

Supporting Information

Quantum-chemical insights into a design of molecule-modified Pt catalysts for the oxygen reduction reaction

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Supplementary Note 1: Computational procedure

The Perdew–Burke–Ernzerhof (PBE) exchange–correlation functional [s1] was employed for the DFT calculations. Grimme’s dispersion corrections (DFT-D3 with Becke-Jonson damping) were applied [s2,s3]. Core electrons were treated using the projector-augmented plane-wave method [s4,s5]. The numbers of valence electrons were Pt (10), N (5), O (6), C (4), and H (1). The cut-off energy of plane-wave was set to 400 eV. Sampling of the k -points was performed at the Γ -point. The Vienna Ab initio Simulation Package (VASP) [s6–s9] was used for the DFT calculations, and the VESTA program [s10] was employed to visualise the results. The surface–molecule interaction energy (E_{int}) was calculated: $E_{\text{int}} = E(\text{ads/surf}) - E(\text{ads}) - E(\text{surf})$, where $E(\text{ads/surf})$ is the total energy of the adsorption system after geometry optimisation; $E(\text{ads})$ and $E(\text{surf})$ are the total energies of the molecule and the Pt(111) surface, respectively, with the adsorption geometry fixed. For molecular orbital analysis, calculations were performed using the Gaussian16 program [s11] with the 6-311+G(d,p) basis set.

The Pt(111) slab model with a vacuum region ($> 20 \text{ \AA}$) employed in this study was identical to that used in our previous work [s12], and the specific atomic coordinates can be found in the previous work. In the earlier study [s12], exhaustive DFT calculations exceeding 10,000 configurations were performed to optimise the most stable structures by scanning the xy positions, tilt angles, rotation angles, and the distance between the molecule and the surface. In the present study, by contrast, the tilt angle was fixed at 0° (i.e. only horizontal adsorption structures were considered) during the scanning process to reduce computational cost, while the rotation angles and surface–molecule distance were varied. Based on the energy landscapes obtained from these scans, geometry optimisations were carried out from the local minima at each surface distance, yielding stable adsorption structures (these are summarised in Figs. S1–S5). Figs. S1 and S2 show the stable adsorption structures of melamine and diamino-triazine. Although these molecules can adopt adsorption geometries tilted relative to the surface, the approach employed here (horizontal scanning followed by subsequent optimisation) successfully yielded the most stable adsorption structures (Figs. 1(a) and 1(b)), which are consistent with those reported previously [s12,s13]. The atomic coordinates of the most stable structures reported in the present study are summarised in this Supporting Information (see last topic).

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[s4] P.E. Blöchl, *Phys. Rev. B*, 1994, **50**, 17953.

[s5] G. Kresse, D. Joubert, *Phys. Rev. B*, 1999, **59**, 1758.

[s6] G. Kresse, J. Hafner, *Phys. Rev. B*, 1993, **47**, 558.

[s7] G. Kresse, J. Hafner, *Phys. Rev. B*, 1994, **49**, 14251.

[s8] G. Kresse, J. Furthmüller, *Phys. Rev. B*, 1996, **54**, 11169.

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[s12] K. Tada, S. Yamazaki, M. Asahi, T. Ioroi, *Phys. Chem. Chem. Phys.*, 2023, **25**, 23047.

[s13] K. Tada, S. Yamazaki, M. Asahi, T. Ioroi, *Surf. Sci.*, 2025, **762**, 122817.

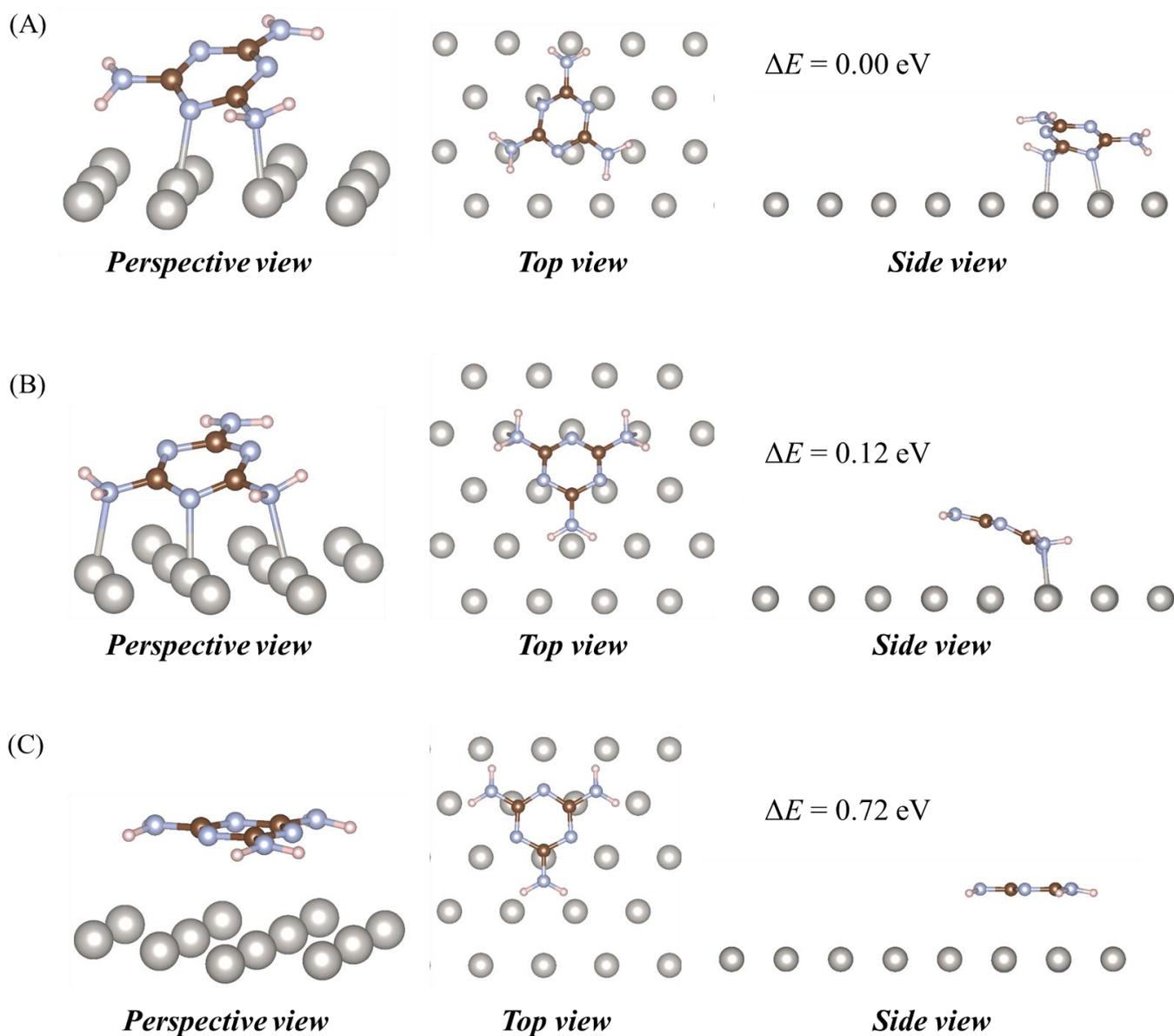
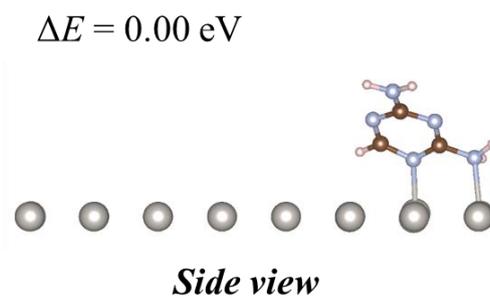
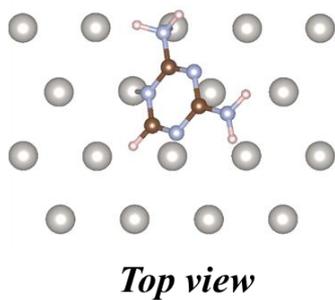
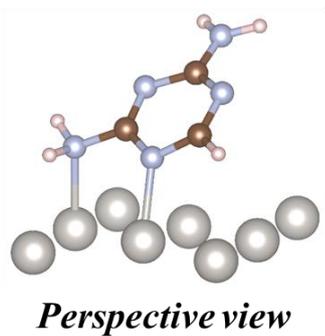


Figure S1. Converged stable structures of melamine. ΔE is relative energy to the most stable structure.

(A)



(B)

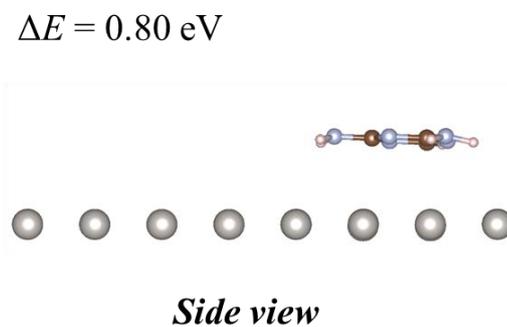
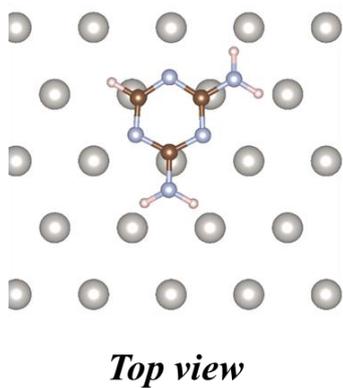
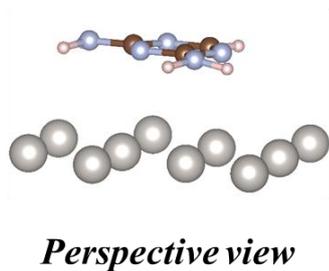
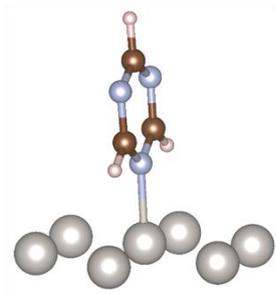
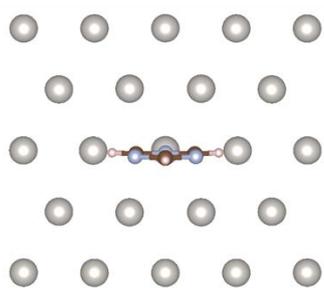


Figure S2. Converged stable structures of diamino-triazine. ΔE is relative energy to the most stable structure.

(A)

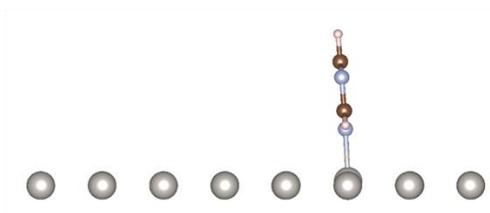


Perspective view



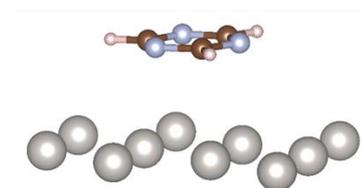
Top view

$\Delta E = 0.00$ eV

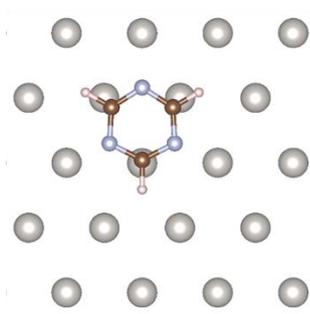


Side view

(B)

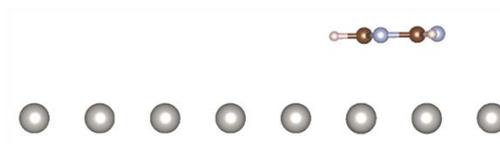


Perspective view



Top view

$\Delta E = 0.66$ eV



Side view

Figure S3. Converged stable structures of triazine. ΔE is relative energy to the most stable structure.

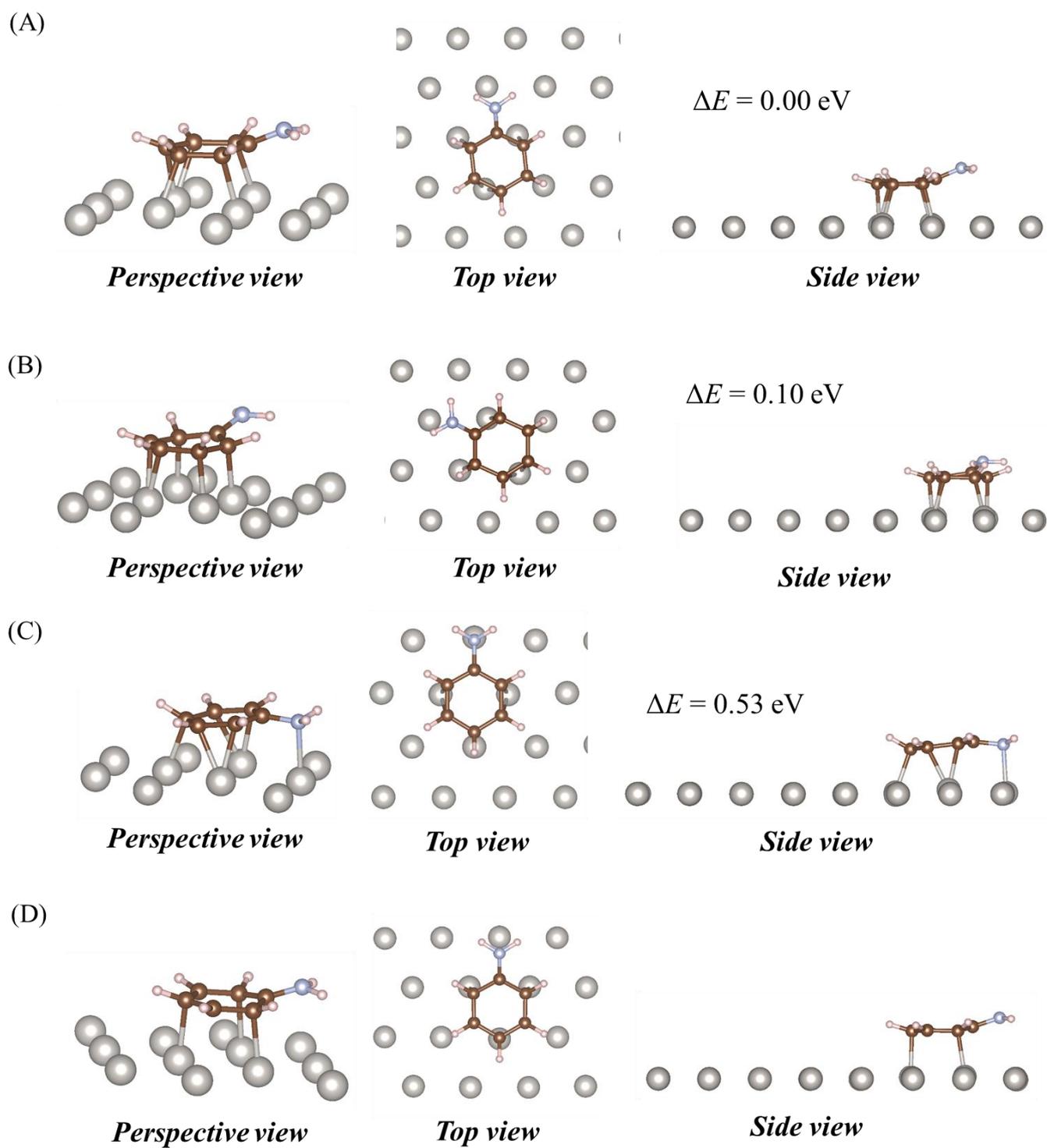


Figure S4. Converged stable structures of aniline. ΔE is relative energy to the most stable structure.

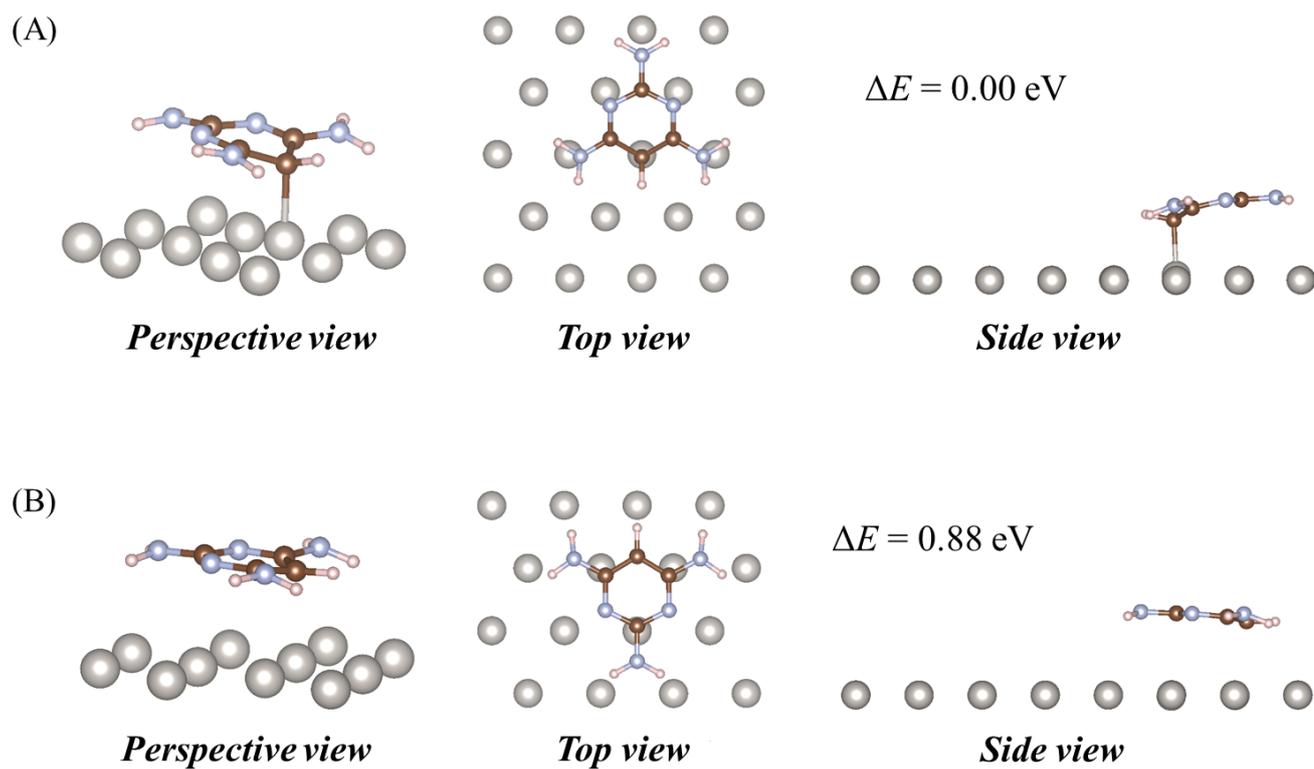


Figure S5. Converged stable structures of triamino-pyrimidine. ΔE is relative energy to the most stable structure.

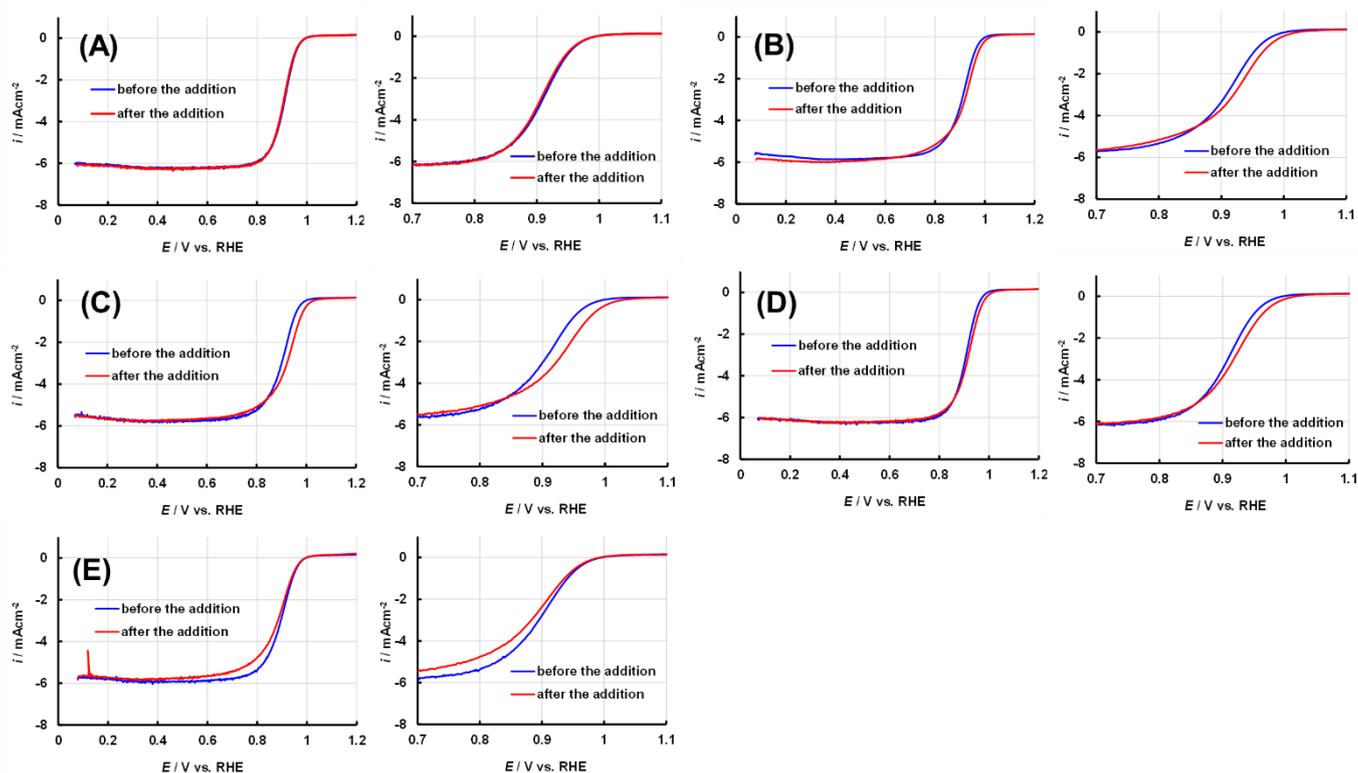


Figure S6. Linear sweep voltammograms (LSVs) of ORR using Pt/C before and after the addition of 1 μM (A) triazine, (B) diamino-triazine, (C) melamine, (D) triamino-pyrimidine, and (E) aniline in 0.1 M HClO_4 . LSV data were acquired in O_2 -saturated 0.1 M HClO_4 at a scan rate of 10 mVs^{-1} at 25°C with electrode rotation at 1600 rpm. The effects of melamine on the ORR activity (C) were examined in Reference [11] in the main text, where R_{ORR} at 0.9 V in the cathodic scan was reported. Right panels are enlarged views of left figures.

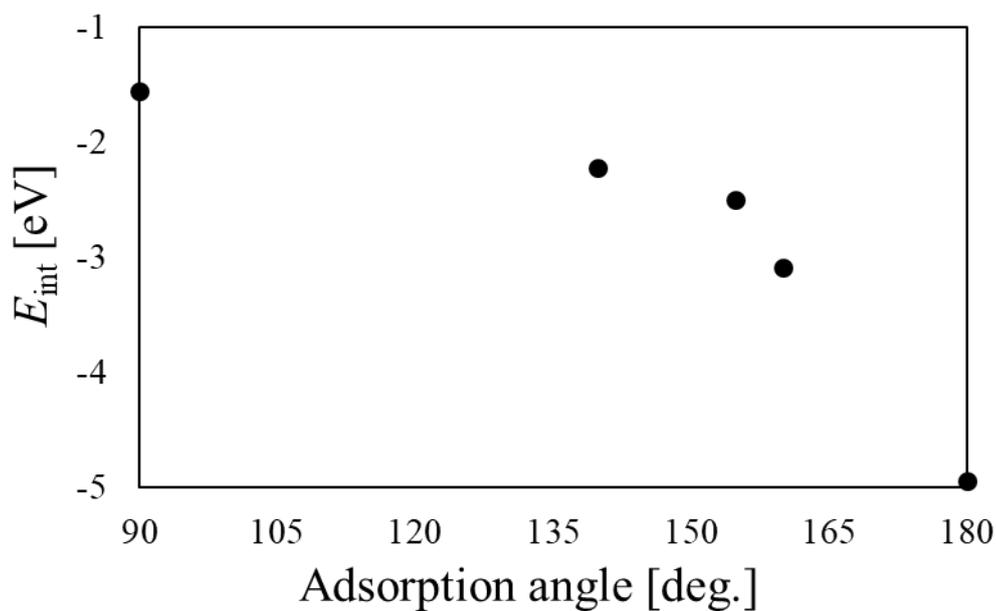
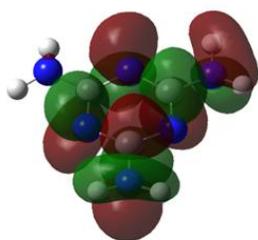
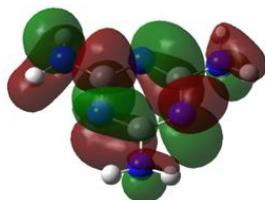


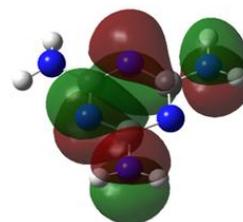
Figure S7. Plot of molecule–Pt interaction energy versus adsorption angle of molecule on Pt.



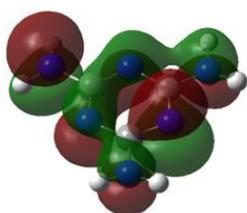
LUMO+1
-0.7706 eV



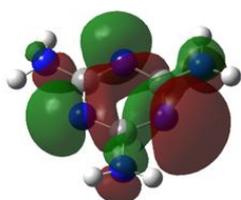
LUMO
-0.7742 eV



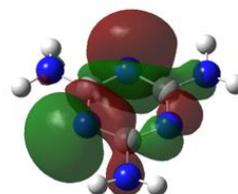
HOMO
-5.7147 eV



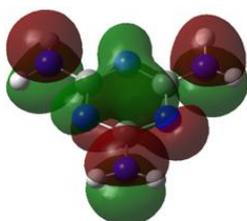
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-5.7204 eV



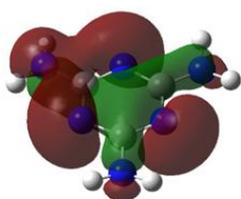
HOMO-2
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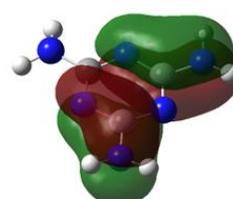
HOMO-3
-6.0067 eV



HOMO-4
-6.1770 eV

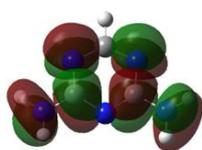


HOMO-5
-8.7738 eV

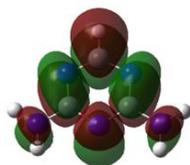


HOMO-6
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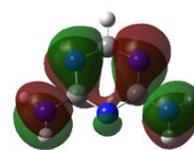
Figure S7. Frontier orbitals and their orbital energies of melamine. Geometry was optimised in gas-phase.



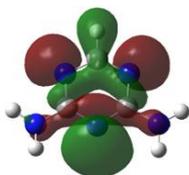
LUMO+1
-1.0248 eV



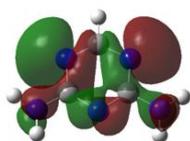
LUMO
-1.6169 eV



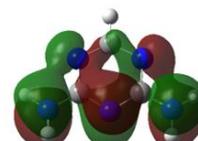
HOMO
-5.9468 eV



HOMO-1
-6.0685 eV



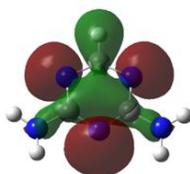
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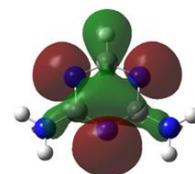
HOMO-3
-6.2633 eV



HOMO-4
-8.2710 eV

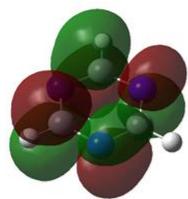


HOMO-5
-8.8231 eV

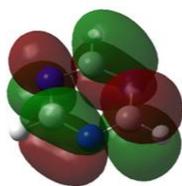


HOMO-6
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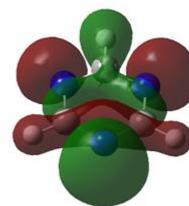
Figure S8. Frontier orbitals of diamino-triazine. Geometry was optimised in gas-phase.



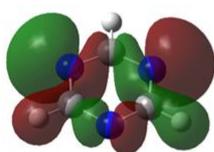
LUMO+1
-2.8442 [eV]



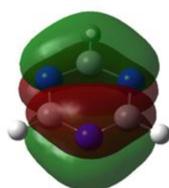
LUMO
-2.8442 eV



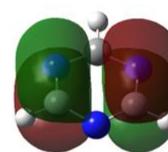
HOMO
-6.6562 eV



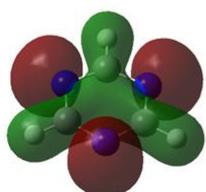
HOMO-1
-6.6562 eV



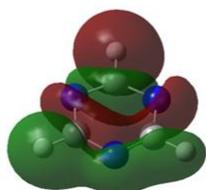
HOMO-2
-8.6511 eV



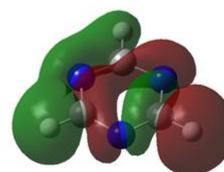
HOMO-3
-8.6511 eV



HOMO-4
-9.2691 eV

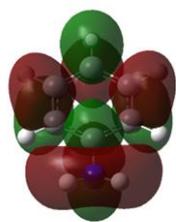


HOMO-5
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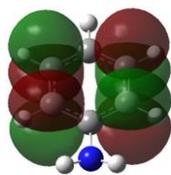


HOMO-6
-10.8308 eV

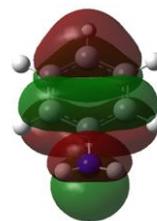
Figure S9. Frontier orbitals of triazine. Geometry was optimised in gas-phase.



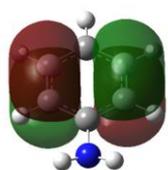
LUMO+1
-0.7135 eV



LUMO
-1.0681 eV



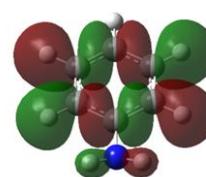
HOMO
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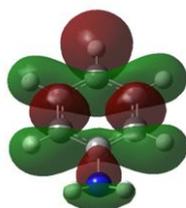
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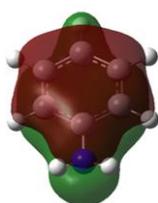
HOMO-2
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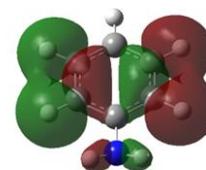
HOMO-3
-8.0770 eV



HOMO-4
-8.5191 eV

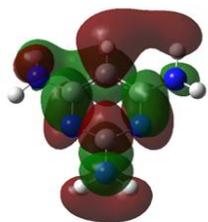


HOMO-5
-9.3099 eV

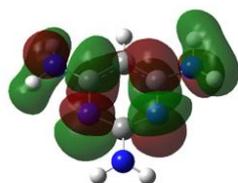


HOMO-6
-10.0463 eV

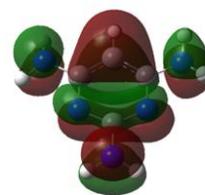
Figure S10. Frontier orbitals of aniline. Geometry was optimised in gas-phase.



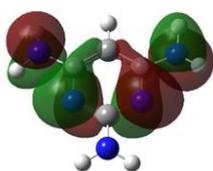
LUMO+1
-0.6038 eV



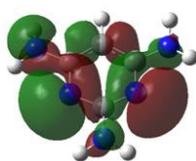
LUMO
-0.7312 eV



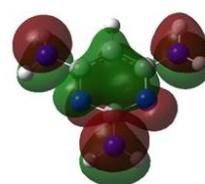
HOMO
-4.9729 eV



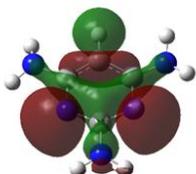
HOMO-1
-5.6263 eV



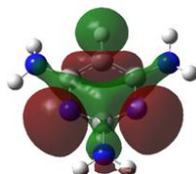
HOMO-2
-5.6728 eV



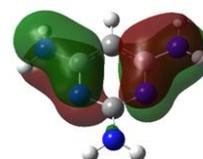
HOMO-3
-6.0007 eV



HOMO-4
-7.0350 eV



HOMO-5
-8.4598 eV



HOMO-6
-8.7377 eV

Figure S11. Frontier orbitals of triamino pyrimidine. Geometry was optimised in gas-phase.

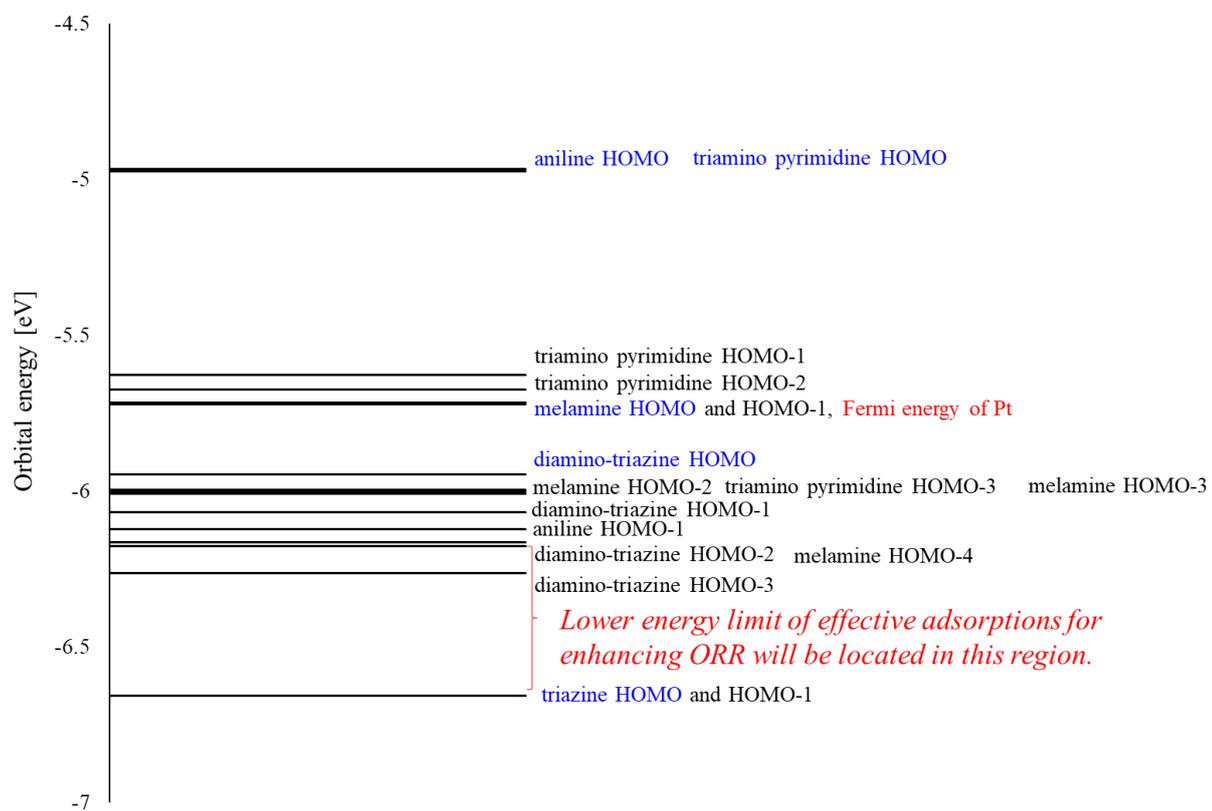


Figure S13. Summary of specific orbital energies of investigated molecules.

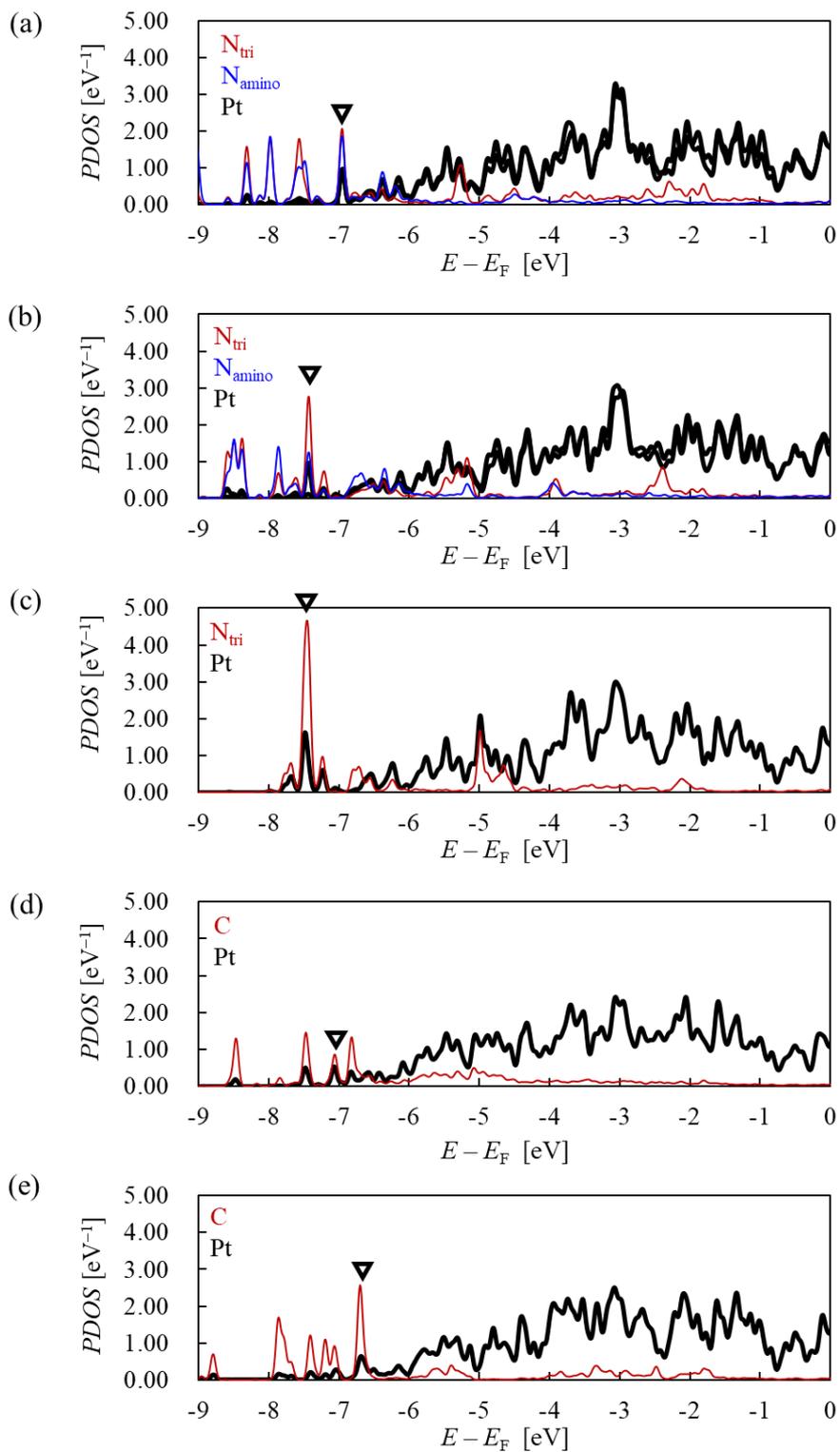


Figure S14. Projected density of states (PDOS) for the most stable adsorption structures of (a) melamine/Pt(111), (b) diamino-triazine/Pt(111), (c) triazine/Pt(111), (d) aniline/Pt(111), and (e) triamino-pyrimidine/Pt(111). Blue lines represent PDOS of N_{amino} , red-brown lines represent PDOS of adsorbed atoms in covalent rings, and black lines represent PDOS of adsorbed Pt atoms.

Supplementary Note 2: Energy alignment scheme

The absolute values of the orbital energies determined from band calculations using plane-wave basis sets and molecular orbital calculations employing atomic-centred basis sets such as Gaussian functions are not generally the same even for a given molecule. This discrepancy arises because it is difficult in the band calculations to correctly set the energy reference point for electrons at infinity. Consequently, a reference energy is required to investigate the relative positions of the bands and molecular orbitals, necessitating careful consideration. In our previous study (Ref. [19] in the main text), the position of the HOMO of melamine relative to the d-band centres of the Pt surfaces were calculated using a supercell where melamine and Pt were positioned at a given distance without orbital correlation, as shown in Fig. S15(a). This approach is effective when the HOMO is below the Fermi energy of Pt. However, when the HOMO is clearly above the Fermi energy, the band of metallic Pt precludes correct determination of the HOMO position.

The HOMO of diamino-triazine and triazine is lower than that of melamine (see Fig. 5 in the main text). Therefore, in this study, the models shown in Figs. S15(a), (b), and (c) were constructed for the three molecules (melamine, diamino-triazine, and triazine), and projected density of states (PDOS) analysis was performed to determine the relative positions of the HOMOs and the d-band centres of Pt(111). Here, the Pt(111) slab and the structure of each molecule in the models shown in Figs. S15(a), (b), and (c) were fixed at their independently optimised geometries. The calculated PDOS results are shown in Figs. S15(d), (e), and (f). As shown in Table S1, the position of the d-band centre remained constant across all systems. Therefore, in Figs. S15(d), (e), and (f), the PDOS is displayed relative to the centre position of the d-band. The energies of the HOMO relative to the d-band centre were 2.07 eV (melamine), 1.89 eV (diamino-triazine), and 1.24 eV (triazine). Table S2 lists the calculated HOMO energies of the molecules in the gas phase. The results obtained with the atomic-centred basis set 6-311+G(d,p) are based on the reference energy when the electron is positioned at infinity. Calculations for the molecules in the gas phase using the plane-wave basis sets were performed for a 3 nm × 3 nm × 3 nm cubic supercell. The obtained orbital energies agreed well with those obtained using the atomic-centre basis set. Therefore, we can assume that the reference energy for the electron was the same for all gas-phase calculations.

The orbital energies of the gas-phase molecules calculated using the plane-wave basis sets are compared with those obtained from the models in Figs. S15(a), (b), and (c). The energy differences were 7.7–7.8 eV. Therefore, adding +7.79 eV to the HOMO energy of the gas-phase molecule yields the orbital energy under the electrostatic potential created by the Pt(111) slab. Because the HOMO of melamine and the Fermi energy of Pt are close, the correction values estimated from the results for triazine and diamino-triazine (7.79 eV) were used. Furthermore, as shown in Table S1, the d-band centres of the Pt atoms on the Pt(111) surface were in the range of –2.09 to –2.13 eV, and the value can be assumed as the constant. This invariant value for the d-band centre was used as the reference for constructing the orbital correlation diagram with one significant digit after the decimal point (Fig. 6(a)).

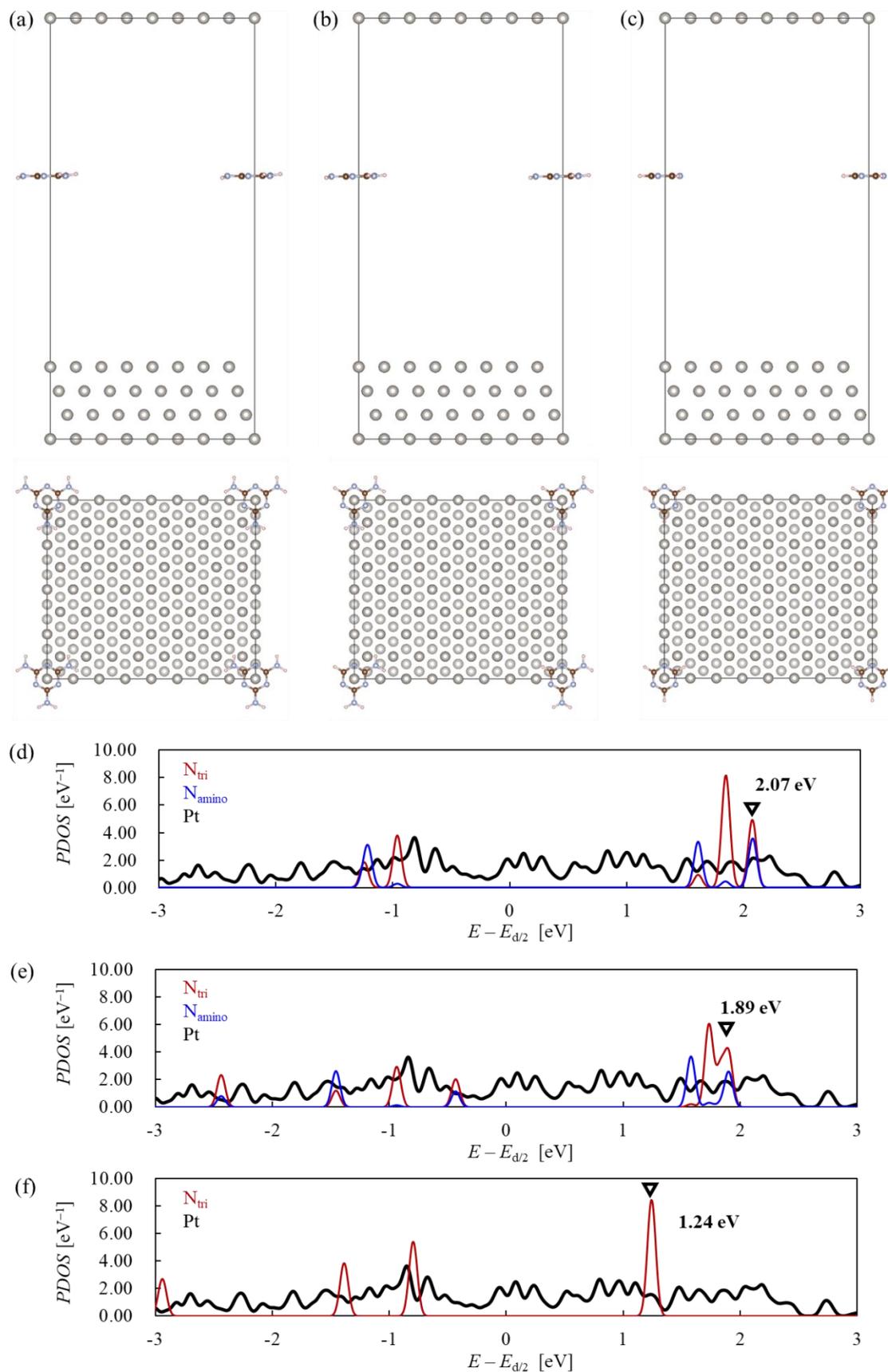


Figure S15. Calculated supercell models of (a) melamine, (b) diamino-triazine, and (c) triazine above Pt(111) slabs. Upper and lower panels are side and top views, respectively. Calculated PDOS data for (a) melamine, (b) diamino-triazine, and (c) triazine above Pt(111) slabs. Blue lines represent PDOS of N_{amino} , red-brown lines represent PDOS of adsorbed atoms in covalent rings, and black lines represent PDOS of Pt atoms. The reference energy was set to the d-band centre of Pt(111) ($E_{d/2}$).

Table S1. Eigenvalues of the band at d-band centre point and on the Fermi level of Pt. The values of the d-band centre (E_{d2}) were estimated using the eigenvalues

System	Eigenvalue of band at d-band centre point [eV]	Eigenvalue of band on the Fermi level of Pt [eV]	E_{d2} [eV]
Melamine above Pt(111)	-3.96	-1.826	-2.13
Melamine on Pt(111)	-3.79	-1.687	-2.10
Diamino-triazine above Pt(111)	-3.98	-1.848	-2.13
Diamino-triazine on Pt(111)	-3.76	-1.668	-2.09
Triazine above Pt(111)	-3.99	-1.862	-2.13
Triazine on Pt(111)	-3.89	-1.795	-2.10
Aniline above Pt(111)	-3.84	-1.709	-2.13
Aniline on Pt(111)	-3.79	-1.692	-2.10
Triamino-pyrimidine above Pt(111)	-3.81	-1.685	-2.13
Triamino-pyrimidine on Pt(111)	-3.83	-1.702	-2.13

Table S2. HOMO energies of gas-phase molecules calculated using atomic-centred and plane-wave basis sets and molecules in the models shown in Fig. S15. The values in parentheses, i.e., values for aniline and triamino-pyrimidine above Pt(111), were estimated using the correction described on page 16 of this file

	Melamine	Diamino-triazine	Triazine	Aniline	Triamino-pyrimidine
Atomic-centred basis set (6-311+G(d,p))	-5.7147	-5.9468	-6.6562	-4.9667	-4.9729
Plane-wave (molecules in vacuum cube)	-5.6502	-5.8953	-6.5512	-4.9405	-4.9181
Plane-wave (molecules above Pt(111))	2.07	1.89	1.24	(2.85)	(2.87)
Differences in calculated plane-wave	7.72	7.79	7.79	(7.79)	(7.79)

Atomic coordinates of the most stable adsorption structures

Here we summarise the specific atomic positions in the most stable structures of melamine/Pt(111), diamino-triazine/Pt(111), triazine/Pt(111), aniline/Pt(111), and triamino-pyrimidine/Pt(111). These calculations were performed using a same super cell: its lattice vectors in real space are (22.1970443726 Å, 0.0000000000 Å, 0.0000000000 Å), (0.0000000000, 19.2232036591 Å, 0.0000000000 Å), and (0.0000000000 Å, 0.0000000000 Å, 40.0000000000 Å). The atomic coordinates are supplied in a direct coordination to the lattice vectors.

Melamine/Pt(111)

N1	0.0067389	0.2515831	0.2285476
N2	0.0983780	0.2476530	0.2600948
N3	0.0378850	0.1451546	0.2540347
N4	0.0550897	0.3528381	0.2459653
N5	0.1377693	0.1382847	0.2698171
N6	0.9446135	0.1517390	0.2273613
C1	0.0543324	0.2831844	0.2450783
C2	0.0911164	0.1783454	0.2608476
C3	0.9994258	0.1839886	0.2374289
H1	0.0937910	0.3767446	0.2531648
H2	0.1790941	0.1603838	0.2720510
H3	0.9418781	0.1026565	0.2373295
H4	0.0251856	0.3801411	0.2315607
H5	0.1341900	0.0859386	0.2671618
H6	0.9074048	0.1812312	0.2331399
Pt1	0.0000000	0.0000000	0.0000000
Pt2	0.1875000	0.1250000	0.0000000
Pt3	0.0625000	0.1250000	0.0000000
Pt4	0.0000000	0.2500000	0.0000000
Pt5	0.0625000	0.3750000	0.0000000
Pt6	0.1875000	0.3750000	0.0000000
Pt7	0.1250000	0.0000000	0.0000000
Pt8	0.1250000	0.2500000	0.0000000
Pt9	0.1872943	0.4645720	0.0575906
Pt10	0.0621632	0.4642486	0.0576119
Pt11	0.9995502	0.0903189	0.0578373
Pt12	0.9997931	0.3389981	0.0584550
Pt13	0.1247488	0.0896427	0.0574861
Pt14	0.0619832	0.2147956	0.0578686
Pt15	0.1871406	0.2146748	0.0575573
Pt16	0.1242203	0.3393703	0.0577585

Pt17	0.1874926	0.3052955	0.1142066
Pt18	0.0617027	0.3046527	0.1158638
Pt19	0.9996242	0.4305506	0.1148817
Pt20	0.9999298	0.1802322	0.1156978
Pt21	0.0625475	0.0541727	0.1141073
Pt22	0.1875273	0.0550571	0.1145597
Pt23	0.1255248	0.1798809	0.1139241
Pt24	0.1250550	0.4300168	0.1142274
Pt25	0.0007121	0.0177501	0.1719308
Pt26	0.1885299	0.1442245	0.1725314
Pt27	0.0656181	0.1423921	0.1705039
Pt28	0.9973757	0.2725757	0.1754472
Pt29	0.0627010	0.3965655	0.1717357
Pt30	0.1873469	0.3944272	0.1722022
Pt31	0.1257208	0.0185071	0.1724385
Pt32	0.1268408	0.2688104	0.1715244
Pt33	0.2500000	0.0000000	0.0000000
Pt34	0.4375000	0.1250000	0.0000000
Pt35	0.3125000	0.1250000	0.0000000
Pt36	0.2500000	0.2500000	0.0000000
Pt37	0.3125000	0.3750000	0.0000000
Pt38	0.4375000	0.3750000	0.0000000
Pt39	0.3750000	0.0000000	0.0000000
Pt40	0.3750000	0.2500000	0.0000000
Pt41	0.4374101	0.4646389	0.0576345
Pt42	0.3123760	0.4648421	0.0576557
Pt43	0.2497725	0.0897853	0.0576788
Pt44	0.2495064	0.3398562	0.0576786
Pt45	0.3749176	0.0897980	0.0576448
Pt46	0.3122582	0.2147536	0.0575562
Pt47	0.4374458	0.2147735	0.0576169
Pt48	0.3748001	0.3396903	0.0575629
Pt49	0.4373889	0.3050701	0.1143636
Pt50	0.3123996	0.3053802	0.1143847
Pt51	0.2500035	0.4303306	0.1145047
Pt52	0.2501144	0.1804564	0.1144340
Pt53	0.3123537	0.0552250	0.1145095
Pt54	0.4374177	0.0550882	0.1144154
Pt55	0.3748700	0.1801440	0.1144858
Pt56	0.3749093	0.4299901	0.1145123
Pt57	0.2503186	0.0190165	0.1724462
Pt58	0.4373836	0.1442794	0.1720706

Pt59	0.3122835	0.1440659	0.1722744
Pt60	0.2505754	0.2697504	0.1723904
Pt61	0.3123958	0.3946054	0.1723413
Pt62	0.4372075	0.3942637	0.1721833
Pt63	0.3749523	0.0194221	0.1721947
Pt64	0.3745143	0.2692867	0.1720977
Pt65	0.5000000	0.0000000	0.0000000
Pt66	0.6875000	0.1250000	0.0000000
Pt67	0.5625000	0.1250000	0.0000000
Pt68	0.5000000	0.2500000	0.0000000
Pt69	0.5625000	0.3750000	0.0000000
Pt70	0.6875000	0.3750000	0.0000000
Pt71	0.6250000	0.0000000	0.0000000
Pt72	0.6250000	0.2500000	0.0000000
Pt73	0.6875739	0.4647072	0.0576721
Pt74	0.5625052	0.4649000	0.0576895
Pt75	0.5000555	0.0899261	0.0577080
Pt76	0.5000862	0.3397143	0.0576222
Pt77	0.6251483	0.0898556	0.0576641
Pt78	0.5627835	0.2148815	0.0576346
Pt79	0.6881321	0.2146627	0.0576194
Pt80	0.6253660	0.3397996	0.0575986
Pt81	0.6873792	0.3054066	0.1143755
Pt82	0.5623624	0.3051976	0.1144489
Pt83	0.4998671	0.4300651	0.1144313
Pt84	0.4999373	0.1800958	0.1143760
Pt85	0.5625778	0.0553395	0.1145807
Pt86	0.6874746	0.0552253	0.1145761
Pt87	0.6251022	0.1805009	0.1143979
Pt88	0.6247300	0.4302792	0.1145539
Pt89	0.4996133	0.0196791	0.1722492
Pt90	0.6864298	0.1445001	0.1722673
Pt91	0.5622281	0.1447420	0.1721904
Pt92	0.4994365	0.2691826	0.1720731
Pt93	0.5617777	0.3942848	0.1722922
Pt94	0.6864996	0.3951662	0.1722809
Pt95	0.6244501	0.0192558	0.1722903
Pt96	0.6244441	0.2698489	0.1721542
Pt97	0.7500000	0.0000000	0.0000000
Pt98	0.9375000	0.1250000	0.0000000
Pt99	0.8125000	0.1250000	0.0000000
Pt100	0.7500000	0.2500000	0.0000000

Pt101	0.8125000	0.3750000	0.0000000
Pt102	0.9375000	0.3750000	0.0000000
Pt103	0.8750000	0.0000000	0.0000000
Pt104	0.8750000	0.2500000	0.0000000
Pt105	0.9375984	0.4643545	0.0577673
Pt106	0.8127315	0.4642231	0.0576004
Pt107	0.7502814	0.0896070	0.0577073
Pt108	0.7506843	0.3394306	0.0576604
Pt109	0.8751562	0.0902621	0.0582101
Pt110	0.8131496	0.2144731	0.0578754
Pt111	0.9375245	0.2148261	0.0587337
Pt112	0.8757870	0.3393343	0.0581014
Pt113	0.9384570	0.3052941	0.1167068
Pt114	0.8125032	0.3049148	0.1143731
Pt115	0.7497198	0.4300898	0.1144720
Pt116	0.7500411	0.1801275	0.1144491
Pt117	0.8123168	0.0551111	0.1148901
Pt118	0.9375055	0.0552815	0.1153162
Pt119	0.8754638	0.1800922	0.1159848
Pt120	0.8747808	0.4299210	0.1146277
Pt121	0.7491278	0.0194767	0.1726264
Pt122	0.9363936	0.1443150	0.1734650
Pt123	0.8099239	0.1443242	0.1726544
Pt124	0.7486632	0.2700714	0.1722636
Pt125	0.8113760	0.3955853	0.1723686
Pt126	0.9361467	0.3977708	0.1731891
Pt127	0.8739960	0.0180825	0.1723768
Pt128	0.8714357	0.2715088	0.1727033
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Pt131	0.0625000	0.6250000	0.0000000
Pt132	0.0000000	0.7500000	0.0000000
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Pt135	0.1250000	0.5000000	0.0000000
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Pt138	0.0623286	0.9647768	0.0576547
Pt139	0.9999626	0.5893821	0.0577206
Pt140	0.9998771	0.8397262	0.0576910
Pt141	0.1248888	0.5893918	0.0576894
Pt142	0.0624680	0.7142893	0.0576659

Pt143	0.1875018	0.7145913	0.0577378
Pt144	0.1249893	0.8393577	0.0576311
Pt145	0.1874600	0.8051357	0.1146495
Pt146	0.0624030	0.8046650	0.1144677
Pt147	0.9996596	0.9294979	0.1143667
Pt148	0.9999523	0.6798576	0.1146203
Pt149	0.0624418	0.5549458	0.1146035
Pt150	0.1876052	0.5551319	0.1144828
Pt151	0.1250346	0.6799012	0.1145909
Pt152	0.1249026	0.9296520	0.1144905
Pt153	0.9995613	0.5210979	0.1726238
Pt154	0.1873554	0.6443156	0.1721830
Pt155	0.0622251	0.6448326	0.1723529
Pt156	0.9998773	0.7695327	0.1723383
Pt157	0.0625896	0.8939486	0.1722775
Pt158	0.1875515	0.8943558	0.1723682
Pt159	0.1249610	0.5198617	0.1722442
Pt160	0.1246873	0.7694889	0.1722445
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Pt163	0.3125000	0.6250000	0.0000000
Pt164	0.2500000	0.7500000	0.0000000
Pt165	0.3125000	0.8750000	0.0000000
Pt166	0.4375000	0.8750000	0.0000000
Pt167	0.3750000	0.5000000	0.0000000
Pt168	0.3750000	0.7500000	0.0000000
Pt169	0.4374478	0.9648196	0.0577212
Pt170	0.3123483	0.9648439	0.0576667
Pt171	0.2499592	0.5898592	0.0576811
Pt172	0.2499080	0.8397773	0.0577267
Pt173	0.3750119	0.5897710	0.0576317
Pt174	0.3124388	0.7149072	0.0577308
Pt175	0.4375429	0.7147671	0.0576000
Pt176	0.3749719	0.8398558	0.0577037
Pt177	0.4373696	0.8051801	0.1144534
Pt178	0.3123363	0.8052693	0.1145569
Pt179	0.2498753	0.9302673	0.1146051
Pt180	0.2500292	0.6802706	0.1145878
Pt181	0.3125681	0.5551809	0.1145005
Pt182	0.4374310	0.5549421	0.1145142
Pt183	0.3749796	0.6801571	0.1144660
Pt184	0.3747601	0.9301704	0.1145580

Pt185	0.2498931	0.5193393	0.1722710
Pt186	0.4371193	0.6443465	0.1721596
Pt187	0.3123434	0.6442177	0.1722681
Pt188	0.2498202	0.7692897	0.1723500
Pt189	0.3123714	0.8941773	0.1723523
Pt190	0.4372562	0.8943852	0.1721845
Pt191	0.3747622	0.5191791	0.1722892
Pt192	0.3746473	0.7692540	0.1721980
Pt193	0.5000000	0.5000000	0.0000000
Pt194	0.6875000	0.6250000	0.0000000
Pt195	0.5625000	0.6250000	0.0000000
Pt196	0.5000000	0.7500000	0.0000000
Pt197	0.5625000	0.8750000	0.0000000
Pt198	0.6875000	0.8750000	0.0000000
Pt199	0.6250000	0.5000000	0.0000000
Pt200	0.6250000	0.7500000	0.0000000
Pt201	0.6876401	0.9648620	0.0577115
Pt202	0.5625237	0.9649374	0.0576938
Pt203	0.4998997	0.5898011	0.0576624
Pt204	0.5000430	0.8399005	0.0576465
Pt205	0.6248887	0.5899679	0.0577047
Pt206	0.5625004	0.7149944	0.0577024
Pt207	0.6874854	0.7148382	0.0577289
Pt208	0.6251544	0.8399870	0.0577013
Pt209	0.6873673	0.8053434	0.1145776
Pt210	0.5624868	0.8053847	0.1145576
Pt211	0.4999183	0.9302386	0.1145124
Pt212	0.4999208	0.6802104	0.1144846
Pt213	0.5622692	0.5551882	0.1145614
Pt214	0.6870537	0.5552865	0.1145527
Pt215	0.6247439	0.6804371	0.1145613
Pt216	0.6249779	0.9303389	0.1145597
Pt217	0.4994895	0.5192973	0.1723053
Pt218	0.6866702	0.6447250	0.1723050
Pt219	0.5619205	0.6443250	0.1722685
Pt220	0.4995468	0.7695450	0.1721663
Pt221	0.5620298	0.8945363	0.1722250
Pt222	0.6868208	0.8945406	0.1724036
Pt223	0.6241412	0.5195973	0.1724117
Pt224	0.6244902	0.7695107	0.1723830
Pt225	0.7500000	0.5000000	0.0000000
Pt226	0.9375000	0.6250000	0.0000000

Pt227	0.8125000	0.6250000	0.0000000
Pt228	0.7500000	0.7500000	0.0000000
Pt229	0.8125000	0.8750000	0.0000000
Pt230	0.9375000	0.8750000	0.0000000
Pt231	0.8750000	0.5000000	0.0000000
Pt232	0.8750000	0.7500000	0.0000000
Pt233	0.9372883	0.9653451	0.0576904
Pt234	0.8124765	0.9649172	0.0576995
Pt235	0.7498776	0.5895562	0.0576811
Pt236	0.7500528	0.8396994	0.0576991
Pt237	0.8750125	0.5893100	0.0576436
Pt238	0.8124967	0.7144077	0.0576939
Pt239	0.9374971	0.7144392	0.0576960
Pt240	0.8749930	0.8397425	0.0577210
Pt241	0.9373428	0.8046960	0.1146068
Pt242	0.8123625	0.8048553	0.1145700
Pt243	0.7499737	0.9301793	0.1146669
Pt244	0.7497095	0.6801133	0.1145735
Pt245	0.8121006	0.5549500	0.1144120
Pt246	0.9372935	0.5551815	0.1146247
Pt247	0.8748018	0.6799046	0.1145479
Pt248	0.8749203	0.9299328	0.1144444
Pt249	0.7491790	0.5200382	0.1722137
Pt250	0.9369323	0.6453092	0.1723881
Pt251	0.8119431	0.6447854	0.1721783
Pt252	0.7492118	0.7697533	0.1722765
Pt253	0.8118507	0.8943481	0.1722942
Pt254	0.9371245	0.8940881	0.1723026
Pt255	0.8742215	0.5206442	0.1722737
Pt256	0.8745399	0.7695945	0.1723243

Diamino-triazine/Pt(111)

N1	0.0229070	0.2754290	0.2264118
N2	0.1001732	0.3172203	0.2624741
N3	0.0706198	0.1971209	0.2641198
N4	0.0485618	0.3947291	0.2281438
N5	0.1567645	0.2354001	0.2907378
C1	0.0575993	0.3264954	0.2398751
C2	0.1086680	0.2501219	0.2718799
C3	0.0296854	0.2118115	0.2413626
H1	0.0746855	0.4294747	0.2410813

H2	0.1876011	0.2729776	0.2956069
H3	0.0038031	0.4093464	0.2274418
H4	0.1650348	0.1851858	0.2970275
H5	0.9977272	0.1716182	0.2336242
Pt1	0.0000000	0.0000000	0.0000000
Pt2	0.1875000	0.1250000	0.0000000
Pt3	0.0625000	0.1250000	0.0000000
Pt4	0.0000000	0.2500000	0.0000000
Pt5	0.0625000	0.3750000	0.0000000
Pt6	0.1875000	0.3750000	0.0000000
Pt7	0.1250000	0.0000000	0.0000000
Pt8	0.1250000	0.2500000	0.0000000
Pt9	0.1868718	0.4666825	0.0582220
Pt10	0.0624245	0.4661612	0.0582966
Pt11	0.9998076	0.0923782	0.0576762
Pt12	0.0001051	0.3415392	0.0588343
Pt13	0.1250023	0.0920728	0.0577932
Pt14	0.0623244	0.2172730	0.0579606
Pt15	0.1875038	0.2170010	0.0576206
Pt16	0.1245008	0.3419067	0.0579506
Pt17	0.1881751	0.3107097	0.1143089
Pt18	0.0624561	0.3100336	0.1161114
Pt19	0.0000151	0.4357881	0.1159021
Pt20	0.0003097	0.1853922	0.1153920
Pt21	0.0623474	0.0600058	0.1145090
Pt22	0.1876002	0.0602826	0.1148320
Pt23	0.1254341	0.1850264	0.1144278
Pt24	0.1238865	0.4350362	0.1160280
Pt25	0.0000366	0.0275296	0.1724986
Pt26	0.1884594	0.1521653	0.1728007
Pt27	0.0636673	0.1514535	0.1719436
Pt28	0.9970138	0.2798467	0.1757365
Pt29	0.0653577	0.4051970	0.1738313
Pt30	0.1899690	0.4030476	0.1729275
Pt31	0.1252947	0.0271031	0.1725626
Pt32	0.1288030	0.2760692	0.1711432
Pt33	0.2500000	0.0000000	0.0000000
Pt34	0.4375000	0.1250000	0.0000000
Pt35	0.3125000	0.1250000	0.0000000
Pt36	0.2500000	0.2500000	0.0000000
Pt37	0.3125000	0.3750000	0.0000000
Pt38	0.4375000	0.3750000	0.0000000

Pt39	0.3750000	0.0000000	0.0000000
Pt40	0.3750000	0.2500000	0.0000000
Pt41	0.4373883	0.4668076	0.0577337
Pt42	0.3119498	0.4669040	0.0578252
Pt43	0.2499597	0.0919911	0.0578122
Pt44	0.2497035	0.3419357	0.0577184
Pt45	0.3749299	0.0919720	0.0577688
Pt46	0.3124420	0.2169546	0.0577658
Pt47	0.4374749	0.2169718	0.0578072
Pt48	0.3749382	0.3419274	0.0576739
Pt49	0.4376426	0.3105517	0.1146945
Pt50	0.3128253	0.3108488	0.1145928
Pt51	0.2499909	0.4356546	0.1147868
Pt52	0.2502562	0.1856104	0.1148050
Pt53	0.3124969	0.0606388	0.1147943
Pt54	0.4373277	0.0605710	0.1147963
Pt55	0.3750791	0.1856119	0.1147872
Pt56	0.3750268	0.4356890	0.1146585
Pt57	0.2503915	0.0275856	0.1727344
Pt58	0.4378852	0.1525176	0.1725955
Pt59	0.3131272	0.1521567	0.1727369
Pt60	0.2516338	0.2777329	0.1728546
Pt61	0.3131921	0.4030182	0.1726751
Pt62	0.4375758	0.4025785	0.1723981
Pt63	0.3751710	0.0276567	0.1726860
Pt64	0.3751555	0.2774861	0.1725177
Pt65	0.5000000	0.0000000	0.0000000
Pt66	0.6875000	0.1250000	0.0000000
Pt67	0.5625000	0.1250000	0.0000000
Pt68	0.5000000	0.2500000	0.0000000
Pt69	0.5625000	0.3750000	0.0000000
Pt70	0.6875000	0.3750000	0.0000000
Pt71	0.6250000	0.0000000	0.0000000
Pt72	0.6250000	0.2500000	0.0000000
Pt73	0.6879456	0.4668019	0.0577079
Pt74	0.5626960	0.4668997	0.0577885
Pt75	0.4999451	0.0919962	0.0578548
Pt76	0.5001925	0.3419186	0.0577427
Pt77	0.6249351	0.0920302	0.0578153
Pt78	0.5625989	0.2170268	0.0578387
Pt79	0.6877267	0.2169179	0.0577297
Pt80	0.6255332	0.3418970	0.0577460

Pt81	0.6878547	0.3107621	0.1146196
Pt82	0.5627297	0.3105237	0.1146762
Pt83	0.5000578	0.4355110	0.1146129
Pt84	0.5001452	0.1854903	0.1147101
Pt85	0.5624965	0.0606326	0.1148030
Pt86	0.6875027	0.0605655	0.1147695
Pt87	0.6252723	0.1856208	0.1147686
Pt88	0.6250941	0.4354863	0.1146923
Pt89	0.5001469	0.0275578	0.1725987
Pt90	0.6872758	0.1521354	0.1726004
Pt91	0.5624587	0.1527346	0.1726250
Pt92	0.5001706	0.2773877	0.1724269
Pt93	0.5624837	0.4023847	0.1724657
Pt94	0.6873872	0.4027957	0.1724570
Pt95	0.6250246	0.0274669	0.1725927
Pt96	0.6251215	0.2775888	0.1724707
Pt97	0.7500000	0.0000000	0.0000000
Pt98	0.9375000	0.1250000	0.0000000
Pt99	0.8125000	0.1250000	0.0000000
Pt100	0.7500000	0.2500000	0.0000000
Pt101	0.8125000	0.3750000	0.0000000
Pt102	0.9375000	0.3750000	0.0000000
Pt103	0.8750000	0.0000000	0.0000000
Pt104	0.8750000	0.2500000	0.0000000
Pt105	0.9382152	0.4664971	0.0577711
Pt106	0.8131559	0.4666087	0.0576481
Pt107	0.7500228	0.0919825	0.0578319
Pt108	0.7510588	0.3416968	0.0578129
Pt109	0.8748849	0.0920761	0.0577867
Pt110	0.8128674	0.2168313	0.0578000
Pt111	0.9376778	0.2172811	0.0583365
Pt112	0.8760620	0.3415207	0.0583103
Pt113	0.9393048	0.3097741	0.1171635
Pt114	0.8129743	0.3104175	0.1148661
Pt115	0.7500873	0.4357085	0.1146183
Pt116	0.7501235	0.1855785	0.1147661
Pt117	0.8124281	0.0606495	0.1148960
Pt118	0.9374456	0.0603925	0.1145951
Pt119	0.8749252	0.1856433	0.1150396
Pt120	0.8749426	0.4352097	0.1143538
Pt121	0.7497123	0.0274078	0.1727202
Pt122	0.9367359	0.1514005	0.1724371

Pt123	0.8118922	0.1524449	0.1728702
Pt124	0.7492779	0.2775030	0.1726574
Pt125	0.8111798	0.4035713	0.1727754
Pt126	0.9342338	0.4045748	0.1727367
Pt127	0.8748949	0.0274105	0.1725726
Pt128	0.8722273	0.2775646	0.1732445
Pt129	0.0000000	0.5000000	0.0000000
Pt130	0.1875000	0.6250000	0.0000000
Pt131	0.0625000	0.6250000	0.0000000
Pt132	0.0000000	0.7500000	0.0000000
Pt133	0.0625000	0.8750000	0.0000000
Pt134	0.1875000	0.8750000	0.0000000
Pt135	0.1250000	0.5000000	0.0000000
Pt136	0.1250000	0.7500000	0.0000000
Pt137	0.1875898	0.9667695	0.0577594
Pt138	0.0625275	0.9669915	0.0577928
Pt139	0.0001246	0.5916430	0.0578510
Pt140	0.0000601	0.8417931	0.0577892
Pt141	0.1246011	0.5915441	0.0578176
Pt142	0.0624544	0.7167286	0.0578355
Pt143	0.1874746	0.7167024	0.0577803
Pt144	0.1251250	0.8416525	0.0577814
Pt145	0.1877563	0.8104206	0.1147783
Pt146	0.0626390	0.8103022	0.1147687
Pt147	-0.0001571	0.9351661	0.1147341
Pt148	0.0000779	0.6854479	0.1148790
Pt149	0.0625031	0.5607015	0.1151199
Pt150	0.1875220	0.5601481	0.1147542
Pt151	0.1252306	0.6853621	0.1147552
Pt152	0.1249936	0.9351761	0.1147058
Pt153	0.9994770	0.5301687	0.1727014
Pt154	0.1879258	0.6531647	0.1724992
Pt155	0.0626320	0.6538693	0.1728517
Pt156	0.0001229	0.7782230	0.1727279
Pt157	0.0624923	0.9026217	0.1725952
Pt158	0.1875338	0.9029244	0.1725941
Pt159	0.1260155	0.5300304	0.1731457
Pt160	0.1251792	0.7778990	0.1725575
Pt161	0.2500000	0.5000000	0.0000000
Pt162	0.4375000	0.6250000	0.0000000
Pt163	0.3125000	0.6250000	0.0000000
Pt164	0.2500000	0.7500000	0.0000000

Pt165	0.3125000	0.8750000	0.0000000
Pt166	0.4375000	0.8750000	0.0000000
Pt167	0.3750000	0.5000000	0.0000000
Pt168	0.3750000	0.7500000	0.0000000
Pt169	0.4375273	0.9670511	0.0578357
Pt170	0.3124662	0.9669515	0.0578414
Pt171	0.2496663	0.5916928	0.0577409
Pt172	0.2501375	0.8418364	0.0578488
Pt173	0.3747968	0.5918517	0.0578089
Pt174	0.3124960	0.7169396	0.0578173
Pt175	0.4375114	0.7169642	0.0577658
Pt176	0.3750789	0.8420602	0.0578542
Pt177	0.4376933	0.8106152	0.1147497
Pt178	0.3127899	0.8106428	0.1147928
Pt179	0.2500094	0.9356089	0.1148747
Pt180	0.2503536	0.6855004	0.1147221
Pt181	0.3125241	0.5606242	0.1147897
Pt182	0.4374944	0.5603986	0.1147964
Pt183	0.3753271	0.6855013	0.1147772
Pt184	0.3749913	0.9356373	0.1147968
Pt185	0.2506551	0.5283425	0.1727912
Pt186	0.4378325	0.6526044	0.1726656
Pt187	0.3131127	0.6527342	0.1726742
Pt188	0.2502112	0.7777807	0.1725020
Pt189	0.3129118	0.9024860	0.1726605
Pt190	0.4375638	0.9025787	0.1725774
Pt191	0.3755430	0.5277959	0.1727160
Pt192	0.3752164	0.7775290	0.1726406
Pt193	0.5000000	0.5000000	0.0000000
Pt194	0.6875000	0.6250000	0.0000000
Pt195	0.5625000	0.6250000	0.0000000
Pt196	0.5000000	0.7500000	0.0000000
Pt197	0.5625000	0.8750000	0.0000000
Pt198	0.6875000	0.8750000	0.0000000
Pt199	0.6250000	0.5000000	0.0000000
Pt200	0.6250000	0.7500000	0.0000000
Pt201	0.6876497	0.9670449	0.0578133
Pt202	0.5625909	0.9669831	0.0577867
Pt203	0.4998104	0.5918946	0.0577919
Pt204	0.5001023	0.8419856	0.0577349
Pt205	0.6249214	0.5919727	0.0577923
Pt206	0.5624603	0.7169942	0.0578181

Pt207	0.6873949	0.7170382	0.0578175
Pt208	0.6251246	0.8420825	0.0577940
Pt209	0.6873751	0.8105963	0.1147541
Pt210	0.5626248	0.8106489	0.1147611
Pt211	0.4999779	0.9356505	0.1147293
Pt212	0.5000787	0.6854585	0.1147467
Pt213	0.5623791	0.5604045	0.1147101
Pt214	0.6871818	0.5605549	0.1147374
Pt215	0.6248187	0.6855243	0.1148149
Pt216	0.6250786	0.9356811	0.1147636
Pt217	0.5001819	0.5272503	0.1726537
Pt218	0.6872025	0.6525257	0.1726677
Pt219	0.5623907	0.6524129	0.1726450
Pt220	0.5000953	0.7774908	0.1725287
Pt221	0.5624420	0.9026907	0.1725079
Pt222	0.6874971	0.9023575	0.1726410
Pt223	0.6246621	0.5276166	0.1726282
Pt224	0.6250036	0.7775749	0.1726337
Pt225	0.7500000	0.5000000	0.0000000
Pt226	0.9375000	0.6250000	0.0000000
Pt227	0.8125000	0.6250000	0.0000000
Pt228	0.7500000	0.7500000	0.0000000
Pt229	0.8125000	0.8750000	0.0000000
Pt230	0.9375000	0.8750000	0.0000000
Pt231	0.8750000	0.5000000	0.0000000
Pt232	0.8750000	0.7500000	0.0000000
Pt233	0.9374633	0.9669704	0.0578129
Pt234	0.8124894	0.9669446	0.0578359
Pt235	0.7499725	0.5918970	0.0577590
Pt236	0.7501034	0.8418841	0.0578539
Pt237	0.8751919	0.5915903	0.0576930
Pt238	0.8124510	0.7167735	0.0578015
Pt239	0.9375609	0.7166580	0.0578256
Pt240	0.8750517	0.8417716	0.0578144
Pt241	0.9375093	0.8102543	0.1147885
Pt242	0.8124381	0.8104391	0.1148347
Pt243	0.7500116	0.9355671	0.1148206
Pt244	0.7497377	0.6855727	0.1147489
Pt245	0.8121742	0.5605404	0.1146133
Pt246	0.9372328	0.5604935	0.1146416
Pt247	0.8748422	0.6854323	0.1147013
Pt248	0.8748689	0.9353621	0.1147916

Pt249	0.7494152	0.5283901	0.1725975
Pt250	0.9371986	0.6534375	0.1726260
Pt251	0.8123084	0.6530554	0.1725065
Pt252	0.7495812	0.7776378	0.1726219
Pt253	0.8124753	0.9027654	0.1726240
Pt254	0.9374910	0.9025114	0.1725764
Pt255	0.8744980	0.5283288	0.1724878
Pt256	0.8750154	0.7776311	0.1725521

Triazine/Pt(111)

N1	0.0624997	0.1375308	0.2278684
N2	0.1161331	0.1297665	0.2789295
N3	0.0088619	0.1298786	0.2789340
C1	0.1143400	0.1350076	0.2458856
C2	0.0624938	0.1270150	0.2942775
C3	0.0106538	0.1351078	0.2458870
H1	0.1565025	0.1375087	0.2315878
H2	0.0624936	0.1221633	0.3215119
H3	0.9684953	0.1376866	0.2315920
Pt1	0.0000000	0.0000000	0.0000000
Pt2	0.1875000	0.1250000	0.0000000
Pt3	0.0625000	0.1250000	0.0000000
Pt4	0.0000000	0.2500000	0.0000000
Pt5	0.0625000	0.3750000	0.0000000
Pt6	0.1875000	0.3750000	0.0000000
Pt7	0.1250000	0.0000000	0.0000000
Pt8	0.1250000	0.2500000	0.0000000
Pt9	0.1874787	0.4639856	0.0575975
Pt10	0.0625022	0.4640564	0.0576352
Pt11	0.0002617	0.0894790	0.0583448
Pt12	0.0001709	0.3388276	0.0575647
Pt13	0.1247421	0.0894747	0.0583456
Pt14	0.0625040	0.2136154	0.0585960
Pt15	0.1869176	0.2138384	0.0577820
Pt16	0.1248284	0.3388251	0.0575636
Pt17	0.1874456	0.3036439	0.1143156
Pt18	0.0625029	0.3041975	0.1147066
Pt19	0.9999491	0.4289479	0.1143929
Pt20	0.0009480	0.1785310	0.1164037
Pt21	0.0625038	0.0542761	0.1157197
Pt22	0.1877644	0.0537934	0.1146626

Pt23	0.1240564	0.1785373	0.1164097
Pt24	0.1250552	0.4289398	0.1143966
Pt25	0.9993140	0.0155868	0.1719457
Pt26	0.1899491	0.1420290	0.1718770
Pt27	0.0625017	0.1428939	0.1763808
Pt28	0.9993132	0.2690175	0.1722986
Pt29	0.0625014	0.3929906	0.1721305
Pt30	0.1876726	0.3925901	0.1720159
Pt31	0.1257040	0.0155930	0.1719525
Pt32	0.1256865	0.2690174	0.1723079
Pt33	0.2500000	0.0000000	0.0000000
Pt34	0.4375000	0.1250000	0.0000000
Pt35	0.3125000	0.1250000	0.0000000
Pt36	0.2500000	0.2500000	0.0000000
Pt37	0.3125000	0.3750000	0.0000000
Pt38	0.4375000	0.3750000	0.0000000
Pt39	0.3750000	0.0000000	0.0000000
Pt40	0.3750000	0.2500000	0.0000000
Pt41	0.4375506	0.4642686	0.0576525
Pt42	0.3125661	0.4641797	0.0576180
Pt43	0.2498256	0.0890410	0.0576075
Pt44	0.2498009	0.3388811	0.0575809
Pt45	0.3749184	0.0892126	0.0575914
Pt46	0.3120805	0.2141425	0.0575970
Pt47	0.4373228	0.2142281	0.0576013
Pt48	0.3748944	0.3391877	0.0576382
Pt49	0.4375430	0.3039352	0.1145079
Pt50	0.3125161	0.3039098	0.1144661
Pt51	0.2501902	0.4288155	0.1143371
Pt52	0.2498889	0.1788951	0.1141691
Pt53	0.3125737	0.0539375	0.1144999
Pt54	0.4374125	0.0539887	0.1144717
Pt55	0.3749753	0.1791675	0.1143091
Pt56	0.3751649	0.4289399	0.1144687
Pt57	0.2504416	0.0169299	0.1723719
Pt58	0.4373746	0.1422785	0.1720248
Pt59	0.3132395	0.1424157	0.1720860
Pt60	0.2503637	0.2675743	0.1721588
Pt61	0.3126960	0.3924832	0.1721093
Pt62	0.4377064	0.3922855	0.1722164
Pt63	0.3752131	0.0169710	0.1721583
Pt64	0.3752886	0.2675542	0.1721641

Pt65	0.5000000	0.0000000	0.0000000
Pt66	0.6875000	0.1250000	0.0000000
Pt67	0.5625000	0.1250000	0.0000000
Pt68	0.5000000	0.2500000	0.0000000
Pt69	0.5625000	0.3750000	0.0000000
Pt70	0.6875000	0.3750000	0.0000000
Pt71	0.6250000	0.0000000	0.0000000
Pt72	0.6250000	0.2500000	0.0000000
Pt73	0.6874511	0.4642688	0.0576487
Pt74	0.5624980	0.4642366	0.0576468
Pt75	0.4999668	0.0892785	0.0576339
Pt76	0.4999539	0.3392125	0.0576465
Pt77	0.6250359	0.0892753	0.0576319
Pt78	0.5625017	0.2142393	0.0575872
Pt79	0.6876778	0.2142260	0.0576009
Pt80	0.6250485	0.3392152	0.0576438
Pt81	0.6874607	0.3039372	0.1145045
Pt82	0.5625012	0.3039681	0.1144162
Pt83	0.5000570	0.4288903	0.1145083
Pt84	0.4999966	0.1789409	0.1143900
Pt85	0.5625047	0.0538646	0.1143967
Pt86	0.6875890	0.0539998	0.1144735
Pt87	0.6250041	0.1789426	0.1143901
Pt88	0.6249557	0.4288814	0.1145014
Pt89	0.5001195	0.0173899	0.1721415
Pt90	0.6876295	0.1422874	0.1720280
Pt91	0.5625003	0.1422167	0.1719080
Pt92	0.5001443	0.2672308	0.1721303
Pt93	0.5625083	0.3923061	0.1722549
Pt94	0.6873115	0.3922946	0.1722123
Pt95	0.6248939	0.0173776	0.1721348
Pt96	0.6248643	0.2672353	0.1721254
Pt97	0.7500000	0.0000000	0.0000000
Pt98	0.9375000	0.1250000	0.0000000
Pt99	0.8125000	0.1250000	0.0000000
Pt100	0.7500000	0.2500000	0.0000000
Pt101	0.8125000	0.3750000	0.0000000
Pt102	0.9375000	0.3750000	0.0000000
Pt103	0.8750000	0.0000000	0.0000000
Pt104	0.8750000	0.2500000	0.0000000
Pt105	0.9375239	0.4639843	0.0575975
Pt106	0.8124324	0.4641953	0.0576222

Pt107	0.7500836	0.0892157	0.0575944
Pt108	0.7500993	0.3391947	0.0576370
Pt109	0.8751789	0.0890380	0.0576112
Pt110	0.8129219	0.2141436	0.0575964
Pt111	0.9380872	0.2138414	0.0577814
Pt112	0.8752011	0.3388899	0.0575838
Pt113	0.9375567	0.3036360	0.1143116
Pt114	0.8124848	0.3039155	0.1144648
Pt115	0.7498537	0.4289577	0.1144696
Pt116	0.7500229	0.1791764	0.1143109
Pt117	0.8124289	0.0539484	0.1145023
Pt118	0.9372435	0.0537834	0.1146666
Pt119	0.8751072	0.1788958	0.1141700
Pt120	0.8748190	0.4288111	0.1143381
Pt121	0.7497867	0.0169616	0.1721566
Pt122	0.9350575	0.1420251	0.1718732
Pt123	0.8117649	0.1424156	0.1720926
Pt124	0.7497219	0.2675674	0.1721644
Pt125	0.8123230	0.3924937	0.1721097
Pt126	0.9373324	0.3925989	0.1720125
Pt127	0.8745654	0.0169384	0.1723735
Pt128	0.8746472	0.2675698	0.1721556
Pt129	0.0000000	0.5000000	0.0000000
Pt130	0.1875000	0.6250000	0.0000000
Pt131	0.0625000	0.6250000	0.0000000
Pt132	0.0000000	0.7500000	0.0000000
Pt133	0.0625000	0.8750000	0.0000000
Pt134	0.1875000	0.8750000	0.0000000
Pt135	0.1250000	0.5000000	0.0000000
Pt136	0.1250000	0.7500000	0.0000000
Pt137	0.1874798	0.9643769	0.0576152
Pt138	0.0625038	0.9647832	0.0575541
Pt139	0.0000226	0.5890500	0.0576628
Pt140	0.0000133	0.8393853	0.0576537
Pt141	0.1249851	0.5890512	0.0576658
Pt142	0.0625037	0.7142593	0.0576416
Pt143	0.1875132	0.7140904	0.0576579
Pt144	0.1249905	0.8393847	0.0576529
Pt145	0.1874791	0.8037426	0.1144163
Pt146	0.0625004	0.8037021	0.1144942
Pt147	0.0000830	0.9288466	0.1142075
Pt148	0.9999872	0.6787291	0.1145026

Pt149	0.0625000	0.5538931	0.1145371
Pt150	0.1875695	0.5538498	0.1144645
Pt151	0.1250159	0.6787359	0.1145045
Pt152	0.1249234	0.9288407	0.1142104
Pt153	0.9999562	0.5175457	0.1721397
Pt154	0.1875268	0.6422279	0.1721644
Pt155	0.0625059	0.6423814	0.1722699
Pt156	0.9999389	0.7669967	0.1721714
Pt157	0.0625090	0.8917665	0.1720577
Pt158	0.1877456	0.8917682	0.1720996
Pt159	0.1250523	0.5175345	0.1721394
Pt160	0.1250723	0.7670013	0.1721752
Pt161	0.2500000	0.5000000	0.0000000
Pt162	0.4375000	0.6250000	0.0000000
Pt163	0.3125000	0.6250000	0.0000000
Pt164	0.2500000	0.7500000	0.0000000
Pt165	0.3125000	0.8750000	0.0000000
Pt166	0.4375000	0.8750000	0.0000000
Pt167	0.3750000	0.5000000	0.0000000
Pt168	0.3750000	0.7500000	0.0000000
Pt169	0.4375224	0.9642756	0.0576478
Pt170	0.3124581	0.9642873	0.0576662
Pt171	0.2500056	0.5890782	0.0576684
Pt172	0.2500331	0.8392106	0.0576132
Pt173	0.3749952	0.5892881	0.0576528
Pt174	0.3124814	0.7142184	0.0576699
Pt175	0.4374714	0.7143177	0.0576666
Pt176	0.3749388	0.8392571	0.0576431
Pt177	0.4374166	0.8039816	0.1145336
Pt178	0.3124722	0.8039514	0.1145480
Pt179	0.2500297	0.9288506	0.1145050
Pt180	0.2500607	0.6788509	0.1145340
Pt181	0.3126347	0.5539592	0.1144926
Pt182	0.4376112	0.5539876	0.1144897
Pt183	0.3750352	0.6789757	0.1144646
Pt184	0.3750116	0.9288891	0.1144754
Pt185	0.2500480	0.5171901	0.1720009
Pt186	0.4374516	0.6423395	0.1721673
Pt187	0.3126740	0.6422994	0.1721204
Pt188	0.2500220	0.7673759	0.1721533
Pt189	0.3127344	0.8921292	0.1722229
Pt190	0.4375294	0.8922820	0.1722188

Pt191	0.3752553	0.5172587	0.1721522
Pt192	0.3751023	0.7672000	0.1722429
Pt193	0.5000000	0.5000000	0.0000000
Pt194	0.6875000	0.6250000	0.0000000
Pt195	0.5625000	0.6250000	0.0000000
Pt196	0.5000000	0.7500000	0.0000000
Pt197	0.5625000	0.8750000	0.0000000
Pt198	0.6875000	0.8750000	0.0000000
Pt199	0.6250000	0.5000000	0.0000000
Pt200	0.6250000	0.7500000	0.0000000
Pt201	0.6874827	0.9642792	0.0576434
Pt202	0.5625061	0.9642825	0.0577020
Pt203	0.5000241	0.5892577	0.0576251
Pt204	0.4999712	0.8392623	0.0576818
Pt205	0.6249800	0.5892529	0.0576256
Pt206	0.5624993	0.7142682	0.0576142
Pt207	0.6875250	0.7143159	0.0576672
Pt208	0.6250271	0.8392602	0.0576823
Pt209	0.6876004	0.8039739	0.1145360
Pt210	0.5625090	0.8039318	0.1144825
Pt211	0.4999764	0.9289161	0.1145397
Pt212	0.4999619	0.6790039	0.1144668
Pt213	0.5625044	0.5539421	0.1144626
Pt214	0.6873956	0.5539890	0.1144898
Pt215	0.6250498	0.6789941	0.1144661
Pt216	0.6250437	0.9289147	0.1145344
Pt217	0.5001431	0.5173328	0.1721714
Pt218	0.6875625	0.6423267	0.1721664
Pt219	0.5625033	0.6424167	0.1720834
Pt220	0.5000583	0.7674271	0.1721308
Pt221	0.5625011	0.8923907	0.1722114
Pt222	0.6874815	0.8922618	0.1722171
Pt223	0.6248792	0.5173319	0.1721650
Pt224	0.6249512	0.7674049	0.1721297
Pt225	0.7500000	0.5000000	0.0000000
Pt226	0.9375000	0.6250000	0.0000000
Pt227	0.8125000	0.6250000	0.0000000
Pt228	0.7500000	0.7500000	0.0000000
Pt229	0.8125000	0.8750000	0.0000000
Pt230	0.9375000	0.8750000	0.0000000
Pt231	0.8750000	0.5000000	0.0000000
Pt232	0.8750000	0.7500000	0.0000000

Pt233	0.9375231	0.9643811	0.0576169
Pt234	0.8125478	0.9642902	0.0576676
Pt235	0.7500062	0.5892931	0.0576537
Pt236	0.7500647	0.8392560	0.0576451
Pt237	0.8749986	0.5890829	0.0576635
Pt238	0.8125208	0.7142192	0.0576688
Pt239	0.9374845	0.7140957	0.0576616
Pt240	0.8749713	0.8392150	0.0576143
Pt241	0.9375226	0.8037469	0.1144151
Pt242	0.8125374	0.8039614	0.1145496
Pt243	0.7499956	0.9288880	0.1144734
Pt244	0.7499739	0.6789833	0.1144648
Pt245	0.8123729	0.5539658	0.1144926
Pt246	0.9374307	0.5538574	0.1144609
Pt247	0.8749439	0.6788631	0.1145351
Pt248	0.8749757	0.9288649	0.1145089
Pt249	0.7497640	0.5172632	0.1721660
Pt250	0.9374802	0.6422161	0.1721576
Pt251	0.8123335	0.6423060	0.1721207
Pt252	0.7499126	0.7671938	0.1722511
Pt253	0.8122879	0.8921365	0.1722263
Pt254	0.9372733	0.8917684	0.1720971
Pt255	0.8749669	0.5171925	0.1720023
Pt256	0.8749868	0.7673842	0.1721587

Aniline/Pt(111)

N1	0.0186824	0.2265643	0.2452582
C1	0.0222583	0.1621804	0.2318898
C2	0.0804446	0.1304389	0.2260444
C3	0.0878085	0.0536235	0.2250499
C4	0.0313451	0.0138847	0.2258479
C5	0.9734111	0.0470041	0.2257881
C6	0.9659935	0.1234537	0.2263443
H1	0.1191972	0.1592650	0.2357299
H2	0.1241825	0.0331012	0.2408112
H3	0.0339739	0.9596328	0.2337969
H4	0.9346049	0.0164699	0.2339482
H5	0.9281357	0.1414460	0.2417028
H6	0.0560971	0.2573014	0.2448844
H7	0.9789830	0.2529239	0.2428645
Pt1	0.0000000	0.0000000	0.0000000

Pt2	0.1875000	0.1250000	0.0000000
Pt3	0.0625000	0.1250000	0.0000000
Pt4	0.0000000	0.2500000	0.0000000
Pt5	0.0625000	0.3750000	0.0000000
Pt6	0.1875000	0.3750000	0.0000000
Pt7	0.1250000	0.0000000	0.0000000
Pt8	0.1250000	0.2500000	0.0000000
Pt9	0.1877112	0.4663671	0.0577247
Pt10	0.0626476	0.4660070	0.0577737
Pt11	0.0000650	0.0918497	0.0589154
Pt12	0.0000753	0.3409058	0.0576735
Pt13	0.1243285	0.0917230	0.0586421
Pt14	0.0617263	0.2159467	0.0580690
Pt15	0.1863098	0.2162787	0.0575698
Pt16	0.1247765	0.3410775	0.0576538
Pt17	0.1881480	0.3099632	0.1142661
Pt18	0.0629941	0.3105331	0.1146781
Pt19	-0.0000377	0.4346509	0.1147523
Pt20	0.0004292	0.1851395	0.1170180
Pt21	0.0615072	0.0599175	0.1169285
Pt22	0.1855867	0.0598483	0.1163363
Pt23	0.1239426	0.1851528	0.1154384
Pt24	0.1253005	0.4349882	0.1146763
Pt25	0.9953458	0.0197312	0.1747482
Pt26	0.1914229	0.1535923	0.1720188
Pt27	0.0669300	0.1564633	0.1742700
Pt28	0.0002681	0.2805864	0.1718426
Pt29	0.0629072	0.4033057	0.1727935
Pt30	0.1883002	0.4028572	0.1723509
Pt31	0.1244854	0.0280455	0.1767270
Pt32	0.1272338	0.2806704	0.1726935
Pt33	0.2500000	0.0000000	0.0000000
Pt34	0.4375000	0.1250000	0.0000000
Pt35	0.3125000	0.1250000	0.0000000
Pt36	0.2500000	0.2500000	0.0000000
Pt37	0.3125000	0.3750000	0.0000000
Pt38	0.4375000	0.3750000	0.0000000
Pt39	0.3750000	0.0000000	0.0000000
Pt40	0.3750000	0.2500000	0.0000000
Pt41	0.4377609	0.4668744	0.0577274
Pt42	0.3127252	0.4667043	0.0577765
Pt43	0.2487811	0.0913194	0.0577464

Pt44	0.2500347	0.3413626	0.0575706
Pt45	0.3739388	0.0915191	0.0577254
Pt46	0.3115581	0.2163393	0.0575806
Pt47	0.4371086	0.2165249	0.0576580
Pt48	0.3751977	0.3416246	0.0577203
Pt49	0.4378200	0.3101894	0.1146320
Pt50	0.3130692	0.3101295	0.1145316
Pt51	0.2505359	0.4350885	0.1145775
Pt52	0.2497156	0.1848848	0.1139511
Pt53	0.3113703	0.0601990	0.1146460
Pt54	0.4369571	0.0604743	0.1144473
Pt55	0.3749788	0.1852852	0.1144000
Pt56	0.3754664	0.4353779	0.1146636
Pt57	0.2506562	0.0264476	0.1729336
Pt58	0.4376843	0.1521797	0.1722338
Pt59	0.3134714	0.1525496	0.1721849
Pt60	0.2513048	0.2780802	0.1723468
Pt61	0.3134615	0.4023501	0.1725411
Pt62	0.4378898	0.4020503	0.1726477
Pt63	0.3750769	0.0271601	0.1723312
Pt64	0.3758943	0.2775630	0.1725454
Pt65	0.5000000	0.0000000	0.0000000
Pt66	0.6875000	0.1250000	0.0000000
Pt67	0.5625000	0.1250000	0.0000000
Pt68	0.5000000	0.2500000	0.0000000
Pt69	0.5625000	0.3750000	0.0000000
Pt70	0.6875000	0.3750000	0.0000000
Pt71	0.6250000	0.0000000	0.0000000
Pt72	0.6250000	0.2500000	0.0000000
Pt73	0.6875528	0.4667430	0.0577855
Pt74	0.5627143	0.4667565	0.0577432
Pt75	0.4995789	0.0918145	0.0577207
Pt76	0.5002378	0.3416225	0.0577402
Pt77	0.6251434	0.0917755	0.0576736
Pt78	0.5627902	0.2165741	0.0577302
Pt79	0.6884300	0.2164165	0.0577707
Pt80	0.6254708	0.3415668	0.0577521
Pt81	0.6877630	0.3096893	0.1147439
Pt82	0.5627203	0.3100118	0.1146009
Pt83	0.5001515	0.4351611	0.1146691
Pt84	0.5000954	0.1852515	0.1145325
Pt85	0.5622464	0.0602878	0.1146026

Pt86	0.6873176	0.0604574	0.1145549
Pt87	0.6251983	0.1851921	0.1145282
Pt88	0.6248808	0.4349564	0.1147049
Pt89	0.4994829	0.0270529	0.1722641
Pt90	0.6870245	0.1518827	0.1724117
Pt91	0.5626081	0.1519588	0.1723673
Pt92	0.5002337	0.2766954	0.1725316
Pt93	0.5623523	0.4018194	0.1725660
Pt94	0.6872175	0.4012272	0.1725928
Pt95	0.6244473	0.0266730	0.1722881
Pt96	0.6248174	0.2768319	0.1725407
Pt97	0.7500000	0.0000000	0.0000000
Pt98	0.9375000	0.1250000	0.0000000
Pt99	0.8125000	0.1250000	0.0000000
Pt100	0.7500000	0.2500000	0.0000000
Pt101	0.8125000	0.3750000	0.0000000
Pt102	0.9375000	0.3750000	0.0000000
Pt103	0.8750000	0.0000000	0.0000000
Pt104	0.8750000	0.2500000	0.0000000
Pt105	0.9375188	0.4659514	0.0577441
Pt106	0.8124333	0.4663422	0.0577599
Pt107	0.7506434	0.0916421	0.0577283
Pt108	0.7504776	0.3412987	0.0577126
Pt109	0.8756542	0.0921417	0.0582366
Pt110	0.8135489	0.2163156	0.0580509
Pt111	0.9376025	0.2160002	0.0585897
Pt112	0.8753966	0.3410358	0.0577004
Pt113	0.9373755	0.3099437	0.1147228
Pt114	0.8127642	0.3092461	0.1147121
Pt115	0.7496071	0.4347247	0.1146721
Pt116	0.7508507	0.1848686	0.1147416
Pt117	0.8122817	0.0601298	0.1144982
Pt118	0.9381266	0.0594215	0.1163229
Pt119	0.8772315	0.1839233	0.1168494
Pt120	0.8746231	0.4345872	0.1146343
Pt121	0.7483456	0.0261914	0.1725453
Pt122	0.9371696	0.1501758	0.1766825
Pt123	0.8112007	0.1511560	0.1729385
Pt124	0.7499187	0.2765643	0.1726648
Pt125	0.8123941	0.4009941	0.1723653
Pt126	0.9371181	0.4023264	0.1725974
Pt127	0.8701526	0.0236995	0.1717391

Pt128	0.8750454	0.2763365	0.1730214
Pt129	0.0000000	0.5000000	0.0000000
Pt130	0.1875000	0.6250000	0.0000000
Pt131	0.0625000	0.6250000	0.0000000
Pt132	0.0000000	0.7500000	0.0000000
Pt133	0.0625000	0.8750000	0.0000000
Pt134	0.1875000	0.8750000	0.0000000
Pt135	0.1250000	0.5000000	0.0000000
Pt136	0.1250000	0.7500000	0.0000000
Pt137	0.1870121	0.9673381	0.0583387
Pt138	0.0624523	0.9675912	0.0584249
Pt139	-0.0001931	0.5910867	0.0577142
Pt140	0.0000445	0.8425731	0.0575875
Pt141	0.1248122	0.5914633	0.0577655
Pt142	0.0624673	0.7170418	0.0577698
Pt143	0.1873811	0.7169734	0.0578007
Pt144	0.1252555	0.8426049	0.0577058
Pt145	0.1874283	0.8103461	0.1147510
Pt146	0.0625190	0.8094249	0.1141679
Pt147	-0.0004706	0.9345744	0.1153845
Pt148	0.0000047	0.6837286	0.1144796
Pt149	0.0624532	0.5593558	0.1146647
Pt150	0.1876305	0.5598490	0.1147136
Pt151	0.1251247	0.6844690	0.1146784
Pt152	0.1247234	0.9358930	0.1158087
Pt153	0.0000964	0.5266479	0.1726136
Pt154	0.1876957	0.6515700	0.1725366
Pt155	0.0623430	0.6505966	0.1724690
Pt156	-0.0005180	0.7739152	0.1721414
Pt157	0.0630307	0.8963669	0.1718309
Pt158	0.1876124	0.9014675	0.1729983
Pt159	0.1253373	0.5270486	0.1725674
Pt160	0.1253077	0.7752208	0.1722889
Pt161	0.2500000	0.5000000	0.0000000
Pt162	0.4375000	0.6250000	0.0000000
Pt163	0.3125000	0.6250000	0.0000000
Pt164	0.2500000	0.7500000	0.0000000
Pt165	0.3125000	0.8750000	0.0000000
Pt166	0.4375000	0.8750000	0.0000000
Pt167	0.3750000	0.5000000	0.0000000
Pt168	0.3750000	0.7500000	0.0000000
Pt169	0.4373663	0.9668673	0.0577693

Pt170	0.3121315	0.9667645	0.0577782
Pt171	0.2498291	0.5917433	0.0578418
Pt172	0.2500474	0.8420964	0.0578406
Pt173	0.3748982	0.5918974	0.0577926
Pt174	0.3123250	0.7168535	0.0578227
Pt175	0.4373385	0.7169180	0.0578182
Pt176	0.3749860	0.8419743	0.0578211
Pt177	0.4374441	0.8103033	0.1147381
Pt178	0.3124979	0.8102633	0.1148221
Pt179	0.2496904	0.9352379	0.1149735
Pt180	0.2499628	0.6851441	0.1147633
Pt181	0.3126760	0.5603243	0.1147461
Pt182	0.4374965	0.5604789	0.1146736
Pt183	0.3748860	0.6854313	0.1147711
Pt184	0.3746289	0.9354578	0.1147642
Pt185	0.2504006	0.5268469	0.1724609
Pt186	0.4374342	0.6521830	0.1725720
Pt187	0.3127784	0.6521123	0.1726154
Pt188	0.2501483	0.7765251	0.1725926
Pt189	0.3121268	0.9017949	0.1726820
Pt190	0.4371663	0.9019435	0.1724618
Pt191	0.3752390	0.5272412	0.1725911
Pt192	0.3749734	0.7772576	0.1726503
Pt193	0.5000000	0.5000000	0.0000000
Pt194	0.6875000	0.6250000	0.0000000
Pt195	0.5625000	0.6250000	0.0000000
Pt196	0.5000000	0.7500000	0.0000000
Pt197	0.5625000	0.8750000	0.0000000
Pt198	0.6875000	0.8750000	0.0000000
Pt199	0.6250000	0.5000000	0.0000000
Pt200	0.6250000	0.7500000	0.0000000
Pt201	0.6875898	0.9669410	0.0577398
Pt202	0.5624871	0.9670115	0.0578056
Pt203	0.4999366	0.5918580	0.0577336
Pt204	0.5000829	0.8418656	0.0578501
Pt205	0.6250032	0.5918933	0.0577964
Pt206	0.5624639	0.7168468	0.0577861
Pt207	0.6875014	0.7168514	0.0578494
Pt208	0.6250025	0.8419114	0.0578053
Pt209	0.6875290	0.8100826	0.1147877
Pt210	0.5625766	0.8102042	0.1148128
Pt211	0.4997464	0.9353050	0.1146426

Pt212	0.4999342	0.6853428	0.1147309
Pt213	0.5623891	0.5602672	0.1147042
Pt214	0.6872691	0.5601541	0.1147634
Pt215	0.6250027	0.6852269	0.1147617
Pt216	0.6248771	0.9352081	0.1146428
Pt217	0.4999074	0.5269238	0.1725105
Pt218	0.6871982	0.6511497	0.1726518
Pt219	0.5623555	0.6519815	0.1725157
Pt220	0.4997289	0.7771186	0.1725190
Pt221	0.5620873	0.9021425	0.1724985
Pt222	0.6864135	0.9011196	0.1726029
Pt223	0.6248122	0.5265858	0.1725515
Pt224	0.6246066	0.7765288	0.1726450
Pt225	0.7500000	0.5000000	0.0000000
Pt226	0.9375000	0.6250000	0.0000000
Pt227	0.8125000	0.6250000	0.0000000
Pt228	0.7500000	0.7500000	0.0000000
Pt229	0.8125000	0.8750000	0.0000000
Pt230	0.9375000	0.8750000	0.0000000
Pt231	0.8750000	0.5000000	0.0000000
Pt232	0.8750000	0.7500000	0.0000000
Pt233	0.9378589	0.9676302	0.0579802
Pt234	0.8128091	0.9670453	0.0576901
Pt235	0.7499959	0.5916902	0.0578960
Pt236	0.7499499	0.8419869	0.0577971
Pt237	0.8748309	0.5911939	0.0577554
Pt238	0.8123851	0.7167252	0.0577846
Pt239	0.9373805	0.7167805	0.0576878
Pt240	0.8749011	0.8421942	0.0576845
Pt241	0.9374219	0.8087269	0.1142254
Pt242	0.8122970	0.8095725	0.1147261
Pt243	0.7497148	0.9351005	0.1147014
Pt244	0.7499071	0.6849272	0.1148355
Pt245	0.8121902	0.5596146	0.1148174
Pt246	0.9371803	0.5590288	0.1146964
Pt247	0.8748346	0.6840872	0.1145918
Pt248	0.8744375	0.9342637	0.1145132
Pt249	0.7494903	0.5258147	0.1725312
Pt250	0.9371338	0.6504072	0.1723919
Pt251	0.8120911	0.6508702	0.1725828
Pt252	0.7490380	0.7757393	0.1727483
Pt253	0.8105102	0.8996581	0.1727086

Pt254	0.9347281	0.8959826	0.1720909
Pt255	0.8747194	0.5260879	0.1725554
Pt256	0.8737961	0.7743964	0.1723888

Triamino-pyrimidine/Pt(111)

N1	0.0074677	0.2342500	0.2493759
N2	0.1169912	0.2343849	0.2493925
N3	0.0621341	0.3353058	0.2520479
N4	0.1690323	0.1319690	0.2443201
N5	0.9556133	0.1317213	0.2442838
C1	0.0623304	0.1303713	0.2302484
C2	0.0621983	0.2657740	0.2498265
C3	0.1169587	0.1671119	0.2418045
C4	0.0076347	0.1669766	0.2417840
H1	0.0623799	0.0744025	0.2355859
H2	0.1017135	0.3613445	0.2495534
H3	0.2074984	0.1592256	0.2488344
H4	0.9519611	0.0823877	0.2351095
H5	0.0225062	0.3612411	0.2495359
H6	0.1727667	0.0826433	0.2351482
H7	0.9171001	0.1588873	0.2488049
Pt1	0.0000000	0.0000000	0.0000000
Pt2	0.1875000	0.1250000	0.0000000
Pt3	0.0625000	0.1250000	0.0000000
Pt4	0.0000000	0.2500000	0.0000000
Pt5	0.0625000	0.3750000	0.0000000
Pt6	0.1875000	0.3750000	0.0000000
Pt7	0.1250000	0.0000000	0.0000000
Pt8	0.1250000	0.2500000	0.0000000
Pt9	0.1874579	0.4616408	0.0575444
Pt10	0.0624943	0.4616084	0.0575935
Pt11	0.0002902	0.0870102	0.0583228
Pt12	0.0001893	0.3364979	0.0574516
Pt13	0.1246917	0.0870159	0.0583217
Pt14	0.0624914	0.2112209	0.0582899
Pt15	0.1868201	0.2114293	0.0574506
Pt16	0.1247926	0.3365194	0.0574488
Pt17	0.1875317	0.2988460	0.1138724
Pt18	0.0624903	0.2993635	0.1142516
Pt19	0.9999159	0.4240366	0.1142802
Pt20	0.0007891	0.1735822	0.1158427

Pt21	0.0624665	0.0494436	0.1157412
Pt22	0.1875871	0.0486273	0.1144809
Pt23	0.1241621	0.1735903	0.1158498
Pt24	0.1250495	0.4240784	0.1142871
Pt25	0.9993871	0.0090723	0.1719048
Pt26	0.1896543	0.1355503	0.1711016
Pt27	0.0624042	0.1351109	0.1764456
Pt28	0.9992669	0.2623561	0.1712327
Pt29	0.0624410	0.3868376	0.1718792
Pt30	0.1876010	0.3861747	0.1718515
Pt31	0.1254587	0.0090763	0.1719158
Pt32	0.1255604	0.2623633	0.1712252
Pt33	0.2500000	0.0000000	0.0000000
Pt34	0.4375000	0.1250000	0.0000000
Pt35	0.3125000	0.1250000	0.0000000
Pt36	0.2500000	0.2500000	0.0000000
Pt37	0.3125000	0.3750000	0.0000000
Pt38	0.4375000	0.3750000	0.0000000
Pt39	0.3750000	0.0000000	0.0000000
Pt40	0.3750000	0.2500000	0.0000000
Pt41	0.4375348	0.4618671	0.0574860
Pt42	0.3125317	0.4617696	0.0574540
Pt43	0.2496119	0.0866300	0.0574794
Pt44	0.2496957	0.3365808	0.0574393
Pt45	0.3746925	0.0868753	0.0574555
Pt46	0.3118574	0.2117632	0.0575066
Pt47	0.4371628	0.2118727	0.0574566
Pt48	0.3748425	0.3367894	0.0574486
Pt49	0.4375105	0.2988490	0.1141224
Pt50	0.3125544	0.2989289	0.1140862
Pt51	0.2501520	0.4237673	0.1140856
Pt52	0.2497236	0.1739328	0.1138910
Pt53	0.3123850	0.0490094	0.1142606
Pt54	0.4372841	0.0490294	0.1140367
Pt55	0.3748200	0.1741549	0.1139953
Pt56	0.3751137	0.4238903	0.1140885
Pt57	0.2505363	0.0101684	0.1721195
Pt58	0.4373279	0.1355752	0.1715998
Pt59	0.3133163	0.1357455	0.1717710
Pt60	0.2503415	0.2611440	0.1716772
Pt61	0.3125675	0.3857895	0.1716466
Pt62	0.4376296	0.3855216	0.1716354

Pt63	0.3752341	0.0104207	0.1716964
Pt64	0.3751884	0.2608367	0.1717028
Pt65	0.5000000	0.0000000	0.0000000
Pt66	0.6875000	0.1250000	0.0000000
Pt67	0.5625000	0.1250000	0.0000000
Pt68	0.5000000	0.2500000	0.0000000
Pt69	0.5625000	0.3750000	0.0000000
Pt70	0.6875000	0.3750000	0.0000000
Pt71	0.6250000	0.0000000	0.0000000
Pt72	0.6250000	0.2500000	0.0000000
Pt73	0.6874516	0.4618744	0.0574990
Pt74	0.5624948	0.4618153	0.0574539
Pt75	0.4998488	0.0869362	0.0574053
Pt76	0.4999667	0.3367765	0.0574542
Pt77	0.6251617	0.0869364	0.0574080
Pt78	0.5624976	0.2117859	0.0574265
Pt79	0.6878339	0.2118657	0.0574569
Pt80	0.6250297	0.3367736	0.0574513
Pt81	0.6874481	0.2988308	0.1141195
Pt82	0.5624811	0.2987950	0.1140542
Pt83	0.5000226	0.4237821	0.1140770
Pt84	0.4998764	0.1739074	0.1139975
Pt85	0.5624750	0.0488528	0.1138999
Pt86	0.6876643	0.0490011	0.1140499
Pt87	0.6250514	0.1738909	0.1140040
Pt88	0.6249376	0.4237812	0.1140841
Pt89	0.4999982	0.0107079	0.1715083
Pt90	0.6874439	0.1355617	0.1716025
Pt91	0.5623936	0.1355298	0.1713433
Pt92	0.5000002	0.2604654	0.1716390
Pt93	0.5624306	0.3854968	0.1716617
Pt94	0.6872315	0.3854814	0.1716474
Pt95	0.6247926	0.0107058	0.1715154
Pt96	0.6247924	0.2604260	0.1716387
Pt97	0.7500000	0.0000000	0.0000000
Pt98	0.9375000	0.1250000	0.0000000
Pt99	0.8125000	0.1250000	0.0000000
Pt100	0.7500000	0.2500000	0.0000000
Pt101	0.8125000	0.3750000	0.0000000
Pt102	0.9375000	0.3750000	0.0000000
Pt103	0.8750000	0.0000000	0.0000000
Pt104	0.8750000	0.2500000	0.0000000

Pt105	0.9375314	0.4616366	0.0575521
Pt106	0.8124561	0.4617619	0.0574561
Pt107	0.7502961	0.0868614	0.0574559
Pt108	0.7501493	0.3367897	0.0574506
Pt109	0.8753873	0.0866124	0.0574728
Pt110	0.8131193	0.2117544	0.0574976
Pt111	0.9381544	0.2114229	0.0574491
Pt112	0.8752975	0.3365614	0.0574419
Pt113	0.9374443	0.2988156	0.1138774
Pt114	0.8124131	0.2989085	0.1140719
Pt115	0.7498431	0.4238742	0.1141010
Pt116	0.7501269	0.1741295	0.1139986
Pt117	0.8125508	0.0489817	0.1142564
Pt118	0.9373466	0.0485859	0.1144723
Pt119	0.8752026	0.1738939	0.1138779
Pt120	0.8748128	0.4237445	0.1140913
Pt121	0.7495378	0.0103657	0.1717448
Pt122	0.9351742	0.1355042	0.1710626
Pt123	0.8114932	0.1356130	0.1717665
Pt124	0.7496543	0.2607700	0.1716940
Pt125	0.8122996	0.3856979	0.1716295
Pt126	0.9372940	0.3861464	0.1718580
Pt127	0.8742463	0.0101258	0.1721052
Pt128	0.8745011	0.2610561	0.1716710
Pt129	0.0000000	0.5000000	0.0000000
Pt130	0.1875000	0.6250000	0.0000000
Pt131	0.0625000	0.6250000	0.0000000
Pt132	0.0000000	0.7500000	0.0000000
Pt133	0.0625000	0.8750000	0.0000000
Pt134	0.1875000	0.8750000	0.0000000
Pt135	0.1250000	0.5000000	0.0000000
Pt136	0.1250000	0.7500000	0.0000000
Pt137	0.1873376	0.9620285	0.0575661
Pt138	0.0624908	0.9624710	0.0574910
Pt139	0.0000741	0.5866135	0.0575847
Pt140	0.0000909	0.8370387	0.0574661
Pt141	0.1249231	0.5866063	0.0575828
Pt142	0.0624970	0.7118245	0.0574621
Pt143	0.1874550	0.7117508	0.0575144
Pt144	0.1248989	0.8370373	0.0574672
Pt145	0.1874162	0.7988451	0.1140443
Pt146	0.0624812	0.7988071	0.1141321

Pt147	0.0000851	0.9239436	0.1140252
Pt148	0.0000176	0.6737754	0.1141641
Pt149	0.0624921	0.5489018	0.1143777
Pt150	0.1874858	0.5488030	0.1142063
Pt151	0.1249664	0.6737787	0.1141555
Pt152	0.1248660	0.9239657	0.1140160
Pt153	0.9999169	0.5111960	0.1720033
Pt154	0.1874494	0.6356044	0.1716553
Pt155	0.0624343	0.6360271	0.1719290
Pt156	0.9997901	0.7604706	0.1716802
Pt157	0.0624180	0.8850798	0.1716493
Pt158	0.1876978	0.8852059	0.1716682
Pt159	0.1250048	0.5111818	0.1720025
Pt160	0.1250175	0.7604680	0.1716545
Pt161	0.2500000	0.5000000	0.0000000
Pt162	0.4375000	0.6250000	0.0000000
Pt163	0.3125000	0.6250000	0.0000000
Pt164	0.2500000	0.7500000	0.0000000
Pt165	0.3125000	0.8750000	0.0000000
Pt166	0.4375000	0.8750000	0.0000000
Pt167	0.3750000	0.5000000	0.0000000
Pt168	0.3750000	0.7500000	0.0000000
Pt169	0.4374349	0.9618894	0.0574419
Pt170	0.3122836	0.9619363	0.0575648
Pt171	0.2499412	0.5867259	0.0575346
Pt172	0.2499698	0.8368402	0.0574529
Pt173	0.3749319	0.5868715	0.0574983
Pt174	0.3124341	0.7118565	0.0575172
Pt175	0.4374038	0.7118879	0.0575091
Pt176	0.3748568	0.8369093	0.0575076
Pt177	0.4373902	0.7989487	0.1141324
Pt178	0.3124300	0.7989706	0.1141965
Pt179	0.2499897	0.9238803	0.1142206
Pt180	0.2499877	0.6738355	0.1141798
Pt181	0.3125282	0.5488902	0.1141513
Pt182	0.4375499	0.5489583	0.1140926
Pt183	0.3749459	0.6739516	0.1141150
Pt184	0.3749483	0.9239684	0.1141247
Pt185	0.2499995	0.5105797	0.1716276
Pt186	0.4374610	0.6355107	0.1716394
Pt187	0.3126457	0.6355604	0.1716409
Pt188	0.2500293	0.7606013	0.1716124

Pt189	0.3126733	0.8854922	0.1717305
Pt190	0.4374972	0.8855170	0.1716424
Pt191	0.3751616	0.5105442	0.1716212
Pt192	0.3750732	0.7604927	0.1716968
Pt193	0.5000000	0.5000000	0.0000000
Pt194	0.6875000	0.6250000	0.0000000
Pt195	0.5625000	0.6250000	0.0000000
Pt196	0.5000000	0.7500000	0.0000000
Pt197	0.5625000	0.8750000	0.0000000
Pt198	0.6875000	0.8750000	0.0000000
Pt199	0.6250000	0.5000000	0.0000000
Pt200	0.6250000	0.7500000	0.0000000
Pt201	0.6875607	0.9618745	0.0574576
Pt202	0.5624955	0.9618969	0.0575118
Pt203	0.5000118	0.5868606	0.0574714
Pt204	0.4999573	0.8368235	0.0575016
Pt205	0.6249883	0.5868550	0.0574767
Pt206	0.5625018	0.7118411	0.0574475
Pt207	0.6875987	0.7118928	0.0575137
Pt208	0.6250384	0.8368240	0.0575053
Pt209	0.6875600	0.7989627	0.1141494
Pt210	0.5624680	0.7988755	0.1141071
Pt211	0.4999146	0.9238892	0.1140862
Pt212	0.4999440	0.6739237	0.1140932
Pt213	0.5624918	0.5488453	0.1140752
Pt214	0.6874417	0.5489469	0.1141060
Pt215	0.6250321	0.6739302	0.1140961
Pt216	0.6250251	0.9238700	0.1141022
Pt217	0.5000406	0.5104910	0.1715982
Pt218	0.6873949	0.6355041	0.1716366
Pt219	0.5624257	0.6355727	0.1715773
Pt220	0.4999794	0.7605741	0.1716109
Pt221	0.5623921	0.8856671	0.1716323
Pt222	0.6872752	0.8854826	0.1716657
Pt223	0.6248314	0.5104648	0.1715992
Pt224	0.6248195	0.7605616	0.1716024
Pt225	0.7500000	0.5000000	0.0000000
Pt226	0.9375000	0.6250000	0.0000000
Pt227	0.8125000	0.6250000	0.0000000
Pt228	0.7500000	0.7500000	0.0000000
Pt229	0.8125000	0.8750000	0.0000000
Pt230	0.9375000	0.8750000	0.0000000

Pt231	0.8750000	0.5000000	0.0000000
Pt232	0.8750000	0.7500000	0.0000000
Pt233	0.9376502	0.9620127	0.0575612
Pt234	0.8127043	0.9619252	0.0575716
Pt235	0.7500678	0.5868808	0.0575017
Pt236	0.7501273	0.8369139	0.0575158
Pt237	0.8750566	0.5867243	0.0575347
Pt238	0.8125612	0.7118451	0.0575171
Pt239	0.9375444	0.7117475	0.0575181
Pt240	0.8750188	0.8368228	0.0574531
Pt241	0.9375417	0.7988270	0.1140522
Pt242	0.8125333	0.7989671	0.1141978
Pt243	0.7500118	0.9239548	0.1141514
Pt244	0.7500256	0.6739540	0.1141282
Pt245	0.8124455	0.5488977	0.1141474
Pt246	0.9374978	0.5487837	0.1142083
Pt247	0.8750045	0.6738369	0.1141763
Pt248	0.8749942	0.9238760	0.1142206
Pt249	0.7497405	0.5105086	0.1716295
Pt250	0.9373946	0.6355973	0.1716594
Pt251	0.8122507	0.6355556	0.1716433
Pt252	0.7497851	0.7604822	0.1716914
Pt253	0.8121318	0.8854788	0.1717454
Pt254	0.9371256	0.8851898	0.1716688
Pt255	0.8748719	0.5105400	0.1716187
Pt256	0.8748021	0.7605769	0.1716272