voltage of 3 keV power and at a working distance of 3 mm. Transmission electron microscopy (TEM) images were obtained using a Philips CM120 TEM. XPS measurements were carried out with a Kratos AXIS ULTRA system using a monochromatized Al Kα X-ray source (hν = 1486.6 eV) at 75 W and detection pass energies ranging between 20 and 80 eV. A low-energy electron flood gun (eFG) was applied for charge neutralization. AFM topography images were acquired using a P47 AFM (NT-MDT) equipped with a small scanner. Images were recorded in tapping mode in the air at room temperature (20-23°C) using silicon micro cantilevers (OMCL-AC240TS-W2, Olympus). The set point ratio was adjusted to 0.75–0.8 (corresponding to "light" tapping) and the scan rate was set to 1 Hz. Imaging was carried out in different scan directions and at different scales to verify the consistency and robustness of the evaluated structures. AFM data were processed using the NT-MDT Nova[2] and Gwyddion[3] software. EQCM measurements (CH Instruments, model 400A) were carried out in a Teflon cell, consisting of an Au coated quartz crystal as the working electrode (from CH Instruments), a Pt-wire counter electrode, and an Ag/AgCl, reference electrode. The resonating frequency of the crystal in air was 8 MHz, and the surface area of the Au electrode was 0.205 cm^2. Before the electrochemical experiments, the quartz crystal working electrode was run in double distilled water to obtain a stable frequency versus time plot (i.e. until the frequency stabilized at or around 0 Hz over a period of 400 s).

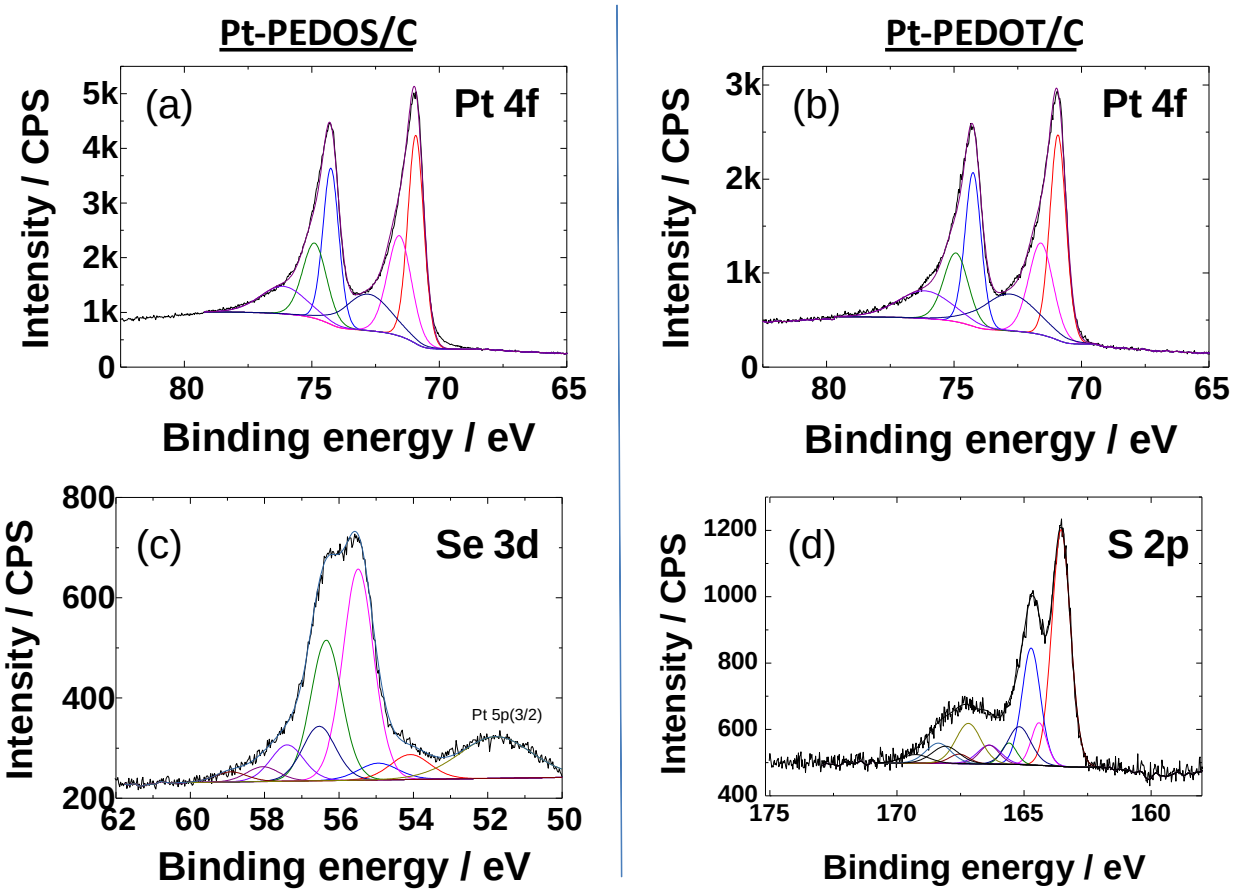


Figure S1. High resolution XPS of (a) the Pt 4f region of Pt-PEDOS/C, (b) the Pt 4f region of Pt-PEDOT/C electrode, (c) the Se 3d region of Pt-PEDOS/C electrode, and (d) the S 2p region of Pt-PEDOT/C electrode.

XPS of Pt NP on PEDOS/C or PEDOT/C (Figure S1a,b) shows major peaks attributed to Pt(0) and minor peaks attributed to Pt(II) (e.g., PtO or $Pt(OH)_2$).[4] These XPS spectra are characteristic to Pt NPs[5]. No substantial contribution from Pt(IV) is observed. XPS of sulfur (Figure S1d) shows some contribution of SO_4^{2-} (from electrolyte).

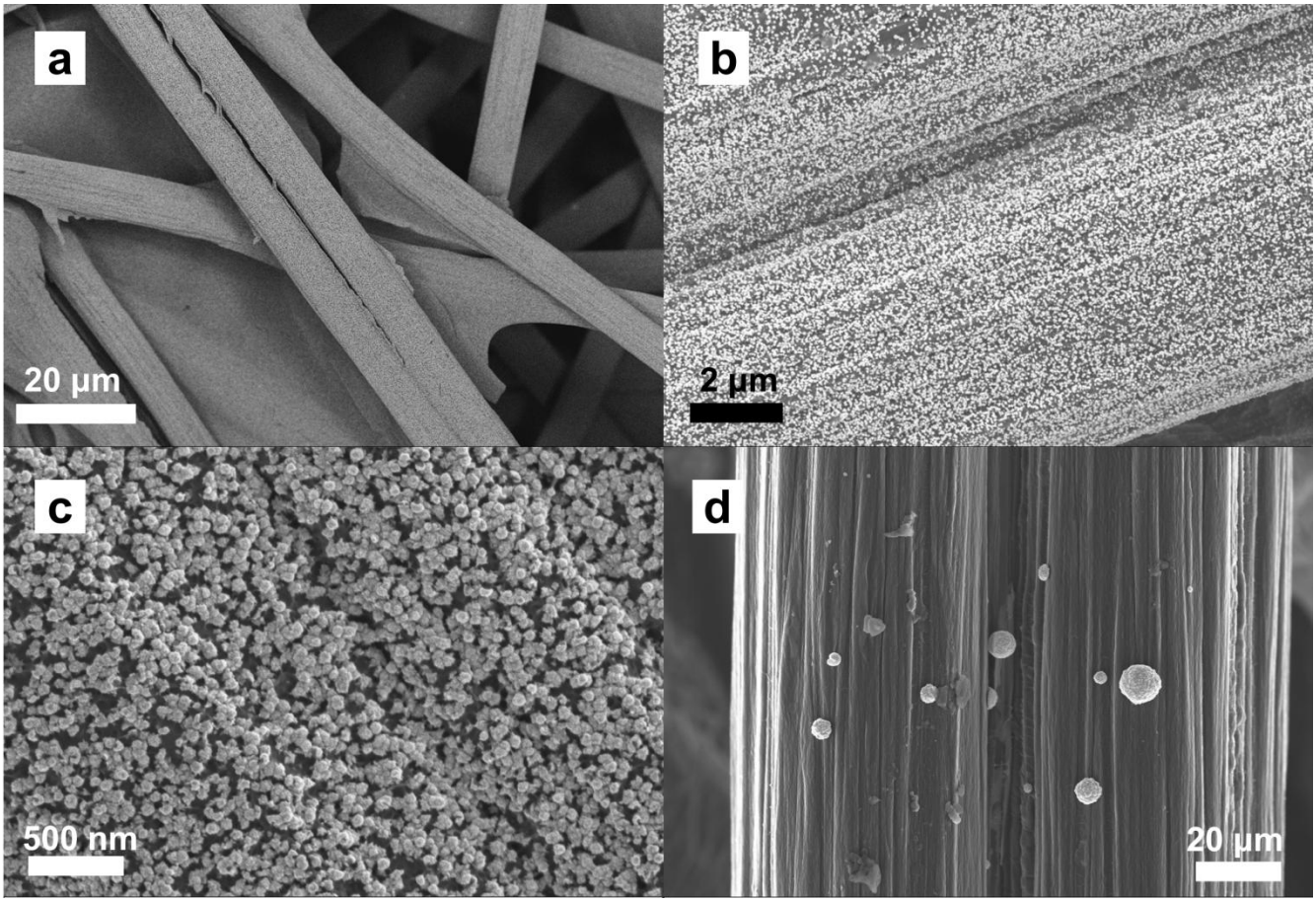


Figure S2. Additional SEM images of Pt nanoparticles on (a-c) PEDOS/C electrode and (d) on bare carbon paper electrode.

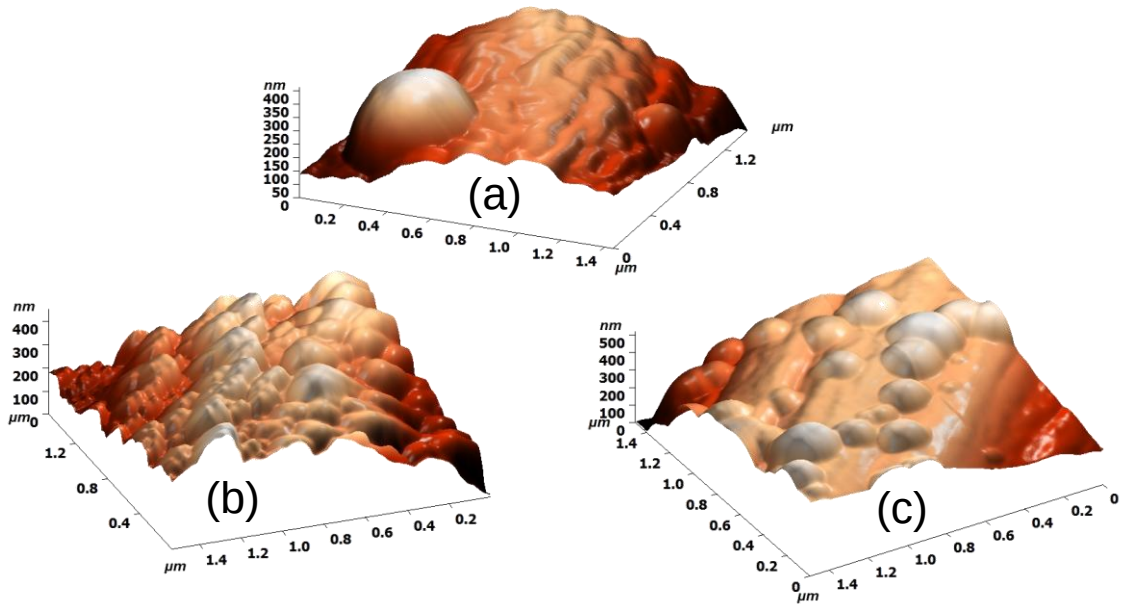


Figure S3. 3D surface AFM images of Pt nanoparticles on (a) bare carbon paper, (b) PEDOS/C and (c) PEDOS/C electrodes (only plane level correction was applied on the raw data).

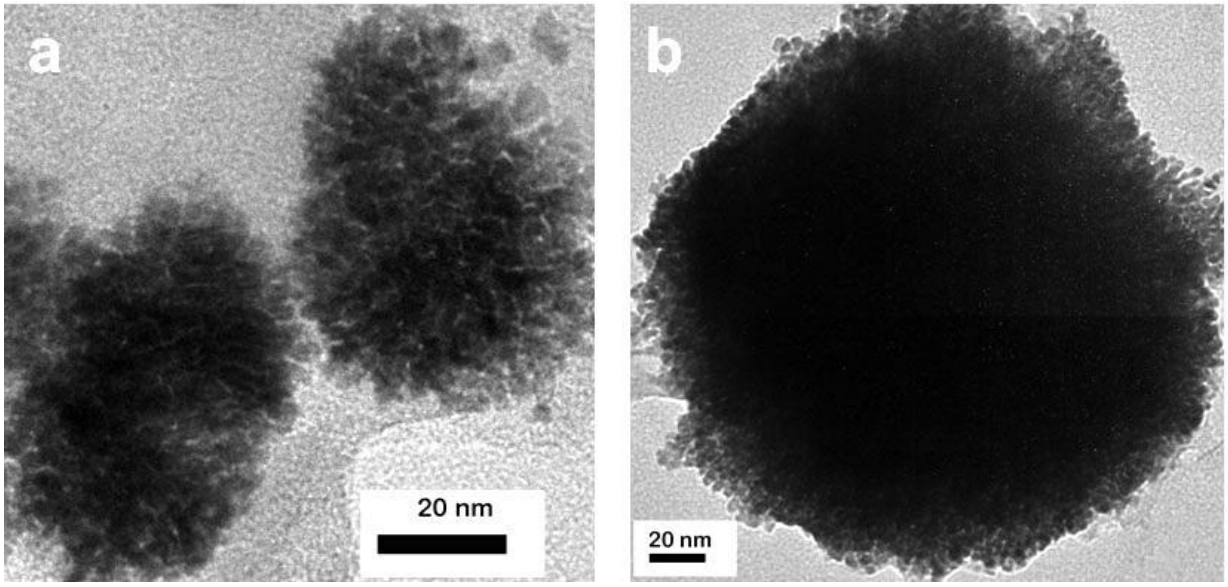


Figure S4. TEM images of Pt nanoparticles deposited on (a) PEDOS/C and (b) PEDOT/C electrodes.

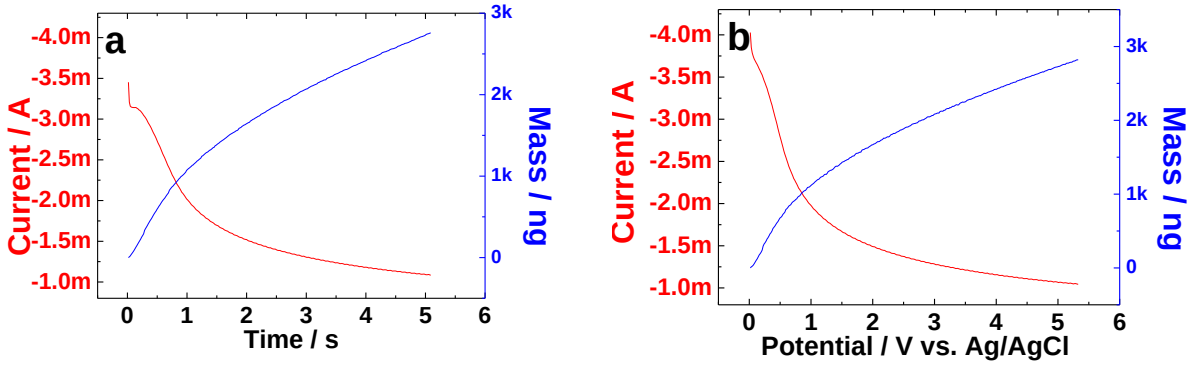


Figure S5. The EQCM study of Pt deposition on (a) PEDOS and (b) PEDOT coated gold crystal. At a deposition charge of 8.5 mC, the deposited mass of Pt on a PEDOS coated gold crystal is 2.76 µg, whereas on a PEDOT surface it is 2.82 µg.

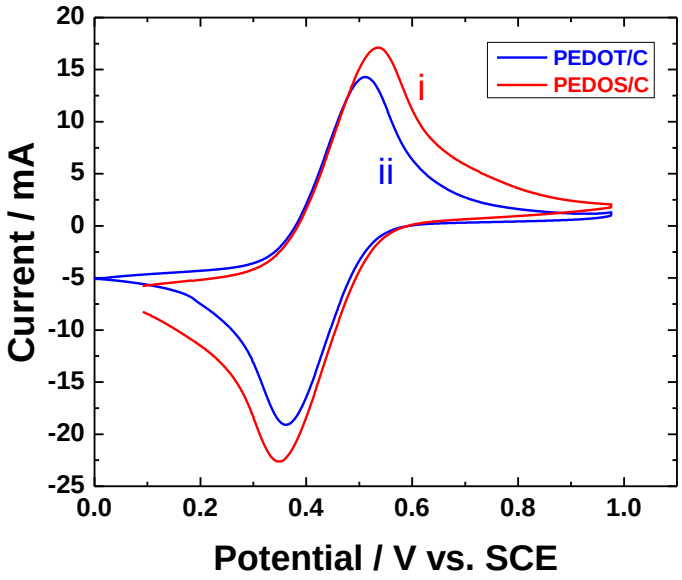
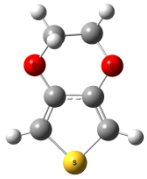


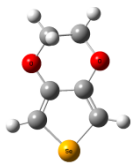
Figure S6. The electrochemical redox reaction on (i) PEDOS/C and (ii) PEDOT/C surface measured in 0.1 $FeCl_3$ and 0.1 HCl. The electrochemically accessible surface area (obtained from integration of the CV curve) of PEDOS/C electrode is 1.4 times larger than that of PEDOT/C electrode.

Computational Details: All calculations were carried out using the Gaussian 09 Revision A.02 software package.[6] The M06L functional[7] was used for all the calculations. Geometry optimizations were carried out with an SDD basis set for all the elements and the optimized structures were confirmed as minima by frequency calculations. The single point calculations on the optimized geometry were performed with the SDB-cc-pVDZ basis set. The SDB-cc-pVDZ basis set combines the Dunning cc-pVDZ basis set on the main group elements and the Stuggart-Dresden basis set-RECP on the transition metals. It includes an additional *f*-type polarization exponent for the transition metals, which is taken as the geometric average of the two *f*-exponents as detailed in ref. 8.



EDOT $E_{SDB\text{-}cc\text{-}pVDZ}$ = -780.8244866 a.u.

6	1.252503000	1.270456000	0.077574000
6	-0.000356000	0.721496000	0.042053000
16	2.506168000	0.000002000	0.000264000
6	-0.000336000	-0.721491000	-0.042101000
8	-1.181506000	1.466098000	0.099105000
6	1.252522000	-1.270433000	-0.077853000
8	-1.181492000	-1.466074000	-0.099396000
1	1.529952000	-2.307655000	-0.136846000
6	-2.350259000	-0.681845000	0.337357000
1	-2.324317000	-0.574365000	1.426902000
1	-3.213913000	-1.275573000	0.045018000
6	-2.350356000	0.681798000	-0.337302000
1	-3.213964000	1.275499000	-0.044759000
1	-2.324697000	0.574297000	-1.426851000
1	1.529929000	2.307694000	0.136267000



EDOS $E_{SDB\text{-}cc\text{-}pVDZ}$ =-755.8302418 a.u.

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6	-0.524236000	-0.723621000	-0.040660000
8	-1.714381000	1.460846000	0.098103000
6	0.712087000	-1.306814000	-0.077004000
8	-1.714405000	-1.460768000	-0.099364000

1	0.929442000	-2.360730000	-0.135960000
6	-2.883700000	-0.680885000	0.338441000
1	-2.858210000	-0.571765000	1.427982000
1	-3.746361000	-1.277015000	0.047311000
6	-2.884296000	0.680738000	-0.337397000
1	-3.746502000	1.276889000	-0.044907000
1	-2.860772000	0.571391000	-1.426973000
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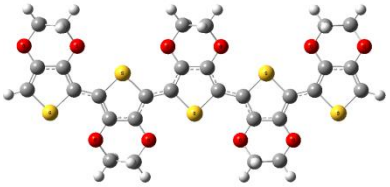
34	2.092295000	0.000025000	0.000068000



$(EDOT)_5$ $E_{SDB\text{-}cc\text{-}pVDZ}$ =-3899.4200935 a.u.

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6	-1.296789000	0.156366000	0.172088000
6	0.707110000	-1.101603000	0.228753000
6	-0.710323000	-1.099279000	0.223685000
6	0.655325000	-3.466895000	-0.061704000
6	-0.667370000	-3.432310000	0.691308000
1	0.484429000	-3.487503000	-1.142984000
1	-0.498061000	-3.360391000	1.770499000
8	-1.465787000	-2.275561000	0.252813000
8	1.459746000	-2.279249000	0.273707000
1	1.267077000	-4.316659000	0.234420000
1	-1.281211000	-4.302441000	0.467877000
6	-2.677858000	0.477169000	0.128984000
6	-3.273502000	1.728282000	0.081968000
6	-4.691491000	1.716104000	0.014062000
6	-5.265370000	0.455860000	-0.007579000
6	2.677986000	0.473325000	0.150556000
6	3.272525000	1.724648000	0.094896000
6	4.689872000	1.713509000	0.016982000
6	5.265018000	0.453794000	0.000136000
6	6.642740000	0.110146000	-0.083412000
6	7.220431000	-1.147975000	-0.104651000
6	8.649687000	-1.156777000	-0.208562000
6	9.205041000	0.092642000	-0.278536000
1	10.244067000	0.360083000	-0.355687000
6	-6.643131000	0.110304000	-0.082832000
6	-7.217126000	-1.149297000	-0.113754000
6	-8.647059000	-1.161787000	-0.206129000
6	-9.206795000	0.086620000	-0.256481000
1	-10.247045000	0.351990000	-0.323420000
6	-3.323620000	4.073691000	-0.331071000
6	-4.678292000	4.071735000	0.364205000
1	-2.729848000	4.942621000	-0.055074000
1	-3.446085000	4.033800000	-1.418242000
1	-5.285627000	4.924379000	0.067573000

1	-4.555651000	4.060189000	1.452022000
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8	-5.453534000	2.887208000	-0.043306000
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6	-8.587242000	-3.511143000	0.181014000
6	4.677343000	4.071080000	0.355142000
6	3.316659000	4.068440000	-0.328301000
6	8.601780000	-3.499544000	0.214183000
6	7.228787000	-3.505296000	-0.443243000
1	9.185653000	-4.373186000	-0.068906000
1	8.506434000	-3.452625000	1.304178000
1	6.630942000	-4.356948000	-0.124934000
1	7.321115000	-3.499821000	-1.534324000
1	-7.319635000	-3.477504000	-1.576950000
1	-6.615979000	-4.355251000	-0.187310000
1	-8.483583000	-3.481995000	1.270914000
1	-9.170203000	-4.382151000	-0.111958000
1	4.564250000	4.064802000	1.444023000
1	5.281397000	4.922708000	0.048985000
1	3.429671000	4.023897000	-1.416300000
1	2.724328000	4.937936000	-0.050991000
8	9.387166000	-2.345311000	-0.254305000
8	6.462964000	-2.320119000	-0.020575000
8	5.450029000	2.885111000	-0.053283000
8	2.528098000	2.907824000	0.119742000
8	-6.455137000	-2.319778000	-0.050168000
8	-9.380825000	-2.352220000	-0.261795000
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16	0.001218000	1.430294000	0.147981000
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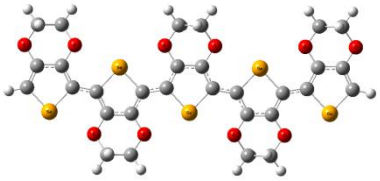

$(EDOS)_5$ $E_{SDB\text{-}cc\text{-}pVDZ}$ =-3774.4731706 a.u.

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6	0.709120000	1.193162000	0.158030000
6	-0.659812000	3.561334000	-0.178451000
6	0.662566000	3.546804000	0.575261000
1	-0.488328000	3.554028000	-1.260006000
1	0.492065000	3.499464000	1.655834000
8	1.459637000	2.381909000	0.162667000
8	-1.459024000	2.382662000	0.189570000
1	-1.270432000	4.419575000	0.095642000
1	1.273641000	4.414074000	0.332521000

6	2.732119000	-0.287159000	0.096162000
6	3.356837000	-1.524529000	0.058164000
6	4.775313000	-1.526162000	0.011239000
6	5.401329000	-0.290840000	-0.007311000
6	-2.732832000	-0.286466000	0.127846000
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6	-4.775951000	-1.525179000	0.040648000
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6	-7.431574000	1.186327000	-0.092078000
6	-8.864376000	1.178654000	-0.168052000
6	-9.441009000	-0.062664000	-0.210237000
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6	8.865371000	1.178966000	-0.149761000
6	9.442414000	-0.062088000	-0.194374000
1	10.498067000	-0.276992000	-0.243263000
6	3.389862000	-3.879532000	-0.358033000
6	4.733089000	-3.893919000	0.357644000
1	2.785046000	-4.745543000	-0.096090000
1	3.529502000	-3.834582000	-1.443156000
1	5.335384000	-4.752825000	0.067839000
1	4.593030000	-3.884574000	1.443545000
8	2.606342000	-2.712964000	0.075352000
8	5.521972000	-2.716030000	-0.035536000
6	7.471684000	3.552642000	-0.438248000
6	8.825371000	3.532835000	0.256028000
6	-4.738469000	-3.888388000	0.412853000
6	-3.389279000	-3.884314000	-0.291757000
6	-8.827597000	3.534476000	0.226108000
6	-7.468468000	3.550913000	-0.457610000
1	-9.426027000	4.400338000	-0.051284000
1	-8.709291000	3.498193000	1.314594000
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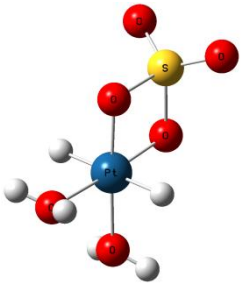
1	-7.581707000	3.534187000	-1.546714000
1	7.593258000	3.541345000	-1.526505000
1	6.874321000	4.412041000	-0.139497000
1	8.698555000	3.491334000	1.343383000
1	9.425922000	4.400019000	-0.012504000
1	-4.607723000	-3.864951000	1.499672000
1	-5.338920000	-4.750551000	0.129016000
1	-3.520231000	-3.854078000	-1.378502000
1	-2.787130000	-4.747087000	-0.013388000
8	-9.606246000	2.370138000	-0.219946000
8	-6.686957000	2.376432000	-0.038211000
8	-5.522705000	-2.715096000	-0.002495000
8	-2.608145000	-2.712499000	0.131623000
8	6.686979000	2.376044000	-0.030870000
8	9.607609000	2.370691000	-0.189383000
34	-8.131992000	-1.446158000	-0.146508000
34	-4.070569000	1.119641000	0.079920000
34	-0.000593000	-1.451244000	0.129389000

34	4.070317000	1.118659000	0.061698000
34	8.133137000	-1.445921000	-0.148342000

H_2O $E_{SDB\text{-}cc\text{-}pVDZ}$ = -76.4131849 a.u.

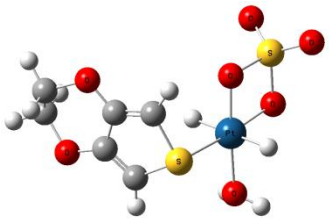
8	0.000000000	0.000000000	0.112783000
1	0.000000000	0.792988000	-0.451132000
1	0.000000000	-0.792988000	-0.451132000

6-coordinate complex



$[Pt(SO_4)(H_2O)_2(H)_2]$ $E_{SDB\text{-}cc\text{-}pVDZ}$ =-972.3655097 a.u.

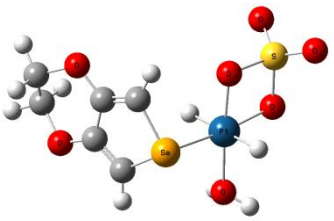
78	0.669376000	-0.000087000	0.000019000
8	-0.861224000	-1.279455000	0.000237000
8	-0.861198000	1.279231000	-0.000440000
16	-2.233312000	-0.000043000	-0.000004000
8	-3.041580000	-0.000360000	-1.366094000
8	-3.041423000	0.000415000	1.366180000
8	2.223632000	1.502298000	-0.000078000
1	2.258371000	2.044057000	-0.807309000
8	2.224473000	-1.501409000	0.000092000
1	2.259865000	-2.043565000	0.807021000
1	2.258601000	2.043731000	0.807362000
1	2.260744000	-2.042281000	-0.807656000
1	0.671505000	-0.000233000	-1.685607000
1	0.671163000	0.000009000	1.685595000



$[Pt(SO_4)(H_2O)(EDOT)(H)_2]$ $E_{SDB\text{-}cc\text{-}pVDZ}$ =-1676.7782313 a.u.

78	-1.015644000	-0.673316000	0.010537000
8	-1.183914000	1.194672000	-0.696201000
8	-2.737133000	-0.061471000	0.905258000
16	-2.778410000	1.626820000	0.168994000
8	-2.555622000	2.754927000	1.266598000
8	-3.975804000	1.795369000	-0.861338000

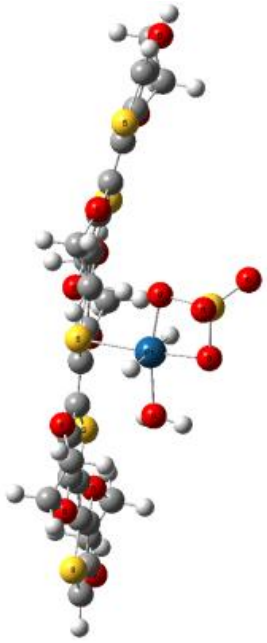
8	-0.988332000	-2.669128000	0.877696000
1	-0.951614000	-2.646040000	1.850950000
1	-1.728638000	-3.216474000	0.558688000
1	-0.122244000	-0.089876000	1.313068000
1	-1.911834000	-1.254473000	-1.287125000
6	1.715929000	0.500453000	-1.466164000
1	1.195618000	1.171396000	-2.125216000
6	2.338233000	-1.528395000	0.017632000
1	2.366494000	-2.491269000	0.494812000
6	2.796005000	0.699720000	-0.667715000
6	3.146062000	-0.448192000	0.177302000
6	4.822255000	1.752471000	0.047135000
6	4.680645000	0.970663000	1.338158000
8	3.507772000	1.883337000	-0.618687000
8	4.220239000	-0.408905000	1.046507000
1	5.141902000	2.775557000	0.228682000
1	5.517213000	1.261244000	-0.640322000
1	5.636289000	0.841467000	1.839881000
1	3.961837000	1.441835000	2.013549000
16	1.079835000	-1.180910000	-1.238096000



$[Pt(SO_4)(H_2O)(EDOS)(H)_2]$ $E_{SDB\text{-}cc\text{-}pVDZ}$= -1651.7928625

78	-1.063579000	-0.583440000	0.188251000
8	-1.406136000	1.099911000	-0.848674000
8	-2.787419000	0.109271000	1.071956000
16	-2.992203000	1.580047000	0.015230000
8	-2.810469000	2.929046000	0.835375000
8	-4.242805000	1.447634000	-0.956925000
8	-0.855525000	-2.355130000	1.444323000
1	-0.677626000	-2.113453000	2.371298000
1	-1.626696000	-2.946296000	1.369520000
1	-0.135285000	0.286498000	1.289486000
1	-1.991477000	-1.455837000	-0.910161000
6	1.674683000	0.597699000	-1.430085000
1	1.179542000	1.264459000	-2.115645000
6	2.360173000	-1.385849000	0.199690000
1	2.458469000	-2.298084000	0.764161000
6	2.723082000	0.846642000	-0.604699000
6	3.096232000	-0.249771000	0.306184000
6	4.677978000	2.028229000	0.141168000
6	4.517730000	1.299250000	1.459194000
8	3.388234000	2.061131000	-0.579902000
8	4.138381000	-0.111021000	1.207754000
1	4.938825000	3.073913000	0.285103000
1	5.425031000	1.542023000	-0.493280000

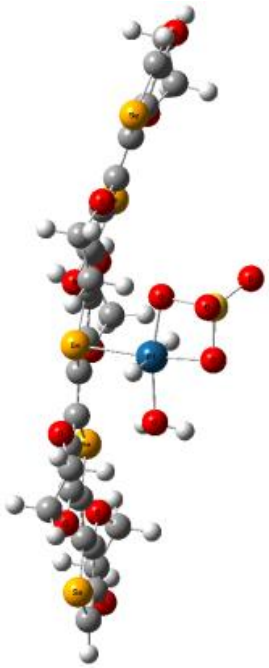
1	5.454443000	1.239745000	2.007768000
1	3.747096000	1.763656000	2.080344000
34	1.010845000	-1.188030000	-1.158700000



$[Pt(SO_4)(H_2O)((EDOT)_5)(H)_2]$ $E_{SDB\text{-}cc\text{-}pVDZ}$ =-4795.398821 a.u.

6	1.554473000	0.846259000	-0.866258000
6	-1.079566000	0.960394000	-0.999501000
6	0.982242000	2.071046000	-0.578912000
6	-0.441595000	2.138169000	-0.668746000
6	0.968007000	4.260586000	0.379227000
6	-0.293022000	4.505714000	-0.432888000
1	0.724157000	3.978932000	1.407303000
1	-0.050005000	4.743692000	-1.473086000
8	-1.151017000	3.307434000	-0.403414000
8	1.758171000	3.169459000	-0.232737000
1	1.630674000	5.122872000	0.372621000
1	-0.900764000	5.298066000	-0.002045000
6	-2.442361000	0.626115000	-1.078936000
6	-2.990983000	-0.603926000	-1.434904000
6	-4.392373000	-0.693254000	-1.287253000
6	-5.001778000	0.462963000	-0.820335000
6	2.907392000	0.426648000	-0.852624000
6	3.408105000	-0.820569000	-1.208056000
6	4.803350000	-0.986150000	-1.021404000
6	5.462801000	0.134014000	-0.537803000
6	6.846704000	0.291697000	-0.257639000
6	7.508732000	1.409875000	0.221274000
6	8.921240000	1.246877000	0.395566000
6	9.374684000	-0.003325000	0.069099000
1	10.380901000	-0.381725000	0.110689000
6	-6.379793000	0.684334000	-0.569936000
6	-6.993863000	1.828785000	-0.085257000
6	-8.412305000	1.731109000	0.074950000

6	-8.920001000	0.507177000	-0.273660000
1	-9.943389000	0.176871000	-0.242013000
6	-2.896834000	-2.961439000	-1.670942000
6	-4.305220000	-2.890221000	-2.239779000
1	-2.285513000	-3.687711000	-2.201546000
1	-2.890350000	-3.174496000	-0.598181000
1	-4.847859000	-3.818225000	-2.072584000
1	-4.287476000	-2.652839000	-3.308055000
8	-2.218565000	-1.659945000	-1.884709000
8	-5.107230000	-1.854900000	-1.550769000
6	-7.052476000	3.905044000	1.077058000
6	-8.459202000	4.071488000	0.521385000
6	4.619434000	-3.147175000	-2.034812000
6	3.196745000	-3.168756000	-1.495320000
6	9.079691000	3.592078000	0.770451000
6	7.663088000	3.519871000	1.321134000
1	9.701977000	4.265471000	1.356157000
1	9.072155000	3.908857000	-0.277519000
1	7.156287000	4.480809000	1.262863000
1	7.665076000	3.159023000	2.354522000
1	-7.076960000	3.500130000	2.093328000
1	-6.496955000	4.840240000	1.061467000
1	-8.425813000	4.431228000	-0.512370000
1	-9.052352000	4.750715000	1.130408000
1	4.631340000	-2.855453000	-3.089093000
1	5.112955000	-4.108552000	-1.909658000
1	3.163934000	-3.417529000	-0.430709000
1	2.562469000	-3.851459000	-2.055717000
8	9.736009000	2.276747000	0.874498000
8	6.845974000	2.606624000	0.498958000
8	5.454447000	-2.191857000	-1.273570000
8	2.584419000	-1.837548000	-1.679414000
8	-6.279365000	2.986746000	0.218209000
8	-9.184139000	2.789025000	0.563610000
16	8.042249000	-1.054414000	-0.492490000
16	4.272209000	1.494474000	-0.296471000
16	0.210276000	-0.348549000	-1.274669000
16	-3.754949000	1.757896000	-0.546186000
16	-7.635771000	-0.601293000	-0.832729000
78	-0.058940000	-1.570917000	0.877078000
1	-0.118734000	-3.022711000	0.037272000
1	-0.000977000	-0.104165000	1.715228000
8	2.104992000	-1.728327000	1.251948000
1	2.196296000	-2.054231000	2.169325000
8	-2.074468000	-1.511166000	0.929406000
8	-0.466982000	-2.604094000	2.601572000
1	2.563511000	-0.868403000	1.134760000
16	-2.279572000	-2.627024000	2.406128000
8	-2.837369000	-4.036835000	1.904014000
8	-2.998653000	-1.928597000	3.638164000

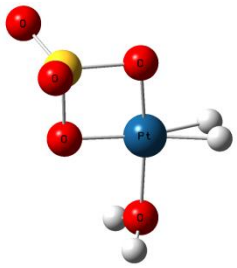


$[Pt(SO_4)(H_2O)((EDOS)_5)(H)_2]$ $E_{SDB\text{-}cc\text{-}pVDZ}$ =-4670.4615968 a.u.

6	1.548161000	0.787878000	-0.937621000
6	-1.158042000	0.883975000	-1.061723000
6	0.932113000	1.996168000	-0.667213000
6	-0.491741000	2.053304000	-0.752961000
6	0.900739000	4.174950000	0.332070000
6	-0.363545000	4.425051000	-0.473674000
1	0.659492000	3.868977000	1.354129000
1	-0.122935000	4.684256000	-1.509504000
8	-1.209401000	3.220262000	-0.464467000
8	1.698586000	3.105427000	-0.304567000
1	1.552801000	5.045517000	0.343798000
1	-0.974801000	5.206437000	-0.027326000
6	-2.534531000	0.610578000	-1.067257000
6	-3.124154000	-0.617584000	-1.361287000
6	-4.515713000	-0.716582000	-1.148967000
6	-5.151690000	0.423937000	-0.674606000
6	2.920752000	0.450187000	-0.856488000
6	3.477278000	-0.791937000	-1.144861000
6	4.865698000	-0.944936000	-0.905057000
6	5.539774000	0.171252000	-0.432065000
6	6.921125000	0.263350000	-0.116198000
6	7.596059000	1.375724000	0.356089000
6	9.000921000	1.224221000	0.600349000
6	9.504535000	-0.024386000	0.347784000
1	10.529873000	-0.337292000	0.466327000
6	-6.531126000	0.560701000	-0.379090000
6	-7.167770000	1.688450000	0.114931000
6	-8.576657000	1.584273000	0.350162000
6	-9.123304000	0.360240000	0.063356000
1	-10.159570000	0.082728000	0.175944000
6	-3.016355000	-2.990945000	-1.538080000
6	-4.447584000	-2.948761000	-2.048637000
1	-2.422721000	-3.729105000	-2.073095000

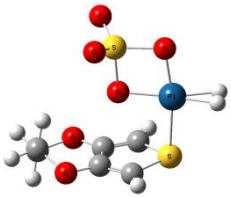
1	-2.960378000	-3.168204000	-0.460397000
1	-4.972244000	-3.877144000	-1.831764000
1	-4.476832000	-2.743315000	-3.123556000
8	-2.365753000	-1.689605000	-1.822570000
8	-5.225960000	-1.900413000	-1.356571000
6	-7.180970000	3.794014000	1.245558000
6	-8.613995000	3.940842000	0.758030000
6	4.719731000	-3.158029000	-1.835946000
6	3.281325000	-3.160860000	-1.340650000
6	9.134445000	3.589989000	0.893332000
6	7.694965000	3.538978000	1.382402000
1	9.729300000	4.290254000	1.476571000
1	9.172531000	3.863332000	-0.166527000
1	7.190364000	4.495601000	1.261656000
1	7.650459000	3.220855000	2.428891000
1	-7.151236000	3.403175000	2.267274000
1	-6.633656000	4.732696000	1.188268000
1	-8.632835000	4.283511000	-0.282115000
1	-9.181149000	4.628036000	1.383200000
1	4.762675000	-2.914214000	-2.901833000
1	5.210131000	-4.112183000	-1.653272000
1	3.214305000	-3.356823000	-0.266606000
1	2.668111000	-3.874282000	-1.886680000
8	9.782311000	2.283650000	1.084666000
8	6.921857000	2.588737000	0.561798000
8	5.524723000	-2.166292000	-1.093324000
8	2.676461000	-1.841398000	-1.610943000
8	-6.451653000	2.866785000	0.360477000
8	-9.323627000	2.656169000	0.860306000
34	8.156944000	-1.216275000	-0.276567000
34	4.308250000	1.666318000	-0.251894000
34	0.171168000	-0.544743000	-1.355941000
34	-3.872946000	1.863287000	-0.450561000
34	-7.818890000	-0.869038000	-0.574827000
78	-0.075352000	-1.586817000	0.948001000
1	-0.090850000	-3.097835000	0.205918000
1	-0.059303000	-0.069013000	1.675826000
8	2.091232000	-1.645778000	1.328226000
1	2.203692000	-1.850644000	2.277148000
8	-2.092948000	-1.556024000	0.984542000
8	-0.505414000	-2.505664000	2.761049000
1	2.527154000	-0.795783000	1.093291000
16	-2.295089000	-2.562499000	2.534579000
8	-2.835043000	-4.009963000	2.127302000
8	-3.059127000	-1.775492000	3.685302000

5-coordinate complex



$[Pt(SO_4)(H_2O)(H)_2]$ $E_{SDB\text{-}cc\text{-}pVDZ}$ =-895.9953918 a.u.

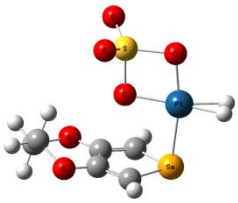
78	0.793552000	-0.205847000	0.000004000
8	-0.851266000	-1.296006000	0.000227000
8	-0.545666000	1.239994000	-0.000232000
16	-2.084559000	0.152658000	-0.000012000
8	-2.883038000	0.262152000	-1.366426000
8	-2.882814000	0.262826000	1.366480000
8	2.479574000	1.177688000	-0.000175000
1	2.569585000	1.720547000	0.803093000
1	2.569157000	1.721636000	-0.802754000
1	1.891551000	-1.500975000	-0.428136000
1	1.891303000	-1.500907000	0.428692000



$[Pt(SO_4)(EDOT)(H)_2]$ $E_{SDB\text{-}cc\text{-}pVDZ}$ =-1600.4144277 a.u.

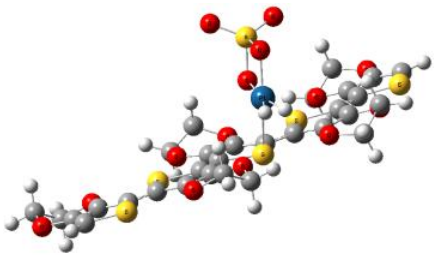
78	1.283147000	-0.772221000	-0.004592000
8	2.650933000	0.718667000	-0.040754000
8	0.109228000	0.836832000	0.006442000
16	1.453290000	2.122693000	-0.039950000
8	1.484792000	2.953554000	1.314377000
8	1.449523000	2.915729000	-1.416560000
1	2.380906000	-2.048208000	0.414543000
1	2.361917000	-2.054208000	-0.452469000
6	-1.559137000	-1.333428000	1.340648000
6	-1.643732000	-1.425463000	-1.253802000
6	-2.368148000	-0.405811000	0.768937000
6	-2.429631000	-0.466023000	-0.697297000
1	-1.469803000	-1.672496000	-2.284803000
1	-1.297676000	-1.487888000	2.371185000
6	-3.410412000	1.714372000	0.636699000
6	-4.108158000	1.257451000	-0.628928000
8	-3.094301000	0.529667000	1.473079000
8	-3.214598000	0.388652000	-1.433179000
1	-4.058868000	2.327922000	1.255898000
1	-2.477340000	2.242249000	0.421106000
1	-5.017191000	0.694618000	-0.399792000
1	-4.342343000	2.090404000	-1.287432000

16	-0.711689000	-2.288355000	0.045895000



$[Pt(SO_4)(EDOS)(H)_2]$ $E_{SDB\text{-}cc\text{-}pVDZ}$ =-1575.4282425 a.u.

78	1.314052000	-0.674042000	0.002567000
8	2.733284000	0.793749000	0.004855000
8	0.198217000	0.979127000	-0.038845000
16	1.584209000	2.215533000	-0.046550000
8	1.578945000	3.058731000	1.301826000
8	1.646228000	3.000256000	-1.427445000
1	2.362221000	-1.966447000	0.472994000
1	2.374345000	-1.979952000	-0.398519000
6	-1.618405000	-1.066313000	1.352309000
6	-1.712411000	-1.103388000	-1.309465000
6	-2.310246000	-0.056259000	0.767212000
6	-2.381424000	-0.085542000	-0.705005000
1	-1.595053000	-1.294953000	-2.362160000
1	-1.393905000	-1.204971000	2.395955000
6	-3.084888000	2.182015000	0.663496000
6	-3.842439000	1.837638000	-0.601308000
8	-2.927104000	0.952672000	1.478674000
8	-3.078175000	0.863549000	-1.416683000
1	-3.643455000	2.866862000	1.295878000
1	-2.090561000	2.584290000	0.450135000
1	-4.818408000	1.400869000	-0.372793000
1	-3.963592000	2.700510000	-1.252126000
34	-0.781978000	-2.159208000	0.002726000

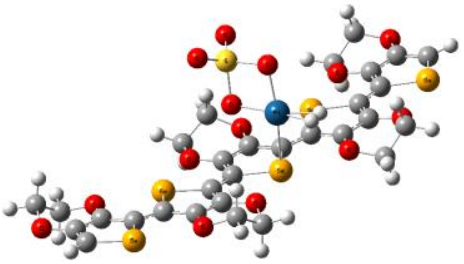


$[Pt(SO_4)((EDOT)_5)(H)_2]$ $E_{SDB\text{-}cc\text{-}pVDZ}$ =-4719.0226355 a.u.

6	-1.496794000	0.510147000	-0.675940000
6	1.137895000	0.581371000	-0.906597000
6	-0.892293000	1.708411000	-0.357745000
6	0.532666000	1.740777000	-0.473324000
6	-0.839073000	4.024175000	0.290348000
6	0.528878000	3.690897000	0.861616000
1	-0.745448000	4.534857000	-0.672288000
1	0.453457000	3.136907000	1.801823000
8	1.268911000	2.861252000	-0.114495000

8	-1.632530000	2.791836000	0.087343000
1	-1.432853000	4.625041000	0.975891000
1	1.136106000	4.582662000	0.995190000
6	2.503684000	0.252960000	-1.026168000
6	3.063834000	-0.982923000	-1.314245000
6	4.478179000	-1.021450000	-1.268893000
6	5.084609000	0.189406000	-0.973960000
6	-2.859174000	0.137910000	-0.689871000
6	-3.412927000	-1.112898000	-0.924365000
6	-4.829070000	-1.157498000	-0.892851000
6	-5.446068000	0.056510000	-0.636812000
6	-6.835497000	0.337939000	-0.542431000
6	-7.450518000	1.551377000	-0.284388000
6	-8.882222000	1.510161000	-0.254935000
6	-9.401050000	0.267217000	-0.502838000
1	-10.433835000	-0.031912000	-0.534318000
6	6.471425000	0.472640000	-0.858097000
6	7.079493000	1.679451000	-0.556168000
6	8.510102000	1.638610000	-0.501600000
6	9.034457000	0.403590000	-0.776106000
1	10.068147000	0.106452000	-0.795370000
6	3.069915000	-3.244130000	-2.096762000
6	4.359385000	-3.389405000	-1.301655000
1	2.422726000	-4.111491000	-1.978976000
1	3.283355000	-3.074510000	-3.156470000
1	4.959047000	-4.223042000	-1.660237000
1	4.151167000	-3.506538000	-0.233566000
8	2.280666000	-2.105471000	-1.586996000
8	5.201100000	-2.194171000	-1.499108000
6	7.185216000	4.053022000	-0.362237000
6	8.470965000	3.831933000	0.420708000
6	-4.716168000	-3.535070000	-0.980000000
6	-3.415038000	-3.354332000	-1.748746000
6	-8.862744000	3.734697000	0.592858000
6	-7.562761000	3.929778000	-0.173200000
1	-9.498021000	4.616038000	0.534206000
1	-8.660913000	3.490248000	1.640826000
1	-6.960075000	4.731197000	0.248811000
1	-7.759710000	4.125958000	-1.231881000
1	7.402230000	4.289163000	-1.408698000
1	6.572499000	4.837035000	0.077656000
1	8.250376000	3.548295000	1.454861000
1	9.105102000	4.715864000	0.406287000
1	-4.520021000	-3.715199000	0.08191200
1	-5.315000000	-4.345717000	-1.389626000
1	-3.610195000	-3.120178000	-2.799403000
1	-2.776773000	-4.233474000	-1.675146000
8	-9.655010000	2.649791000	-0.013885000
8	-6.724167000	2.721190000	-0.060658000
8	-5.552873000	-2.331359000	-1.116842000
8	-2.629226000	-2.254278000	-1.153120000
8	6.347044000	2.840414000	-0.312381000
8	9.276562000	2.771429000	-0.211636000

16	-8.107716000	-0.936979000	-0.775882000
16	-4.185812000	1.346167000	-0.402296000
16	-0.177780000	-0.687039000	-1.184947000
16	3.817039000	1.463001000	-0.704945000
16	7.749243000	-0.793853000	-1.104794000
78	0.108436000	-1.843583000	0.982770000
8	0.465385000	-2.529251000	2.856732000
8	0.989327000	-0.257726000	1.812005000
16	1.280642000	-0.996196000	3.485983000
8	0.420948000	-0.256554000	4.601787000
8	2.831076000	-1.222103000	3.760923000
1	-1.040604000	-3.043352000	0.490039000
1	-0.272140000	-3.368088000	0.251640000



$[Pt(SO_4)((EDOS)_5)(H)_2]$ $E_{SDB\text{-}cc\text{-}pVDZ}$ =-4594.0817657 a.u.

6	-1.346032000	0.253311000	-0.955899000
6	1.373411000	0.263030000	-0.915555000
6	-0.705723000	1.472780000	-0.846437000
6	0.724546000	1.473774000	-0.809794000
6	-0.667723000	3.878304000	-0.622476000
6	0.621483000	3.640159000	0.143127000
1	-0.459954000	4.227497000	-1.638096000
1	0.432929000	3.248343000	1.147032000
8	1.439312000	2.654255000	-0.602135000
8	-1.455855000	2.632329000	-0.713158000
1	-1.318990000	4.584257000	-0.110622000
1	1.230069000	4.539612000	0.193095000
6	2.754592000	-0.014792000	-0.844201000
6	3.361709000	-1.262827000	-0.864587000
6	4.774342000	-1.286107000	-0.759095000
6	5.411450000	-0.058559000	-0.661346000
6	-2.728312000	-0.021921000	-0.915143000
6	-3.329662000	-1.271999000	-0.956846000
6	-4.740828000	-1.302892000	-0.841156000
6	-5.382719000	-0.079842000	-0.723536000
6	-6.780367000	0.134985000	-0.594218000
6	-7.425376000	1.353147000	-0.467861000
6	-8.853448000	1.318917000	-0.341123000
6	-9.412528000	0.069193000	-0.381133000
1	-10.461877000	-0.165275000	-0.297534000
6	6.808327000	0.166072000	-0.541403000
6	7.445415000	1.390435000	-0.433419000
6	8.874252000	1.367957000	-0.312128000
6	9.441798000	0.121702000	-0.339272000

1	10.493233000	-0.104476000	-0.259550000
6	3.415142000	-3.604638000	-1.360111000
6	4.673823000	-3.663604000	-0.507173000
1	2.779871000	-4.474597000	-1.202603000
1	3.666643000	-3.510891000	-2.421042000
1	5.294702000	-4.519114000	-0.765227000
1	4.419965000	-3.694402000	0.557901000
8	2.598514000	-2.445298000	-0.956300000
8	5.510317000	-2.482676000	-0.768518000
6	7.542180000	3.778328000	-0.630993000
6	8.790917000	3.688629000	0.232048000
6	-4.613508000	-3.665032000	-0.533038000
6	-3.363256000	-3.629640000	-1.398737000
6	-8.783845000	3.631364000	0.236744000
6	-7.539019000	3.743106000	-0.629893000
1	-9.423743000	4.505274000	0.130951000
1	-8.511436000	3.494849000	1.288687000
1	-6.911245000	4.581785000	-0.335283000
1	-7.808271000	3.829020000	-1.687495000
1	7.805786000	3.848558000	-1.691015000
1	6.909898000	4.617274000	-0.347326000
1	8.523926000	3.568073000	1.287330000
1	9.424688000	4.564680000	0.108959000
1	-4.353717000	-3.641833000	0.529894000
1	-5.224612000	-4.538859000	-0.749363000
1	-3.628245000	-3.595813000	-2.460157000
1	-2.713548000	-4.480595000	-1.202677000
8	-9.606553000	2.495275000	-0.206475000
8	-6.694493000	2.548506000	-0.449788000
8	-5.465365000	-2.506284000	-0.846653000
8	-2.556948000	-2.440970000	-1.071144000
8	6.706331000	2.580615000	-0.427855000
8	9.619734000	2.550590000	-0.195186000
78	0.166006000	-1.408075000	1.512266000
8	0.255418000	-1.251084000	3.550953000
8	-0.614772000	0.406573000	1.813769000
16	-0.447881000	0.430969000	3.662184000
8	-1.859852000	0.437751000	4.393086000
8	0.619259000	1.532455000	4.097666000
1	0.459933000	-3.107042000	1.397494000
1	1.248693000	-2.739406000	1.328420000
34	8.129710000	-1.247359000	-0.518203000
34	4.099430000	1.368524000	-0.663786000
34	0.009542000	-1.158479000	-1.018743000
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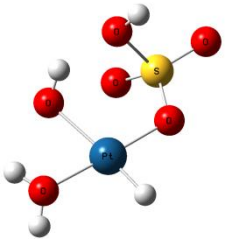
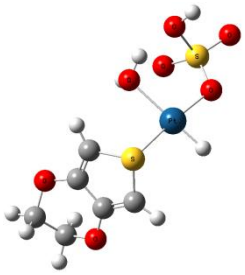
34	-8.091163000	-1.288185000	-0.581914000

4-coordinate complex



$[Pt(HSO_4)(H_2O)_2(H)]$ $E_{SDB\text{-}cc\text{-}pVDZ}$ =-972.4696669 a.u.

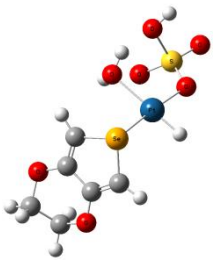
78	-0.930106000	-0.309399000	0.014526000
8	0.892050000	-1.189541000	0.101104000
16	2.211301000	-0.093091000	-0.160720000
8	1.970920000	0.924194000	-1.378284000
8	3.608174000	-0.813011000	0.054201000
8	1.905869000	1.136378000	1.277749000
1	2.213223000	0.724995000	2.118128000
8	-0.298351000	1.891220000	-0.056428000
1	0.322759000	2.001691000	0.707870000
1	0.244876000	2.000910000	-0.870558000
8	-2.814856000	0.644299000	0.004109000
1	-2.691950000	1.609236000	-0.077265000
1	-3.560420000	0.302618000	-0.514696000
1	-1.471518000	-1.765175000	0.055403000



$[Pt(HSO_4)(H_2O)(EDOT)(H)]$ $E_{SDB\text{-}cc\text{-}pVDZ}$ =-1676.8890707 a.u.

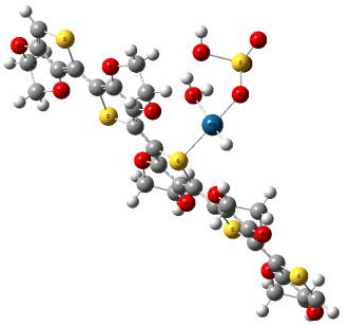
6	-2.098507000	0.117529000	1.437782000
6	-2.500681000	-1.378344000	-0.635961000
6	-3.144636000	0.503573000	0.661130000
1	-1.688041000	0.554309000	2.329666000
6	-3.367388000	-0.339741000	-0.518544000
1	-2.425630000	-2.137711000	-1.392906000
6	-5.191275000	1.636731000	0.148042000
6	-4.915550000	1.299287000	-1.304662000
1	-5.893951000	0.926314000	0.592957000
1	-4.185156000	1.986722000	-1.740761000
16	-1.356525000	-1.397993000	0.774514000
8	-4.395256000	-0.082146000	-1.412161000
8	-3.932359000	1.611884000	0.925904000
1	-5.566805000	2.650552000	0.263706000
1	-5.825632000	1.299498000	-1.899060000
78	0.800962000	-0.792523000	-0.050218000
8	2.685429000	-0.466339000	-0.821502000

16	3.414662000	1.045297000	-0.496197000
8	2.392516000	2.277399000	-0.548190000
8	4.861669000	1.138873000	-1.143162000
8	3.622107000	0.912195000	1.406042000
1	4.431571000	0.387668000	1.602410000
8	0.963965000	0.871163000	1.493779000
1	1.880070000	0.838191000	1.878039000
1	0.879477000	1.727712000	1.023393000
1	0.712529000	-1.911769000	-1.125940000



[Pt(HSO_4)(H_2O)(EDOS)(H)] $E_{SDB\text{-}cc\text{-}pVDZ}$ =-1651.9018967 a.u.

6	-2.029713000	0.030545000	1.424010000
6	-2.488172000	-1.070954000	-0.949978000
6	-3.020446000	0.597536000	0.688192000
1	-1.660724000	0.320368000	2.393473000
6	-3.266645000	-0.006543000	-0.631683000
1	-2.485170000	-1.645275000	-1.861373000
6	-4.974091000	1.956320000	0.343863000
6	-4.678969000	1.863474000	-1.139744000
1	-5.737003000	1.230702000	0.641103000
1	-3.891877000	2.563772000	-1.433712000
8	-4.249620000	0.489306000	-1.477946000
8	-3.743240000	1.700337000	1.122218000
1	-5.281509000	2.957514000	0.636269000
1	-5.568680000	2.032172000	-1.741623000
78	0.886402000	-0.677204000	-0.251087000
8	2.768626000	-0.156900000	-0.989994000
16	3.516571000	1.207894000	-0.306985000
8	2.500724000	2.409049000	-0.001796000
8	4.947136000	1.475400000	-0.943996000
8	3.785340000	0.586868000	1.491933000
1	4.610411000	0.051836000	1.525695000
8	1.145374000	0.525207000	1.665229000
1	2.079340000	0.391904000	1.981476000
1	1.049477000	1.476271000	1.444269000
1	0.716468000	-1.493220000	-1.565196000
34	-1.285934000	-1.495495000	0.504207000



$[Pt(HSO_4)(H_2O)((EDOT)_5)(H)]$ $E_{SDB\text{-}cc\text{-}pVDZ}$ =-4795.4929413 a.u.

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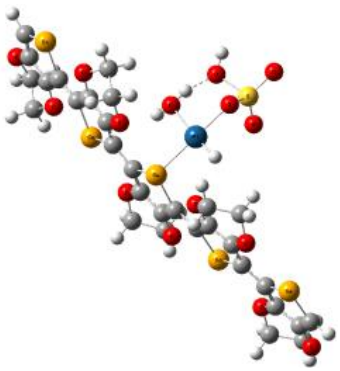
8	0.025550000	-3.929243000	1.191596000
16	-1.071093000	-4.198793000	2.445409000
8	-1.012008000	-3.103431000	3.621884000
8	-1.211671000	-5.738293000	2.821370000
8	-2.723831000	-3.724407000	1.509886000
1	-3.413478000	-4.321316000	1.884196000
8	-1.615217000	-1.260461000	1.546063000
1	-2.385547000	-1.872959000	1.451274000
1	-1.364624000	-1.238172000	2.493189000
1	1.278055000	-2.636974000	-0.545041000
6	-1.134374000	1.049233000	-0.509127000
6	1.510940000	0.997828000	-0.516620000
6	-0.502157000	2.153072000	0.024194000
6	0.925983000	2.115585000	0.040677000
6	-0.394035000	4.434894000	0.731017000
6	0.904205000	4.058061000	1.425828000
1	-0.197021000	4.897196000	-0.241065000
1	0.708536000	3.554284000	2.377223000
8	1.691097000	3.157772000	0.561644000
8	-1.225406000	3.232694000	0.527007000
1	-1.004034000	5.096532000	1.341782000
1	1.543194000	4.923527000	1.586394000
6	2.874642000	0.671628000	-0.686953000
6	3.423225000	-0.399490000	-1.378907000
6	4.836577000	-0.487934000	-1.319872000
6	5.457614000	0.532500000	-0.617108000
6	-2.510813000	0.774036000	-0.658373000
6	-3.101423000	-0.415527000	-1.057845000
6	-4.516960000	-0.426568000	-1.026685000
6	-5.099193000	0.770019000	-0.637904000
6	-6.480414000	1.077506000	-0.509763000
6	-7.069024000	2.279685000	-0.155286000
6	-8.500993000	2.261833000	-0.109356000
6	-9.046185000	1.048782000	-0.435153000
1	-10.084869000	0.772045000	-0.476181000
6	6.847076000	0.734812000	-0.400008000
6	7.472429000	1.752369000	0.301867000
6	8.902115000	1.669213000	0.339813000
6	9.408916000	0.596481000	-0.343808000
1	10.437734000	0.305549000	-0.463589000
6	3.415849000	-2.222174000	-2.932499000

6	4.667386000	-2.684425000	-2.201723000
1	2.741402000	-3.050133000	-3.142892000
1	3.675671000	-1.701964000	-3.859453000
1	5.265227000	-3.355878000	-2.813526000
1	4.410358000	-3.166530000	-1.252952000
8	2.635298000	-1.305282000	-2.081092000
8	5.542863000	-1.526845000	-1.930946000
6	7.618025000	3.910009000	1.306402000
6	8.893453000	3.405767000	1.965631000
6	-4.439857000	-2.792058000	-1.201236000
6	-3.124820000	-2.649358000	-1.949986000
6	-8.433258000	4.434628000	0.867109000
6	-7.137778000	4.646169000	0.097387000
1	-9.053711000	5.328467000	0.860818000
1	-8.223894000	4.134310000	1.899161000
1	-6.517805000	5.415922000	0.552229000
1	-7.342372000	4.898797000	-0.947832000
1	7.848468000	4.489855000	0.406936000
1	7.016457000	4.505785000	1.989737000
1	8.659285000	2.784626000	2.836576000
1	9.542378000	4.227711000	2.261232000
1	-4.249604000	-2.972590000	-0.136845000
1	-5.050398000	-3.591006000	-1.616087000
1	-3.290524000	-2.465587000	-3.015520000
1	-2.490997000	-3.522979000	-1.804021000
8	-9.251567000	3.396034000	0.216583000
8	-6.319732000	3.420149000	0.141458000
8	-5.255000000	-1.566807000	-1.350448000
8	-2.339325000	-1.526329000	-1.400285000
8	6.757603000	2.772342000	0.932964000
8	9.685548000	2.617423000	1.005815000
16	-7.779476000	-0.154819000	-0.814409000
16	-3.802840000	1.988791000	-0.260288000
16	0.162917000	-0.125646000	-1.119751000
16	4.205651000	1.674712000	0.040810000
16	8.106353000	-0.387233000	-1.071892000



$[Pt(HSO_4)(H_2O)((EDOS)_5)(H)]$ $E_{SDB\text{-}cc\text{-}pVDZ}$ =- -4670.5529657 a.u.

78	0.003908000	-2.046398000	0.432150000
8	0.032557000	-3.575499000	1.836437000

16	-0.078367000	-3.177120000	3.485996000
8	0.648347000	-1.825035000	3.906106000
8	0.002892000	-4.480952000	4.402308000
8	-1.961852000	-2.681412000	3.536481000
1	-2.437746000	-3.427559000	3.964595000
8	-2.097942000	-1.618400000	1.172435000
1	-2.235940000	-1.988352000	2.098376000
1	-2.409953000	-0.698423000	1.089096000
1	1.460731000	-2.395883000	0.026976000
6	-1.282342000	0.892779000	-0.818861000
6	1.432640000	0.862395000	-0.780392000
6	-0.633006000	2.005384000	-0.322523000
6	0.794668000	1.981243000	-0.286669000
6	-0.560856000	4.295710000	0.404393000
6	0.733379000	3.921845000	1.107664000
1	-0.357499000	4.778086000	-0.556493000
1	0.535613000	3.395361000	2.046167000
8	1.536830000	3.051544000	0.230100000
8	-1.373211000	3.087597000	0.165376000
1	-1.185707000	4.939330000	1.019924000
1	1.356174000	4.794278000	1.292969000
6	2.816310000	0.599477000	-0.833098000
6	3.433149000	-0.513239000	-1.390942000
6	4.839232000	-0.599599000	-1.241438000
6	5.464892000	0.455883000	-0.595797000
6	-2.672017000	0.649446000	-0.892005000
6	-3.282081000	-0.505387000	-1.368010000
6	-4.687616000	-0.589805000	-1.213586000
6	-5.325261000	0.515417000	-0.672488000
6	-6.714201000	0.659196000	-0.416324000
6	-7.351494000	1.763171000	0.122933000
6	-8.771157000	1.667599000	0.301380000
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6	6.854022000	0.587748000	-0.333898000
6	7.483181000	1.636636000	0.315309000
6	8.905278000	1.539711000	0.471503000
6	9.474451000	0.414664000	-0.063941000
1	10.521427000	0.156721000	-0.044828000
6	3.496806000	-2.508199000	-2.739498000
6	4.700148000	-2.883901000	-1.889912000
1	2.827270000	-3.353770000	-2.887144000
1	3.814856000	-2.105162000	-3.705827000
1	5.321601000	-3.627432000	-2.384213000
1	4.387059000	-3.247702000	-0.905771000
8	2.682177000	-1.490759000	-2.051320000
8	5.566420000	-1.703317000	-1.714666000
6	7.585932000	3.879483000	1.152814000
6	8.797880000	3.413756000	1.945167000
6	-4.487388000	-2.936282000	-1.464654000
6	-3.273192000	-2.713159000	-2.351132000
6	-8.677583000	3.702152000	1.550081000
6	-7.478829000	4.085106000	0.696891000

1	-9.326356000	4.556275000	1.734615000
1	-8.351124000	3.271300000	2.502672000
1	-6.841598000	4.813423000	1.194842000
1	-7.799433000	4.470213000	-0.276317000
1	7.893958000	4.384706000	0.231795000
1	6.942850000	4.532545000	1.739591000
1	8.486348000	2.865562000	2.840675000
1	9.435865000	4.249192000	2.226902000
1	-4.186704000	-3.077533000	-0.422029000
1	-5.081592000	-3.779492000	-1.809216000
1	-3.572854000	-2.551746000	-3.390721000
1	-2.571020000	-3.543338000	-2.285730000
8	-9.518614000	2.728042000	0.836613000
8	-6.621829000	2.904895000	0.484353000
8	-5.382991000	-1.761483000	-1.550437000
8	-2.512136000	-1.533004000	-1.903565000
8	6.743110000	2.722714000	0.802735000
8	9.644551000	2.546645000	1.111460000
34	-8.020878000	-0.715529000	-0.794860000
34	-4.021295000	1.890216000	-0.246499000
34	0.065517000	-0.422871000	-1.410908000
34	4.151983000	1.772669000	-0.053829000
34	8.174122000	-0.722568000	-0.864742000

References:

[1] Patra, A.; Wijsboom, Y. H.; Zade, S. S.; Li, M.; Sheynin, Y.; Leitus, G.; Bendikov, M. *J. Am. Chem. Soc.* **2008**, *130*, 6734-6736.

[2] Nova, Version 1.0.26.1099. http://www.ntmdt.com/

[3] Gwyddion, Version 2.26. http://gwyddion.net/

[4] NIST X-ray Photoelectron Spectroscopy Database, NIST Standard Reference Database 20, Version 3.5 (http://srdata.nist.gov/xps/Default.aspx)

[5] A. Chen and P. Holt-Hindle, *Chem. Rev*., 2010, **110**, 3767.

[6] Frisch, M. J., Trucks, G. W., Schlegel, H. B., Scuseria, G. E., Robb, M. A., Cheeseman, J. R., Scalmani, G., Barone, V., Mennucci, B., Petersson, G. A., Nakatsuji, H., Caricato, M., Li, X., Hratchian, H. P., Izmaylov, A. F., Bloino, J., Zheng, G., Sonnenberg, J. L., Hada, M., Ehara, M., Toyota, K., Fukuda, R., Hasegawa, J., Ishida, M., Nakajima, T., Honda, Y., Kitao, O., Nakai, H., Vreven, T., Montgomery, Jr., J. A., Peralta, J. E., Ogliaro, F., Bearpark, M., Heyd, J. J., Brothers, E., Kudin, K. N., Staroverov, V. N., Kobayashi, R., Normand, J., Raghavachari, K., Rendell, A., Burant, J. C., Iyengar, S. S., Tomasi, J., Cossi, M., Rega, N., Millam, J. M., Klene, M., Knox, J. E., Cross, J. B., Bakken, V., Adamo, C., Jaramillo, J., Gomperts, R., Stratmann, R. E., Yazyev, O., Austin, A. J., Cammi, R., Pomelli, C., Ochterski, J. W., Martin, R. L., Morokuma, K., Zakrzewski, V. G., Voth, G. A., Salvador, P., Dannenberg, J. J., Dapprich, S., Daniels, A. D., Farkas, O., Foresman, J. B., Ortiz, J. V., Cioslowski, J., and Fox, D. J., Gaussian 09, Revision A.02, Gaussian, Inc., Wallingford CT, 2009.

[7] Zhao, Y.; Truhlar, D. G. *J. Chem. Phys.* **2006**, *125*, 194101.

[8] Martin, J. M. L. and Sundermann, A. *J. Chem. Phys.* **2001**, *114*, 3408.