Elucidation of the mechanism of melamine adsorption on Pt(111) surface via density functional theory calculations

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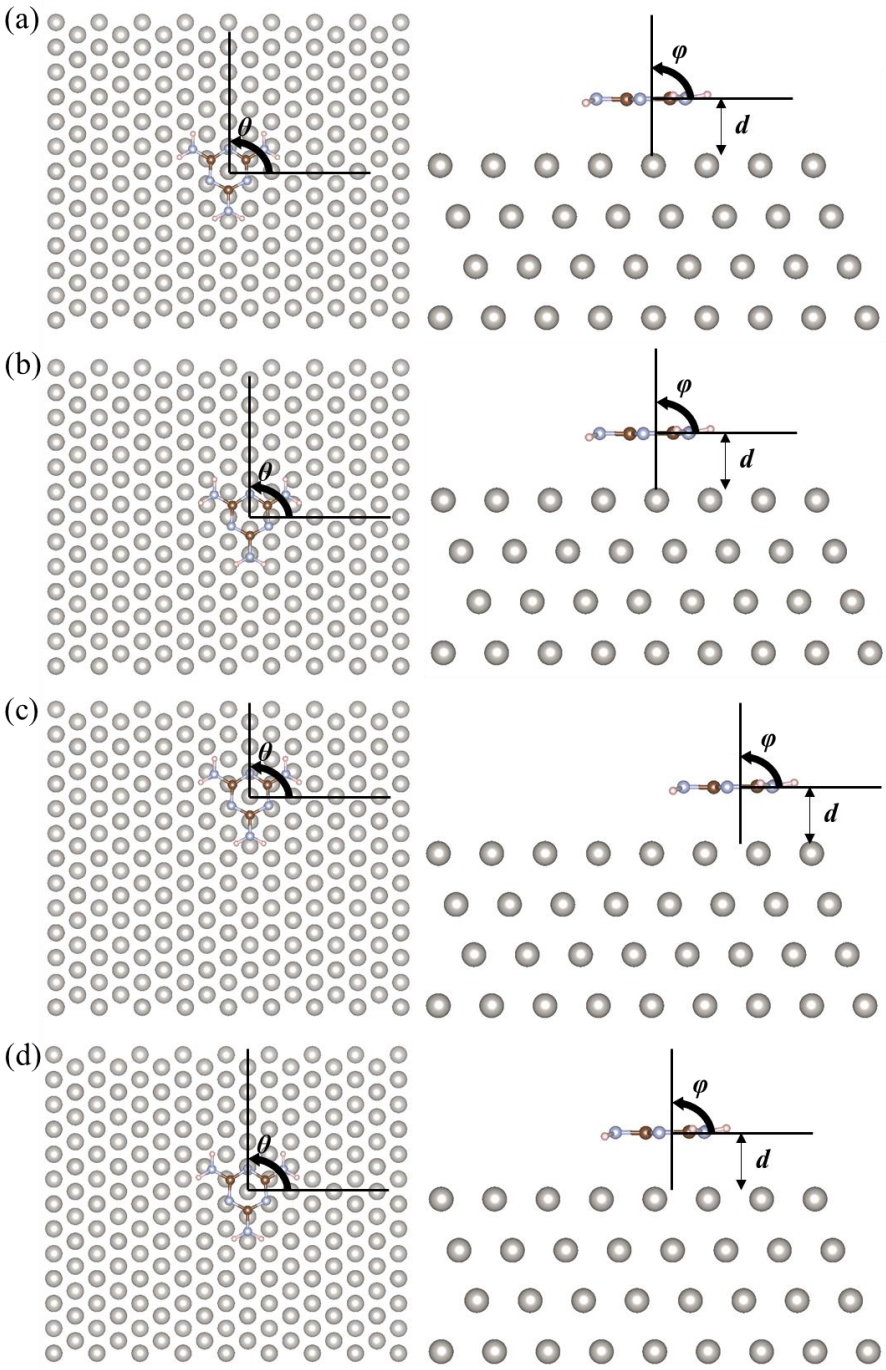

Figure S1. Top (left) and side (right) views of the models for estimating the potential energy map of melamine adsorption on Pt(111) surface: (a) group 1, (b) group 2, (c) group 3, and (d) group 4. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

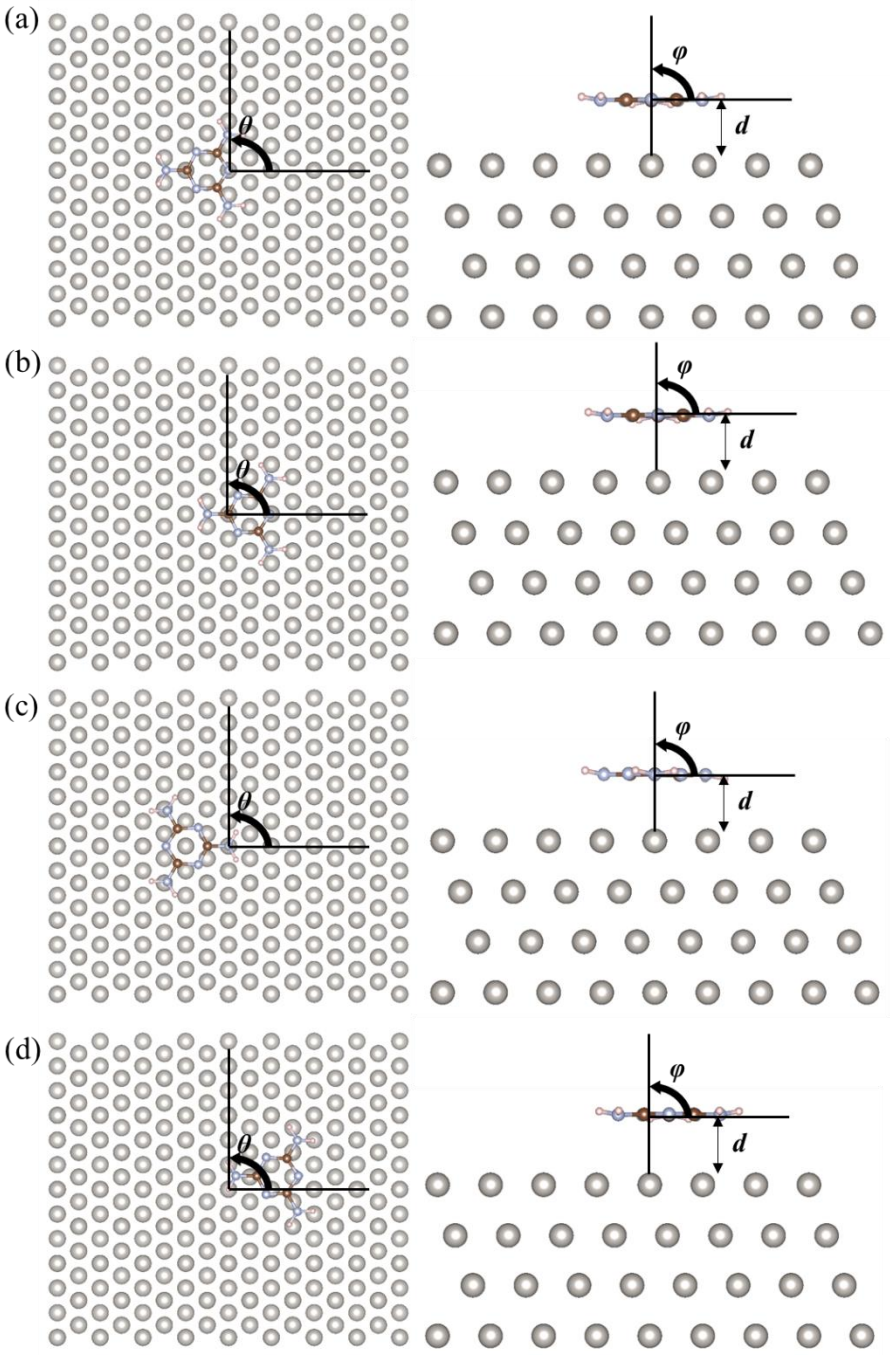

Figure S2. Top (left) and side (right) views of the models for estimating the potential energy map of melamine adsorption on Pt(111) surface: (a) group 5, (b) group 6, (c) group 7, and (d) group 8. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

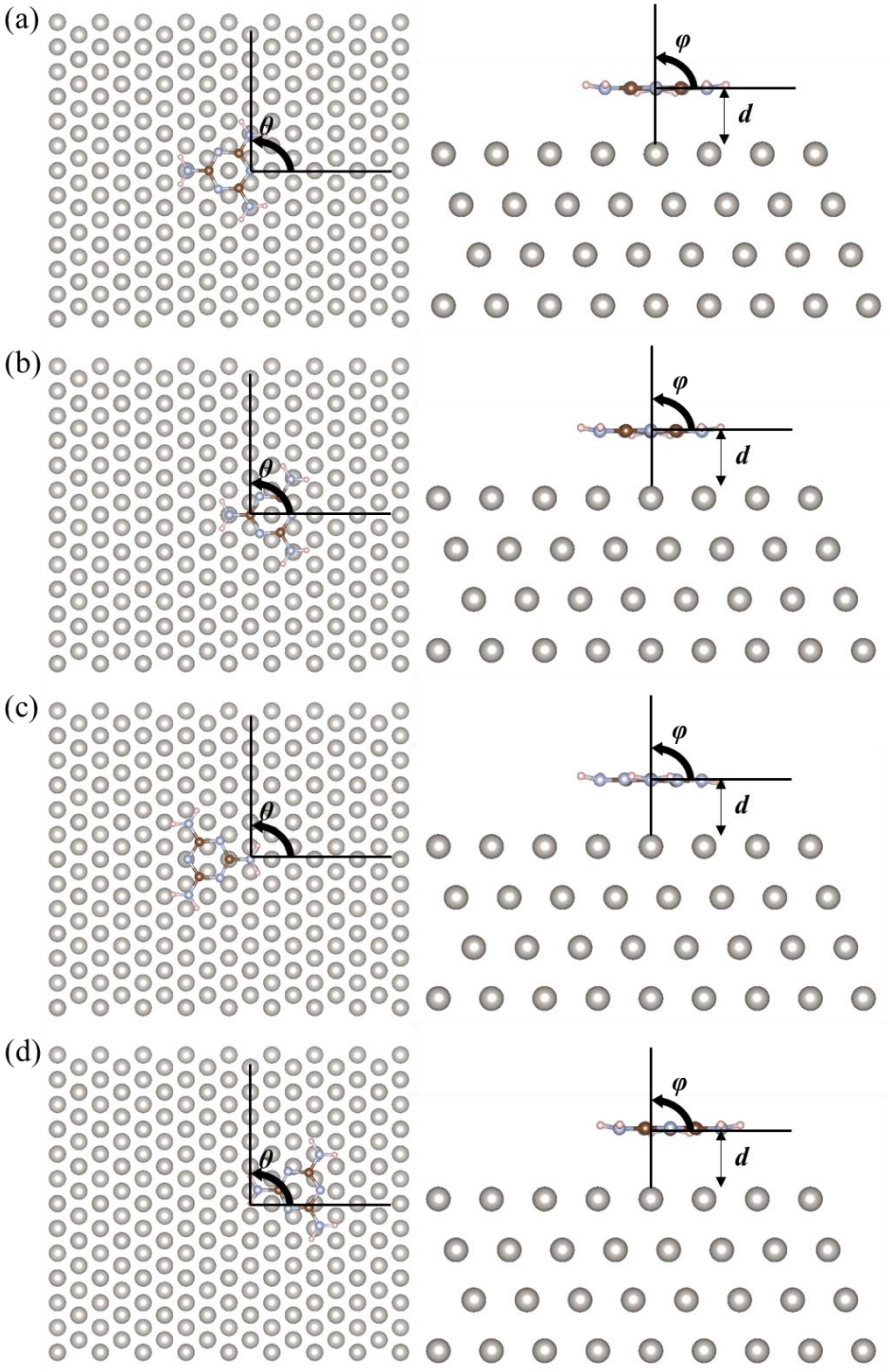

Figure S3. Top (left) and side (right) views of the models for estimating the potential energy map of melamine adsorption on Pt(111) surface: (a) group 9, (b) group 10, (c) group 11, and (d) group 12. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

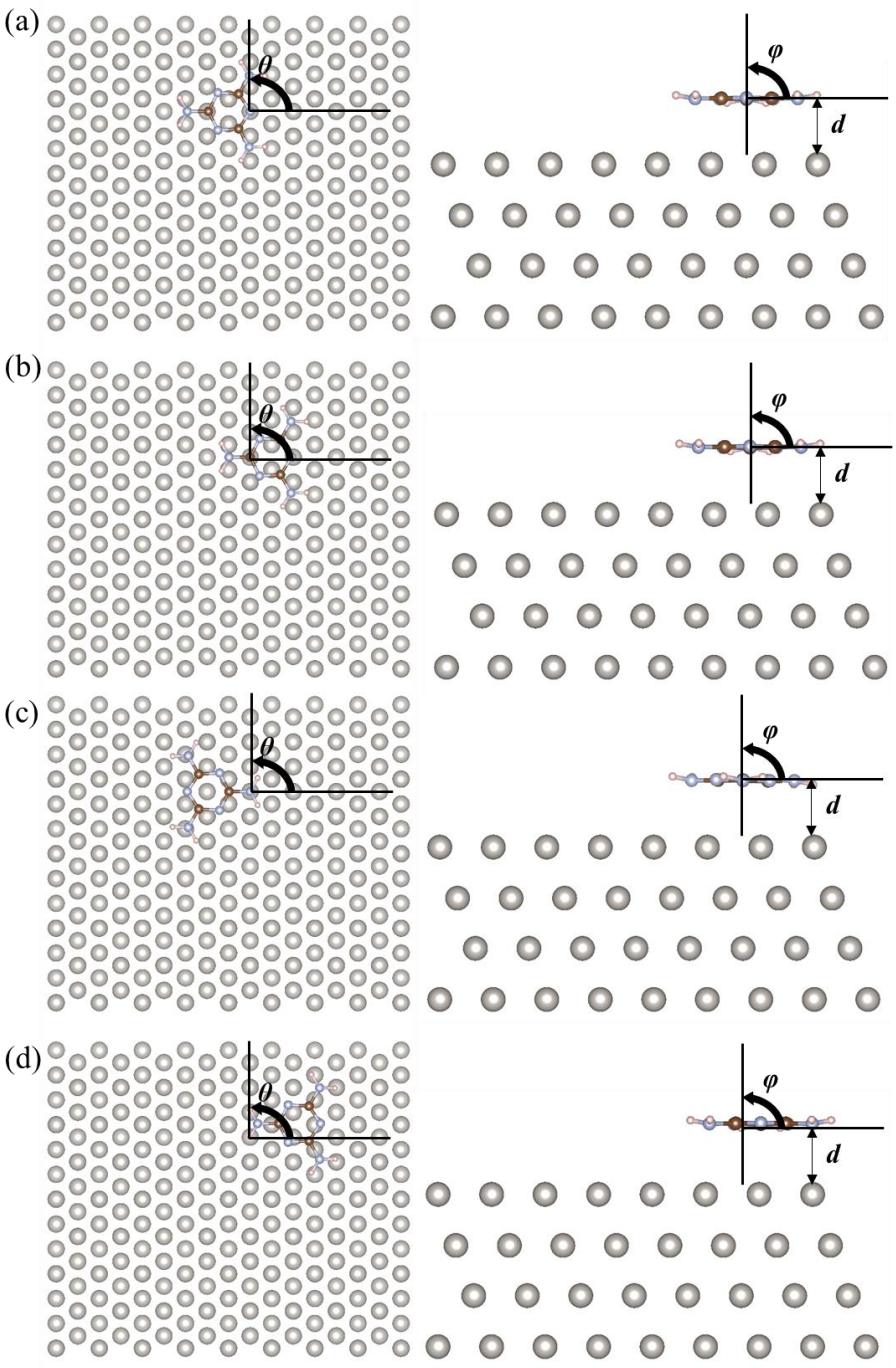

Figure S4. Top (left) and side (right) views of the models for estimating the potential energy map of melamine adsorption on Pt(111) surface: (a) group 13, (b) group 14, (c) group 15, and (d) group 16. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

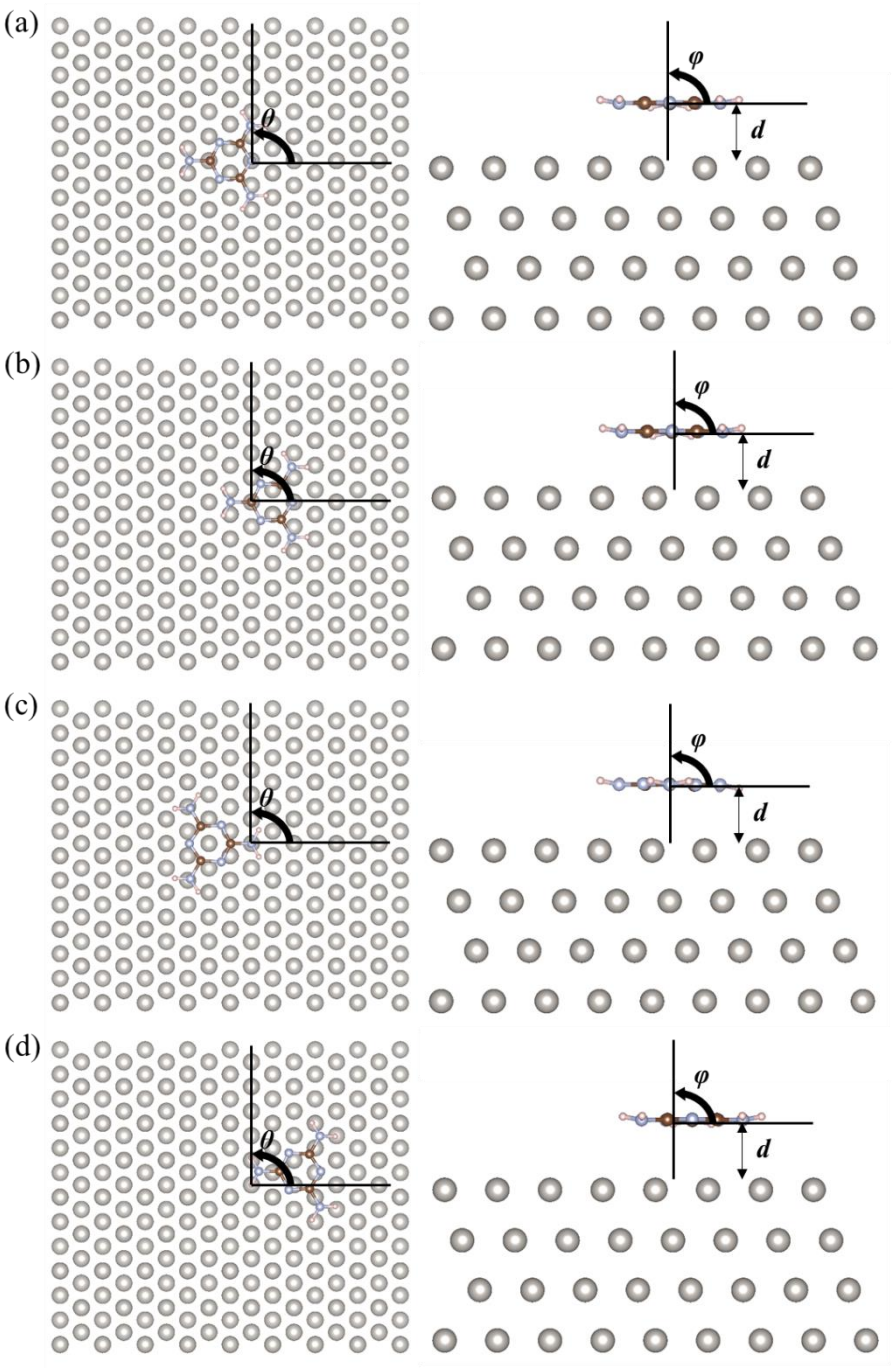

Figure S5. Top (left) and side (right) views of the models for estimating the potential energy map of melamine adsorption on Pt(111) surface: (a) group 17, (b) group 18, (c) group 19, and (d) 20. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

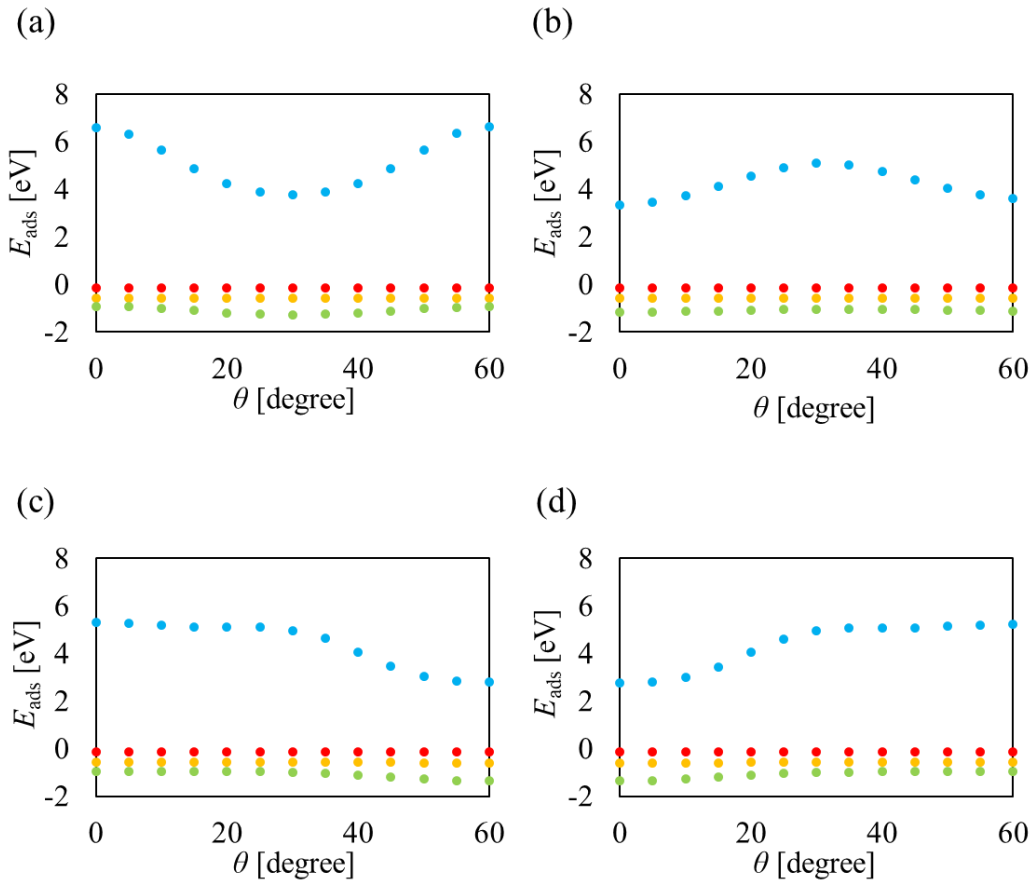

Figure S6. Calculated potential energy mapping of melamine adsorption on Pt(111) surface: (a) group 1, (b) group 2, (c) group 3, and (d) group 4. The red, yellow, green, and blue dots represent the results for d = 5.0, 4.0, 3.0, and 2.0 Å, respectively. E_{ads}, d, and θ are the adsorption energy, distance between melamine and Pt, and molecular rotation angle, respectively.

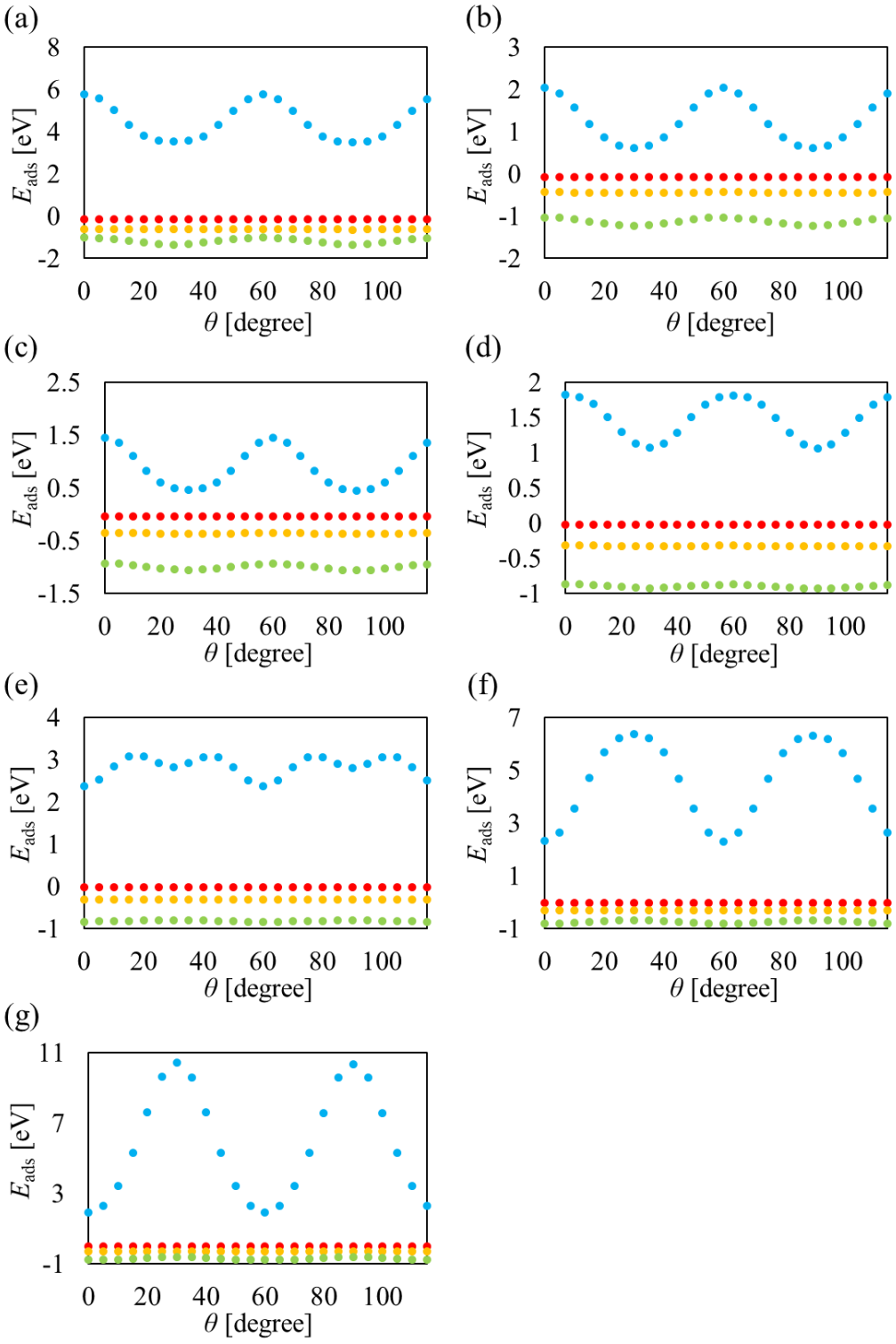

Figure S7. Calculated potential energy mapping of melamine adsorption on Pt(111) surface: group 5. (a) φ = 0, (b) φ = 15, (c) φ = 30, (d) φ = 45, (e) φ = 60, (f) φ = 75, and (g) φ = 90 degrees. The red, yellow, green, and blue dots represent the results for d = 5.0, 4.0, 3.0, and 2.0 Å, respectively. E_{ads}, d, θ, and φ are the adsorption energy, distance between melamine and Pt, molecular rotation angle, and the upright angle of the molecule from the surface, respectively.

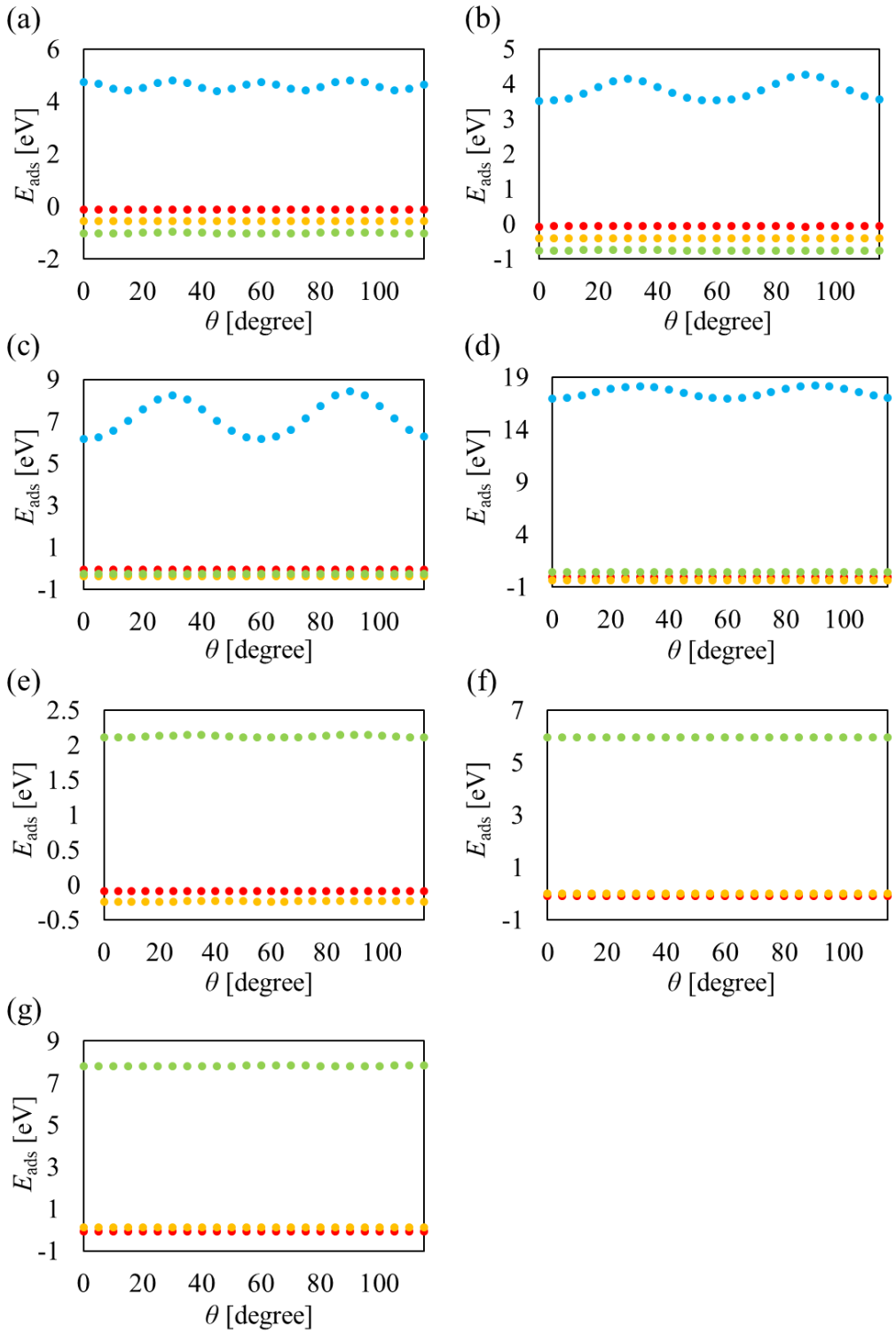

Figure S8. Calculated potential energy mapping of melamine adsorption on Pt(111) surface: group 6. (a) φ = 0, (b) φ = 15, (c) φ = 30, (d) φ = 45, (e) φ = 60, (f) φ = 75, and (g) φ = 90 degrees. The red, yellow, green, and blue dots represent the results for d = 5.0, 4.0, 3.0, and 2.0 Å, respectively. E_{ads}, d, θ, and φ are the adsorption energy, distance between melamine and Pt, molecular rotation angle, and the upright angle of the molecule from the surface, respectively.

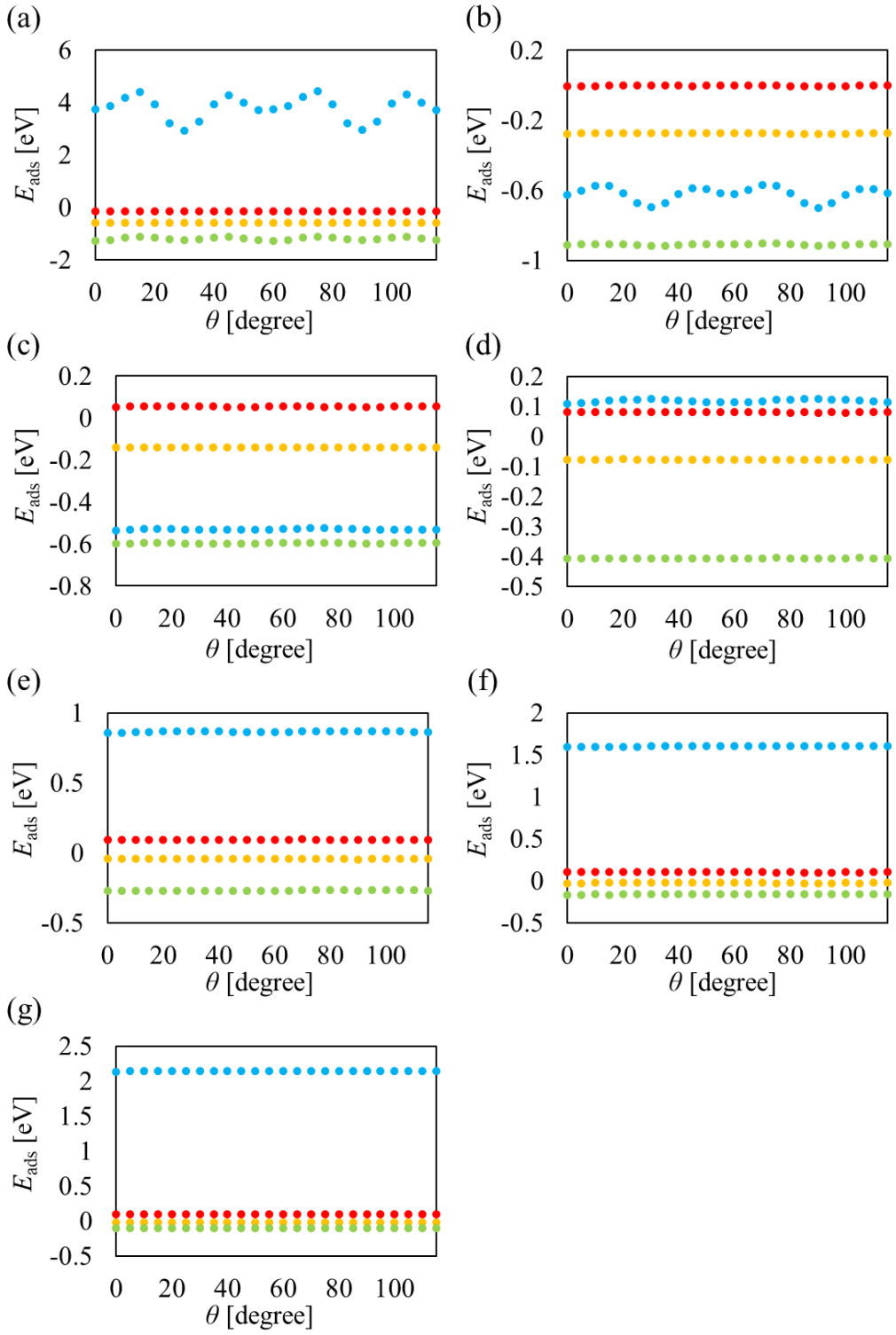

Figure S9. Calculated potential energy mapping of melamine adsorption on Pt(111) surface: group 7. (a) φ = 0, (b) φ = 15, (c) φ = 30, (d) φ = 45, (e) φ = 60, (f) φ = 75, and (g) φ = 90 degrees. The red, yellow, green, and blue dots represent the results for d = 5.0, 4.0, 3.0, and 2.0 Å, respectively. E_{ads}, d, θ, and φ are the adsorption energy, distance between melamine and Pt, molecular rotation angle, and the upright angle of the molecule from the surface, respectively.

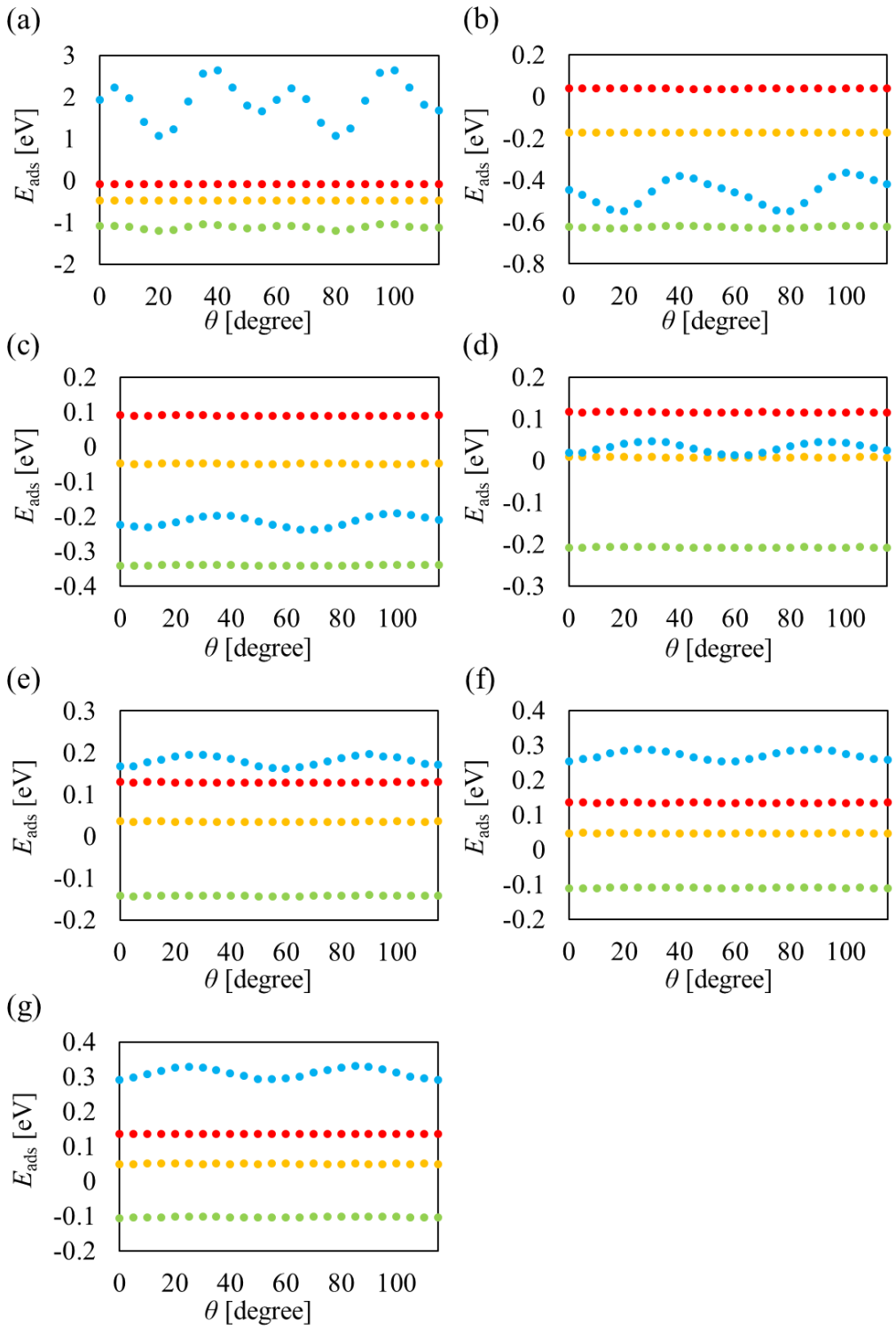

Figure S10. Calculated potential energy mapping of melamine adsorption on Pt(111) surface: group 8. (a) φ = 0, (b) φ = 15, (c) φ = 30, (d) φ = 45, (e) φ = 60, (f) φ = 75, and (g) φ = 90 degrees. The red, yellow, green, and blue dots represent the results for d = 5.0, 4.0, 3.0, and 2.0 Å, respectively. E_{ads}, d, θ, and φ are the adsorption energy, distance between melamine and Pt, molecular rotation angle, and the upright angle of the molecule from the surface, respectively.

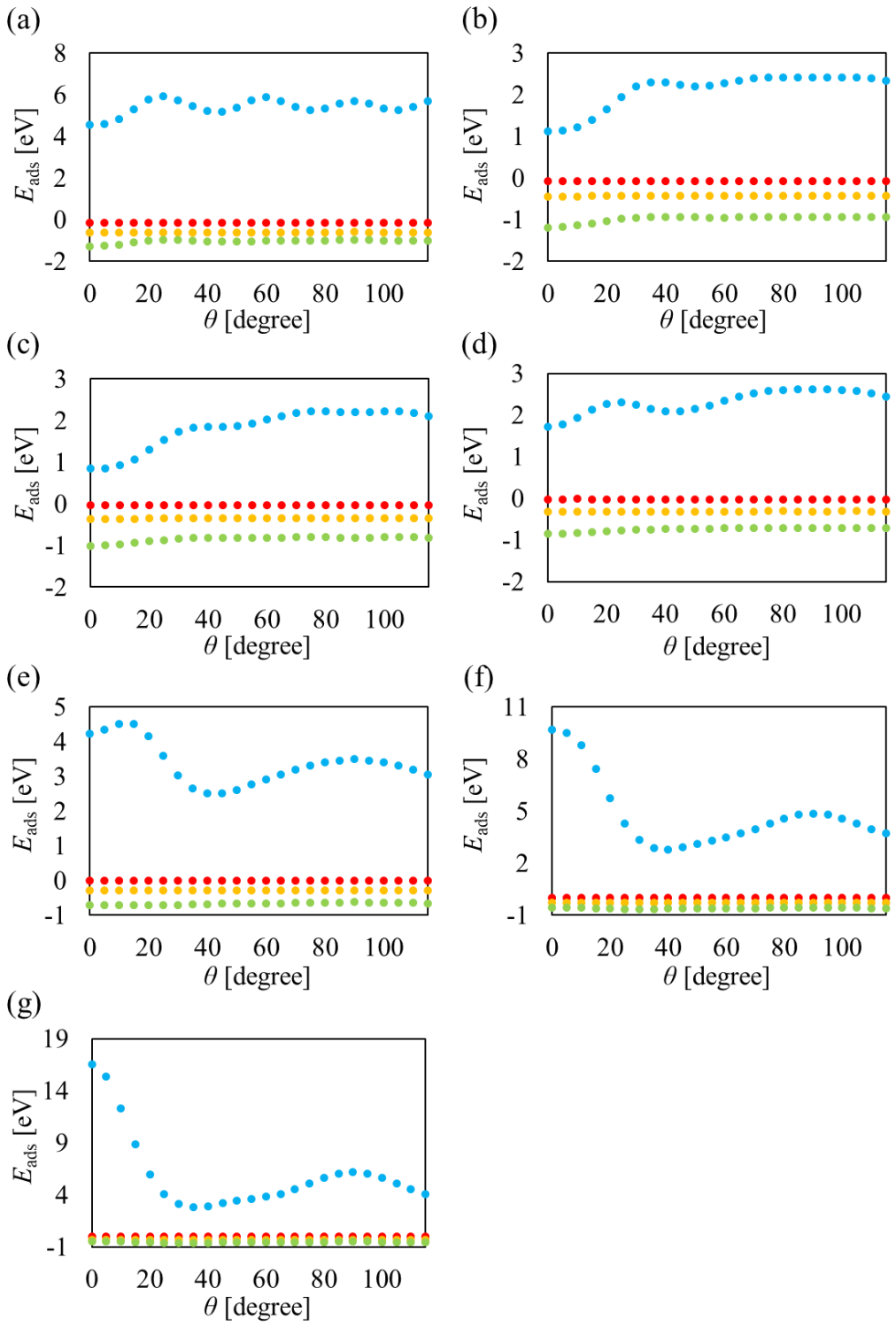

Figure S11. Calculated potential energy mapping of melamine adsorption on Pt(111) surface: group 9. (a) φ = 0, (b) φ = 15, (c) φ = 30, (d) φ = 45, (e) φ = 60, (f) φ = 75, and (g) φ = 90 degrees. The red, yellow, green, and blue dots represent the results for d = 5.0, 4.0, 3.0, and 2.0 Å, respectively. E_{ads}, d, θ, and φ are the adsorption energy, distance between melamine and Pt, molecular rotation angle, and the upright angle of the molecule from the surface, respectively.

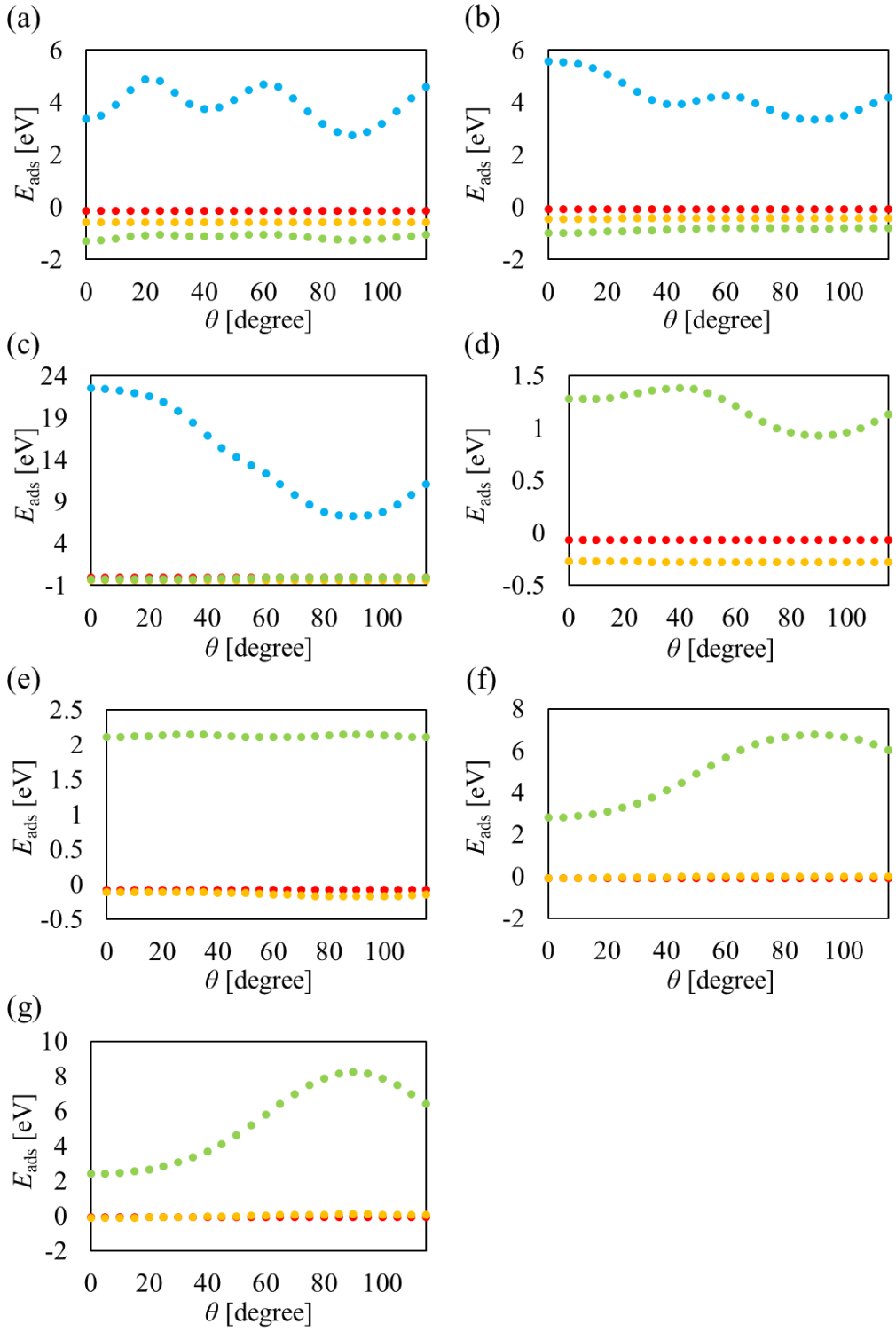

Figure S12. Calculated potential energy mapping of melamine adsorption on Pt(111) surface: group 10. (a) φ = 0, (b) φ = 15, (c) φ = 30, (d) φ = 45, (e) φ = 60, (f) φ = 75, and (g) φ = 90 degrees. The red, yellow, green, and blue dots represent the results for d = 5.0, 4.0, 3.0, and 2.0 Å, respectively. E_{ads}, d, θ, and φ are the adsorption energy, distance between melamine and Pt, molecular rotation angle, and the upright angle of the molecule from the surface, respectively.

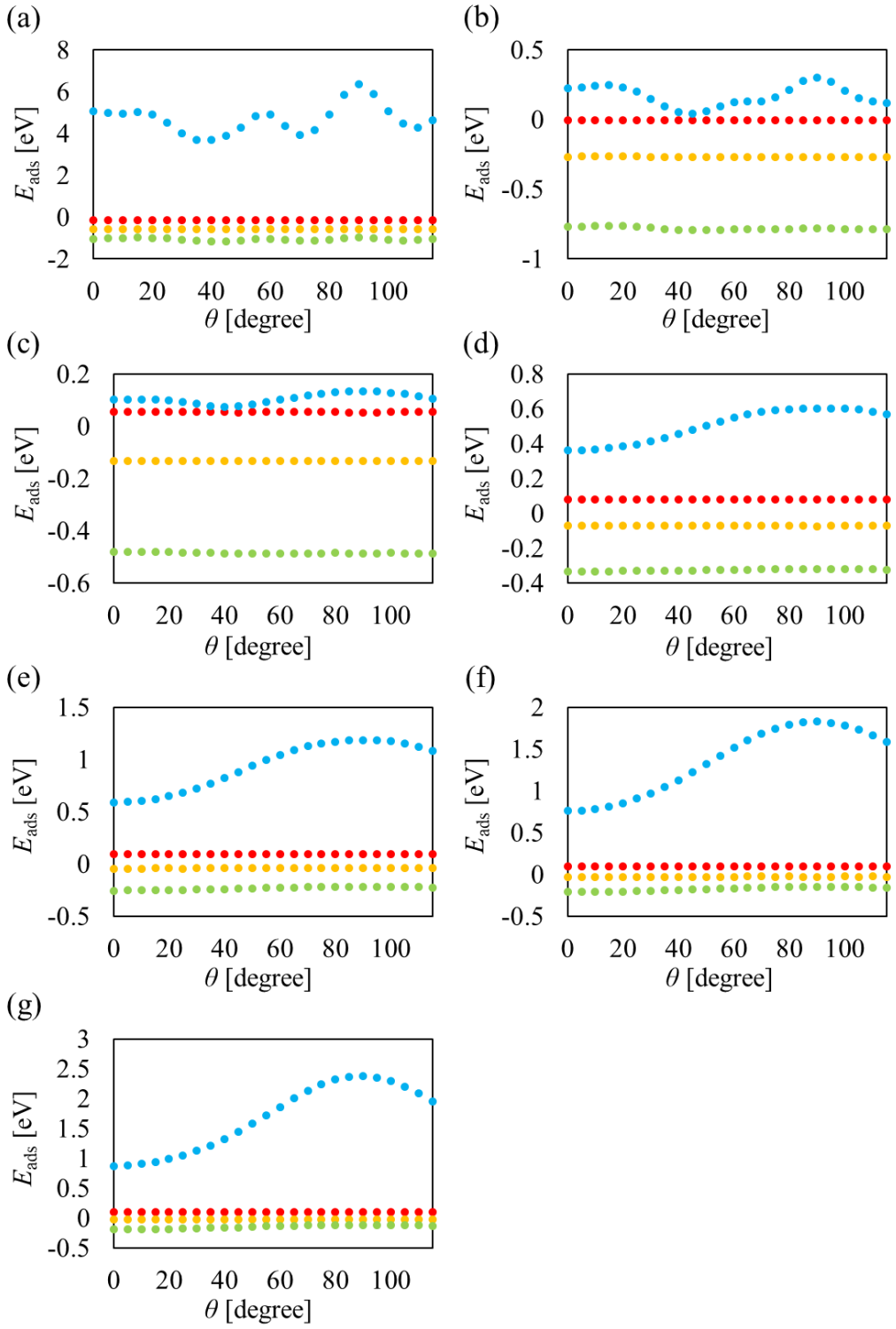

Figure S13. Calculated potential energy mapping of melamine adsorption on Pt(111) surface: group 11. (a) φ = 0, (b) φ = 15, (c) φ = 30, (d) φ = 45, (e) φ = 60, (f) φ = 75, and (g) φ = 90 degrees. The red, yellow, green, and blue dots represent the results for d = 5.0, 4.0, 3.0, and 2.0 Å, respectively. E_{ads}, d, θ, and φ are the adsorption energy, distance between melamine and Pt, molecular rotation angle, and the upright angle of the molecule from the surface, respectively.

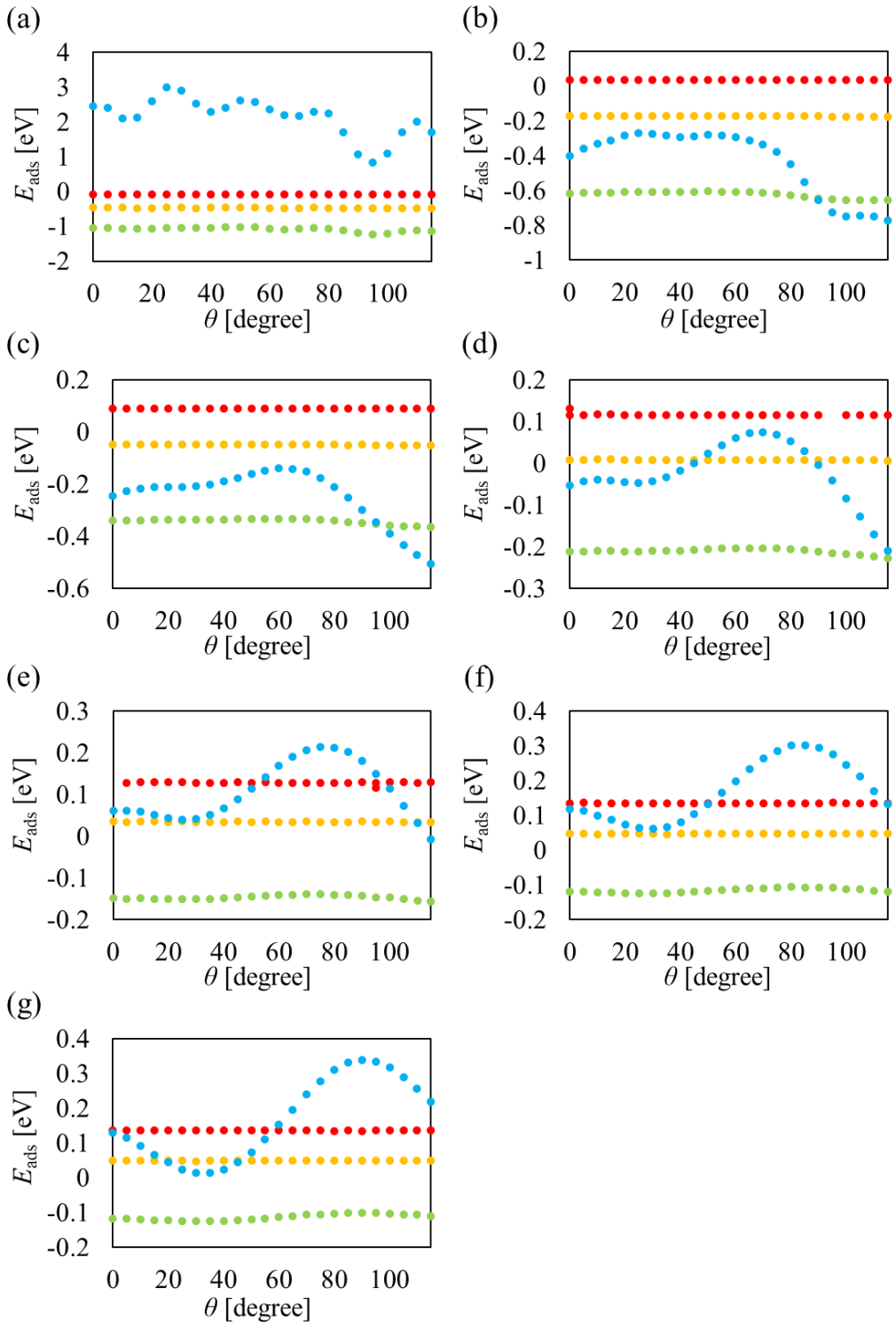

Figure S14. Calculated potential energy mapping of melamine adsorption on Pt(111) surface: group 12. (a) φ = 0, (b) φ = 15, (c) φ = 30, (d) φ = 45, (e) φ = 60, (f) φ = 75, and (g) φ = 90 degrees. The red, yellow, green, and blue dots represent the results for d = 5.0, 4.0, 3.0, and 2.0 Å, respectively. E_{ads}, d, θ, and φ are the adsorption energy, distance between melamine and Pt, molecular rotation angle, and the upright angle of the molecule from the surface, respectively.

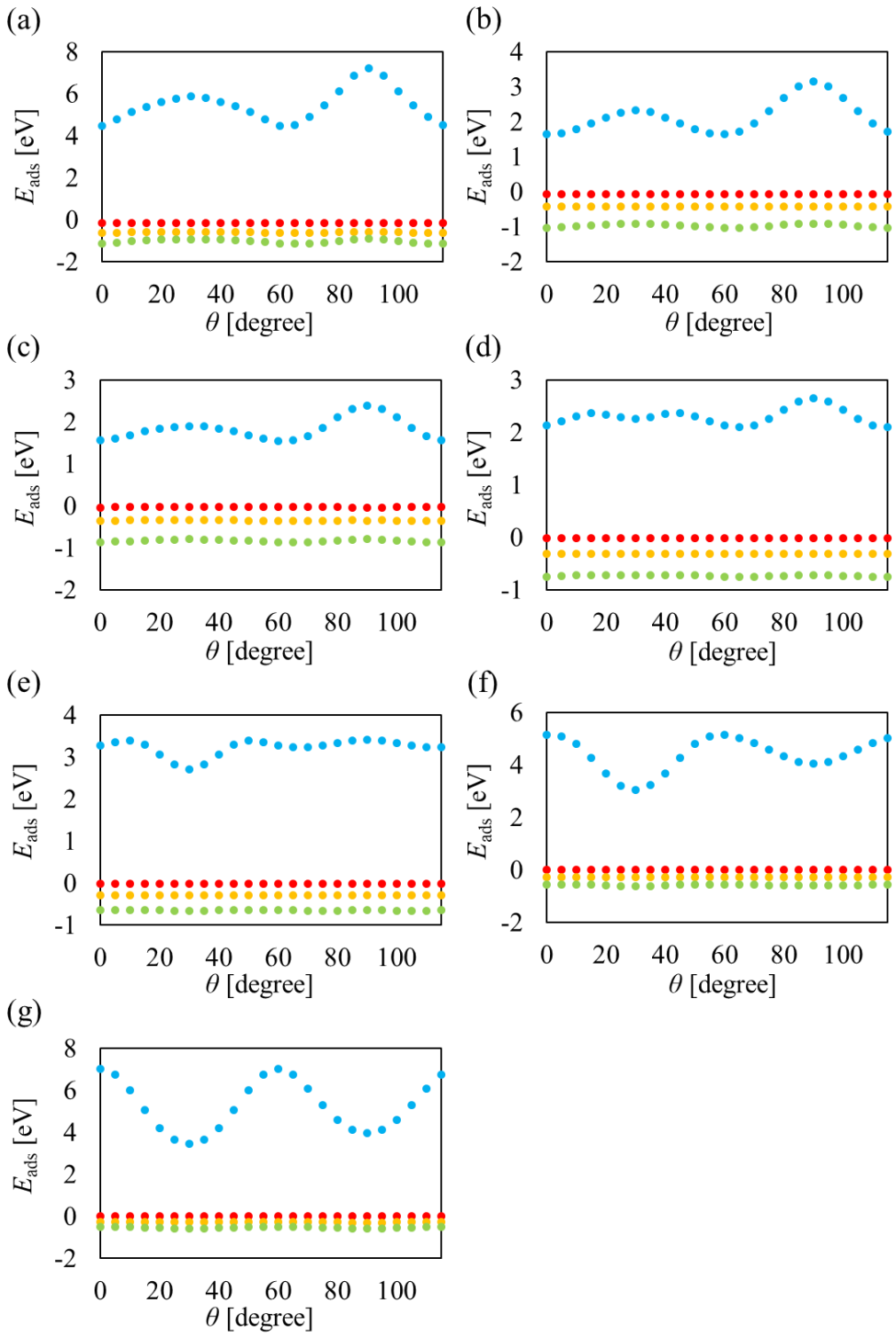

Figure S15. Calculated potential energy mapping of melamine adsorption on Pt(111) surface: group 13. (a) φ = 0, (b) φ = 15, (c) φ = 30, (d) φ = 45, (e) φ = 60, (f) φ = 75, and (g) φ = 90 degrees. The red, yellow, green, and blue dots represent the results for d = 5.0, 4.0, 3.0, and 2.0 Å, respectively. E_{ads}, d, θ, and φ are the adsorption energy, distance between melamine and Pt, molecular rotation angle, and the upright angle of the molecule from the surface, respectively.

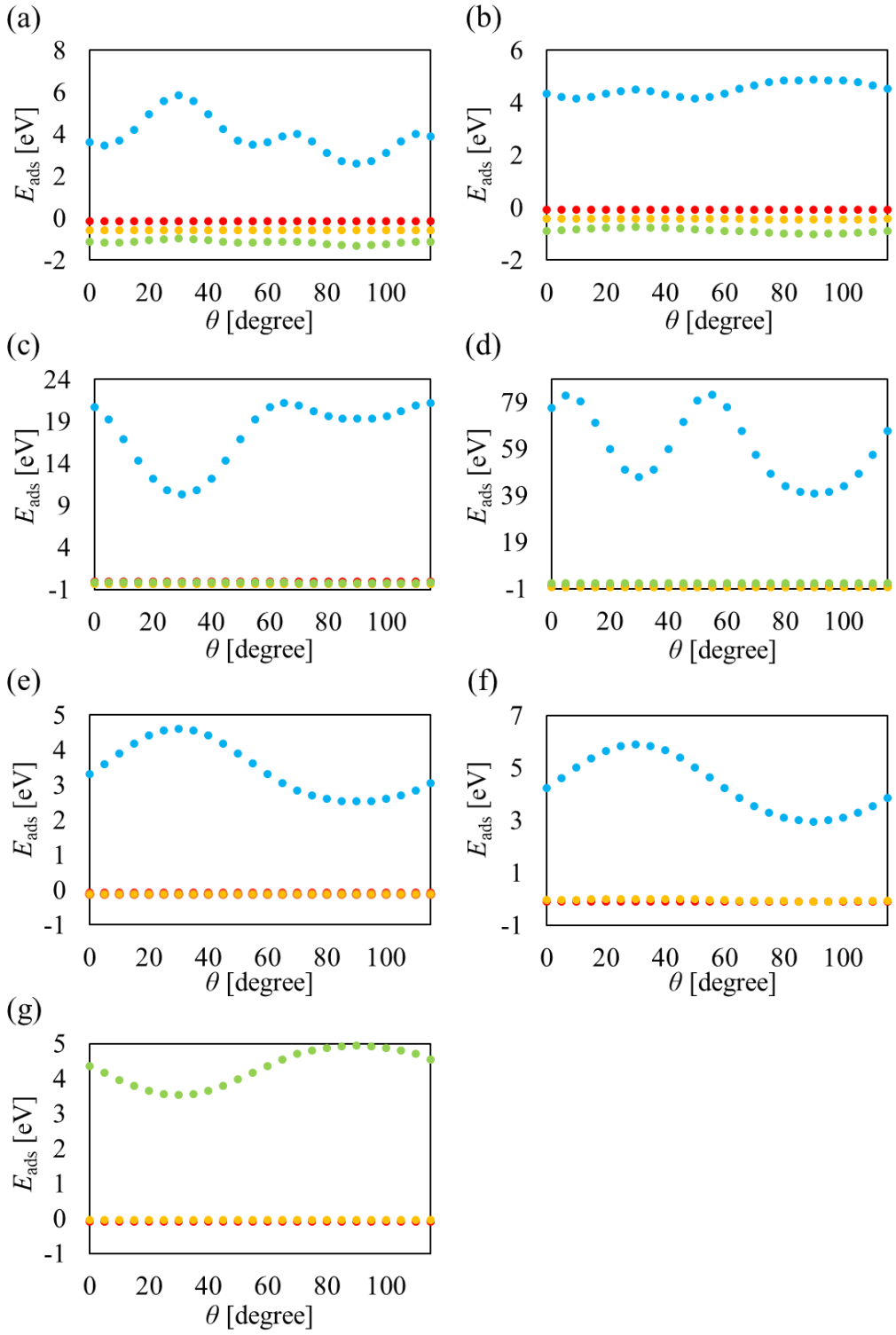

Figure S16. Calculated potential energy mapping of melamine adsorption on Pt(111) surface: group 14. (a) φ = 0, (b) φ = 15, (c) φ = 30, (d) φ = 45, (e) φ = 60, (f) φ = 75, and (g) φ = 90 degrees. The red, yellow, green, and blue dots represent the results for d = 5.0, 4.0, 3.0, and 2.0 Å, respectively. E_{ads}, d, θ, and φ are the adsorption energy, distance between melamine and Pt, molecular rotation angle, and the upright angle of the molecule from the surface, respectively.

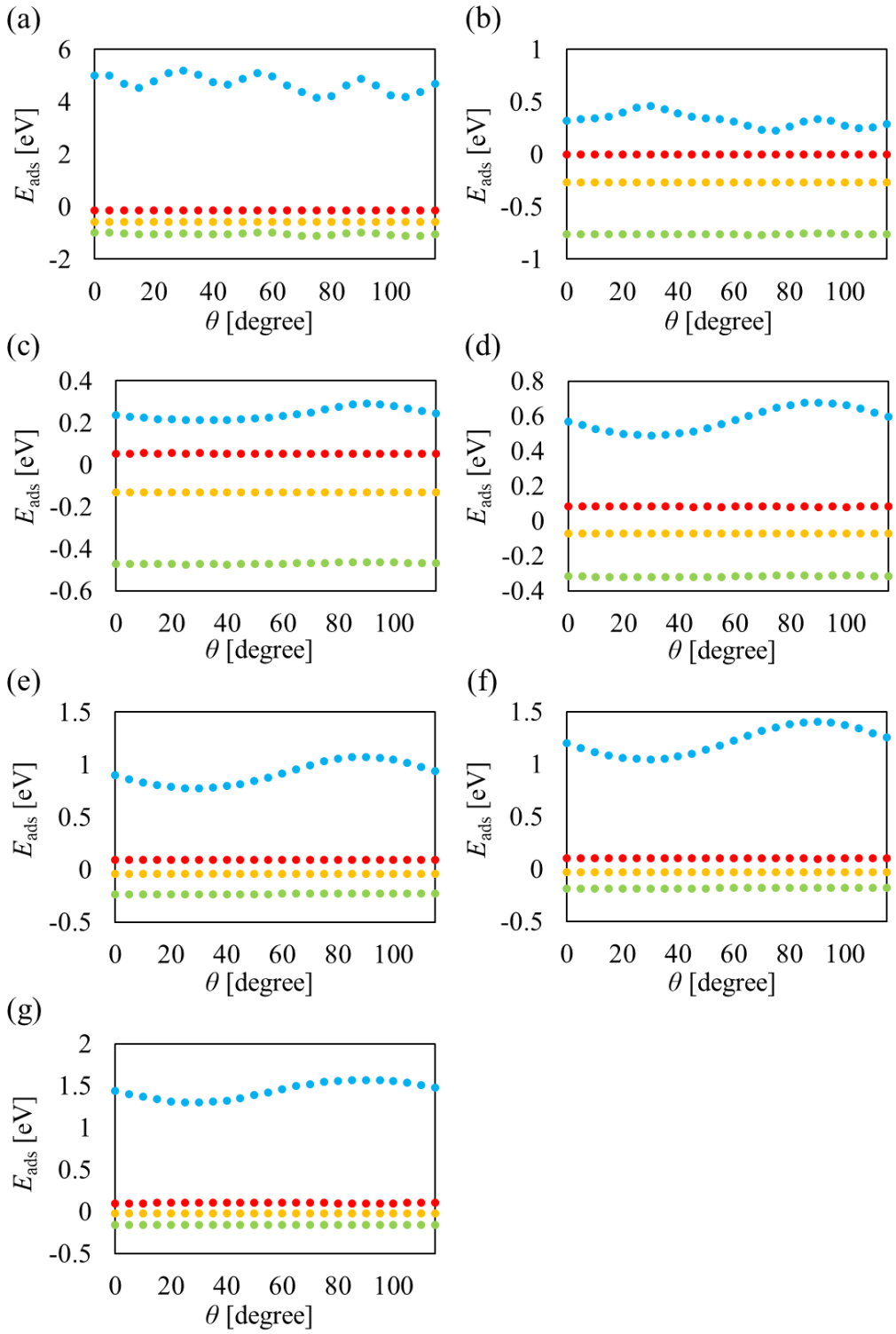

Figure S17. Calculated potential energy mapping of melamine adsorption on Pt(111) surface: group 15. (a) φ = 0, (b) φ = 15, (c) φ = 30, (d) φ = 45, (e) φ = 60, (f) φ = 75, and (g) φ = 90 degrees. The red, yellow, green, and blue dots represent the results for d = 5.0, 4.0, 3.0, and 2.0 Å, respectively. E_{ads}, d, θ, and φ are the adsorption energy, distance between melamine and Pt, molecular rotation angle, and the upright angle of the molecule from the surface, respectively.

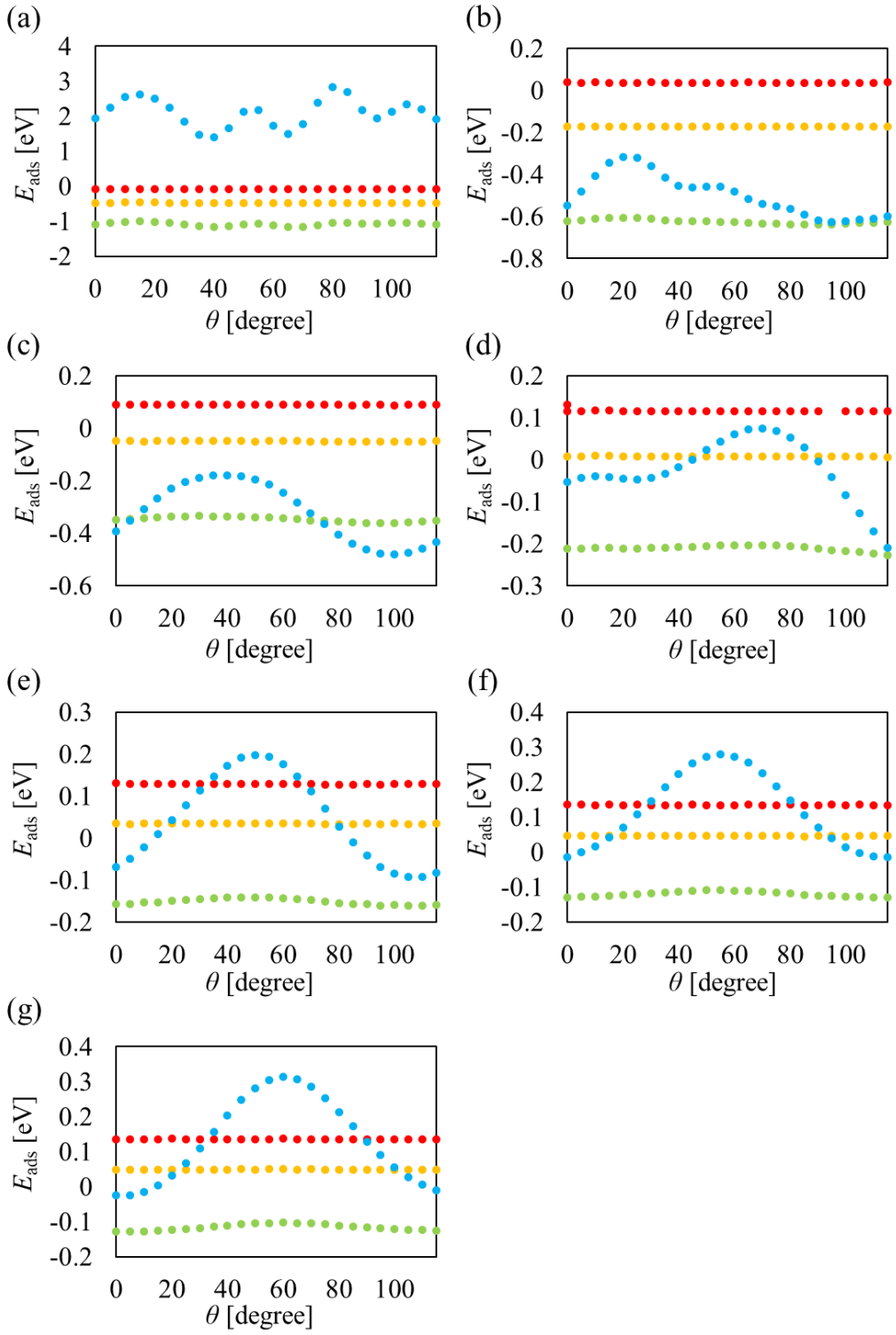

Figure S18. Calculated potential energy mapping of melamine adsorption on Pt(111) surface: group 16. (a) φ = 0, (b) φ = 15, (c) φ = 30, (d) φ = 45, (e) φ = 60, (f) φ = 75, and (g) φ = 90 degrees. The red, yellow, green, and blue dots represent the results for d = 5.0, 4.0, 3.0, and 2.0 Å, respectively. E_{ads}, d, θ, and φ are the adsorption energy, distance between melamine and Pt, molecular rotation angle, and the upright angle of the molecule from the surface, respectively.

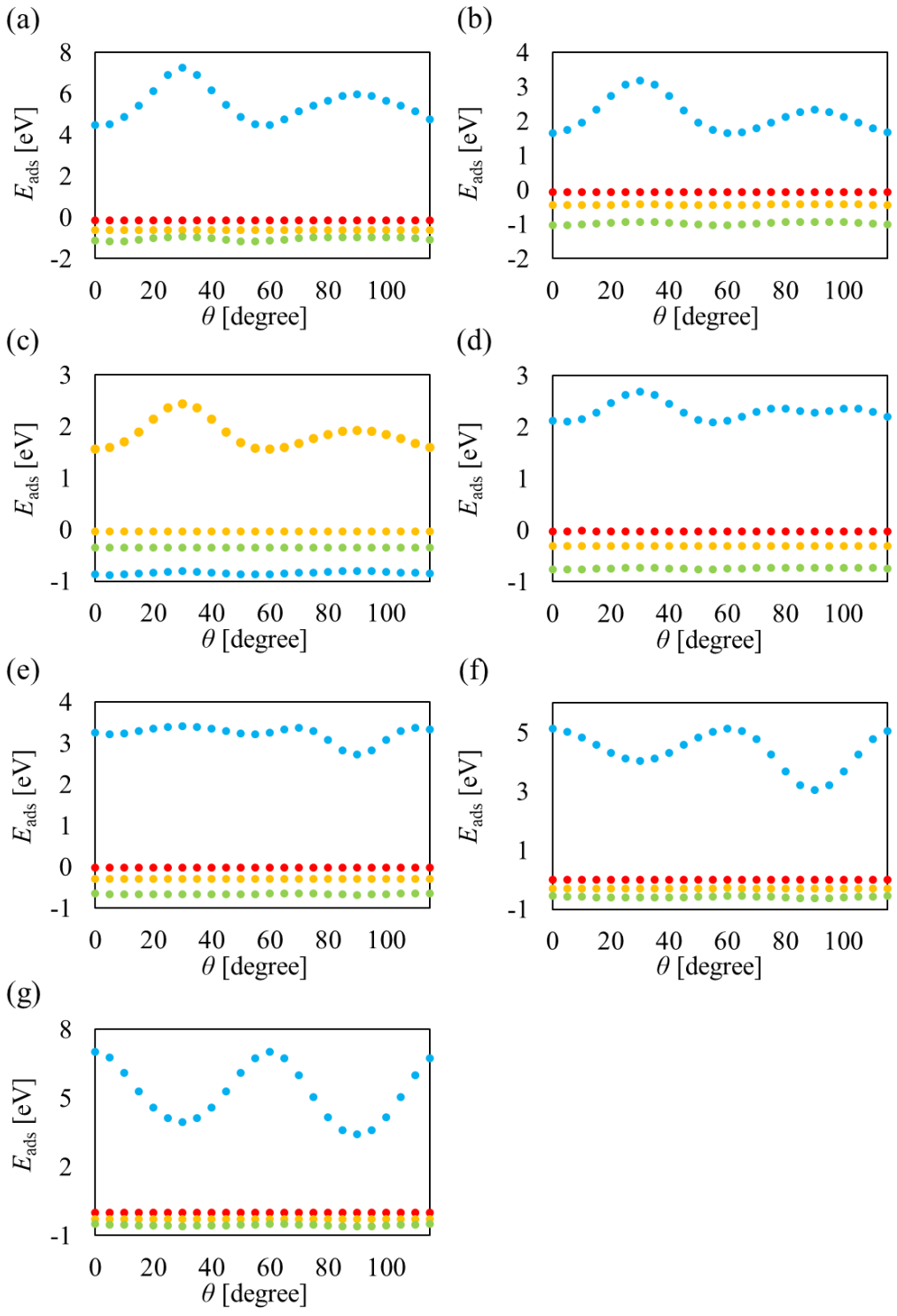

Figure S19. Calculated potential energy mapping of melamine adsorption on Pt(111) surface: group 17. (a) φ = 0, (b) φ = 15, (c) φ = 30, (d) φ = 45, (e) φ = 60, (f) φ = 75, and (g) φ = 90 degrees. The red, yellow, green, and blue dots represent the results for d = 5.0, 4.0, 3.0, and 2.0 Å, respectively. E_{ads}, d, θ, and φ are the adsorption energy, distance between melamine and Pt, molecular rotation angle, and the upright angle of the molecule from the surface, respectively.

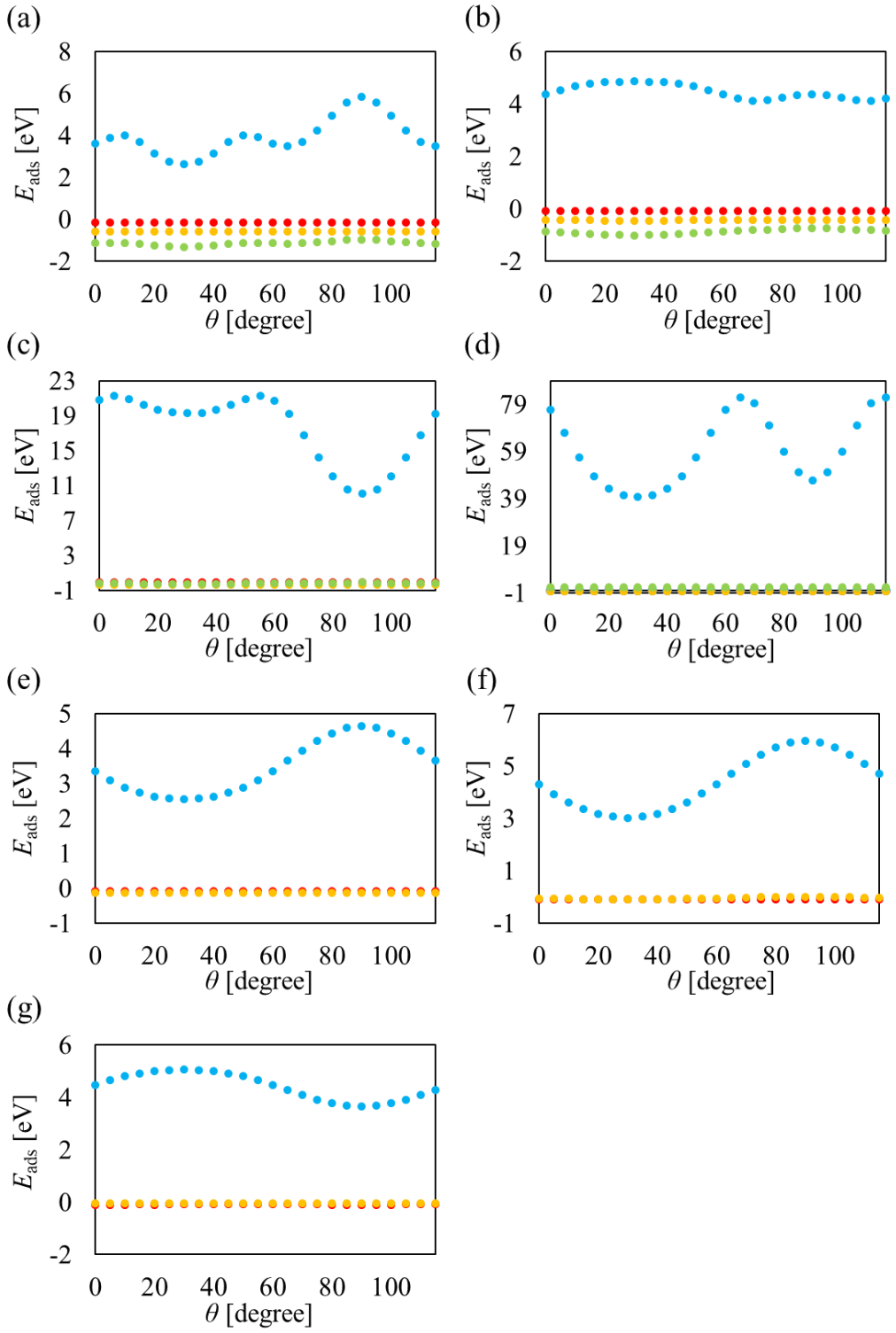

Figure S20. Calculated potential energy mapping of melamine adsorption on Pt(111) surface: group 18. (a) φ = 0, (b) φ = 15, (c) φ = 30, (d) φ = 45, (e) φ = 60, (f) φ = 75, and (g) φ = 90 degrees. The red, yellow, green, and blue dots represent the results for d = 5.0, 4.0, 3.0, and 2.0 Å, respectively. E_{ads}, d, θ, and φ are the adsorption energy, distance between melamine and Pt, molecular rotation angle, and the upright angle of the molecule from the surface, respectively.

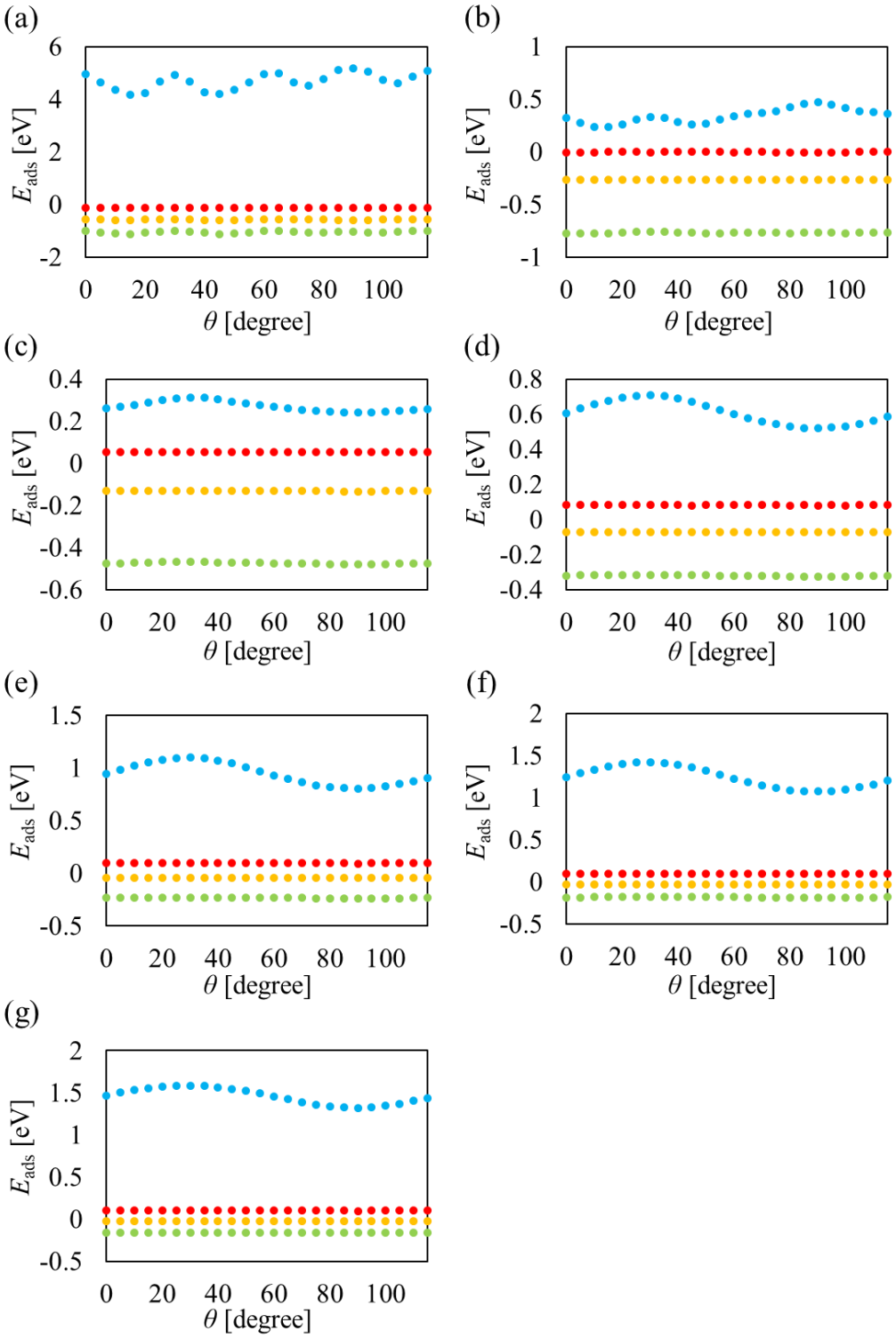

Figure S21. Calculated potential energy mapping of melamine adsorption on Pt(111) surface: group 19. (a) φ = 0, (b) φ = 15, (c) φ = 30, (d) φ = 45, (e) φ = 60, (f) φ = 75, and (g) φ = 90 degrees. The red, yellow, green, and blue dots represent the results for d = 5.0, 4.0, 3.0, and 2.0 Å, respectively. E_{ads}, d, θ, and φ are the adsorption energy, distance between melamine and Pt, molecular rotation angle, and the upright angle of the molecule from the surface, respectively.

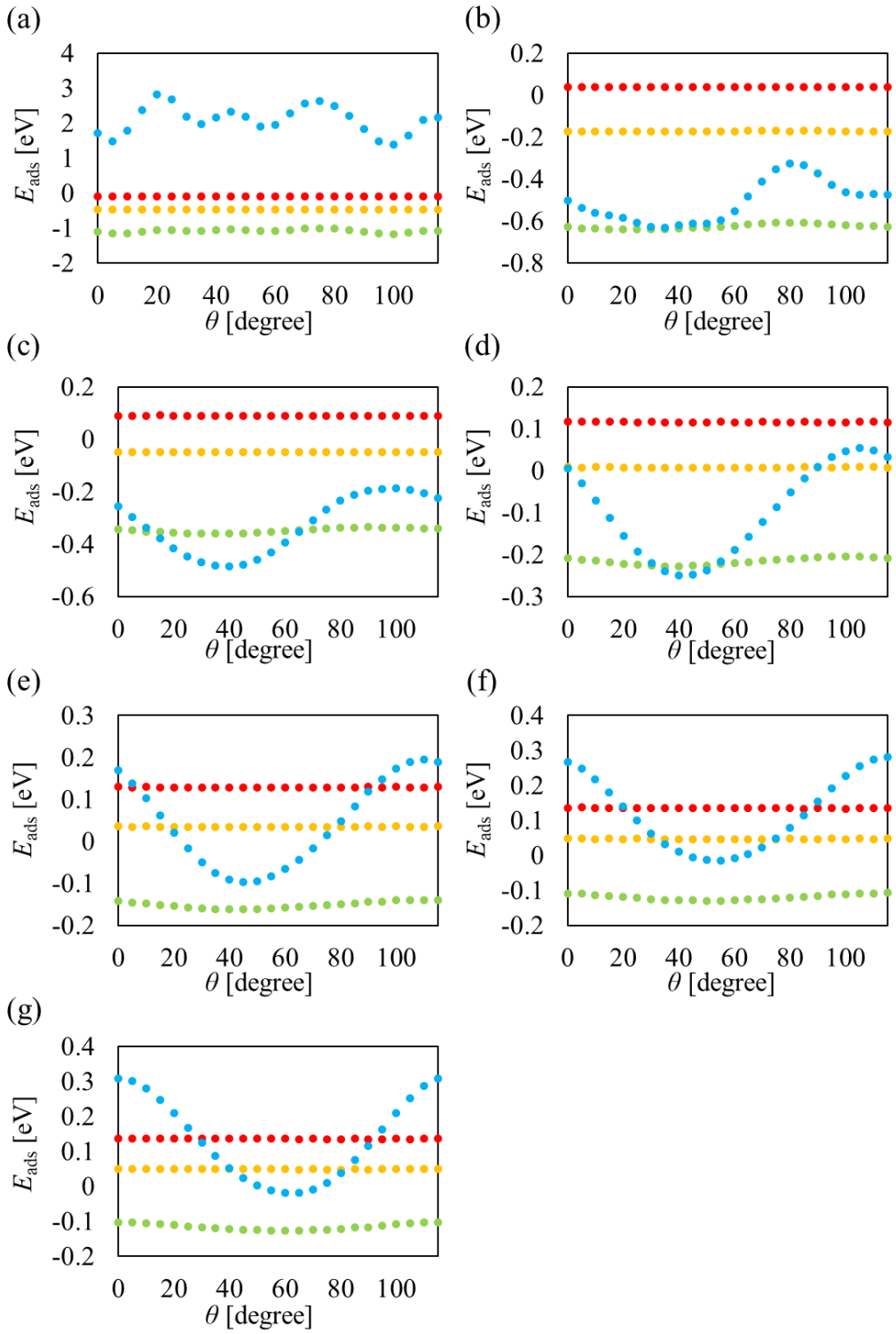

Figure S22. Calculated potential energy mapping of melamine adsorption on Pt(111) surface: group 20. (a) φ = 0, (b) φ = 15, (c) φ = 30, (d) φ = 45, (e) φ = 60, (f) φ = 75, and (g) φ = 90 degrees. The red, yellow, green, and blue dots represent the results for d = 5.0, 4.0, 3.0, and 2.0 Å, respectively. E_{ads}, d, θ, and φ are the adsorption energy, distance between melamine and Pt, molecular rotation angle, and the upright angle of the molecule from the surface, respectively.

Table S1. Initial structure information on the 63 entries

Entry	Map-group	d [Å]	θ [°]	φ [°]	Entry	Map-group	d [Å]	θ [°]	φ [°]
1	5	2.00	30.0	0.0	34	7	3.00	90.0	0.0
2	5	3.00	30.0	0.0	35	7	4.00	90.0	0.0
3	5	4.00	30.0	0.0	36	7	2.00	0.0	15.0
4	5	2.00	30.0	15.0	37	7	3.00	0.0	15.0
5	5	3.00	30.0	15.0	38	7	2.00	30.0	15.0
6	5	2.00	30.0	45.0	39	7	3.00	30.0	15.0
7	5	3.00	30.0	45.0	40	7	2.00	30.0	15.0
8	5	2.00	0.0	60.0	41	7	3.00	60.0	15.0
9	5	3.00	0.0	60.0	42	7	2.00	90.0	15.0
10	5	2.00	30.0	60.0	43	7	3.00	90.0	15.0
11	5	3.00	30.0	60.0	44	2	2.00	0.0	0.0
12	5	2.00	90.0	60.0	45	2	3.00	0.0	0.0
13	5	3.00	90.0	60.0	46	2	4.00	0.0	0.0
14	5	2.00	0.0	75.0	47	2	5.00	0.0	0.0
15	5	3.00	0.0	75.0	48	2	2.00	60.0	0.0
16	5	2.00	90.0	75.0	49	2	3.00	60.0	0.0
17	5	3.00	90.0	75.0	50	2	4.00	60.0	0.0
18	5	2.00	0.0	90.0	51	2	5.00	60.0	0.0
19	5	3.00	0.0	90.0	52	3	2.00	60.0	0.0
20	5	2.00	90.0	90.0	53	3	3.00	60.0	0.0
21	5	3.00	90.0	90.0	54	3	4.00	60.0	0.0
22	7	2.00	0.0	0.0	55	3	5.00	60.0	0.0
23	7	3.00	0.0	0.0	56	4	2.00	0.0	0.0
24	7	4.00	0.0	0.0	57	4	3.00	0.0	0.0
25	7	2.00	30.0	0.0	58	4	4.00	0.0	0.0
26	7	3.00	30.0	0.0	59	4	5.00	0.0	0.0
27	7	4.00	30.0	0.0	60	1	2.00	30.0	0.0
28	7	2.00	55.0	0.0	61	1	3.00	30.0	0.0
29	7	3.00	55.0	0.0	62	1	4.00	30.0	0.0
30	7	2.00	60.0	0.0	63	1	5.00	30.0	0.0
31	7	3.00	60.0	0.0					
32	7	4.00	60.0	0.0					
33	7	2.00	90.0	0.0					

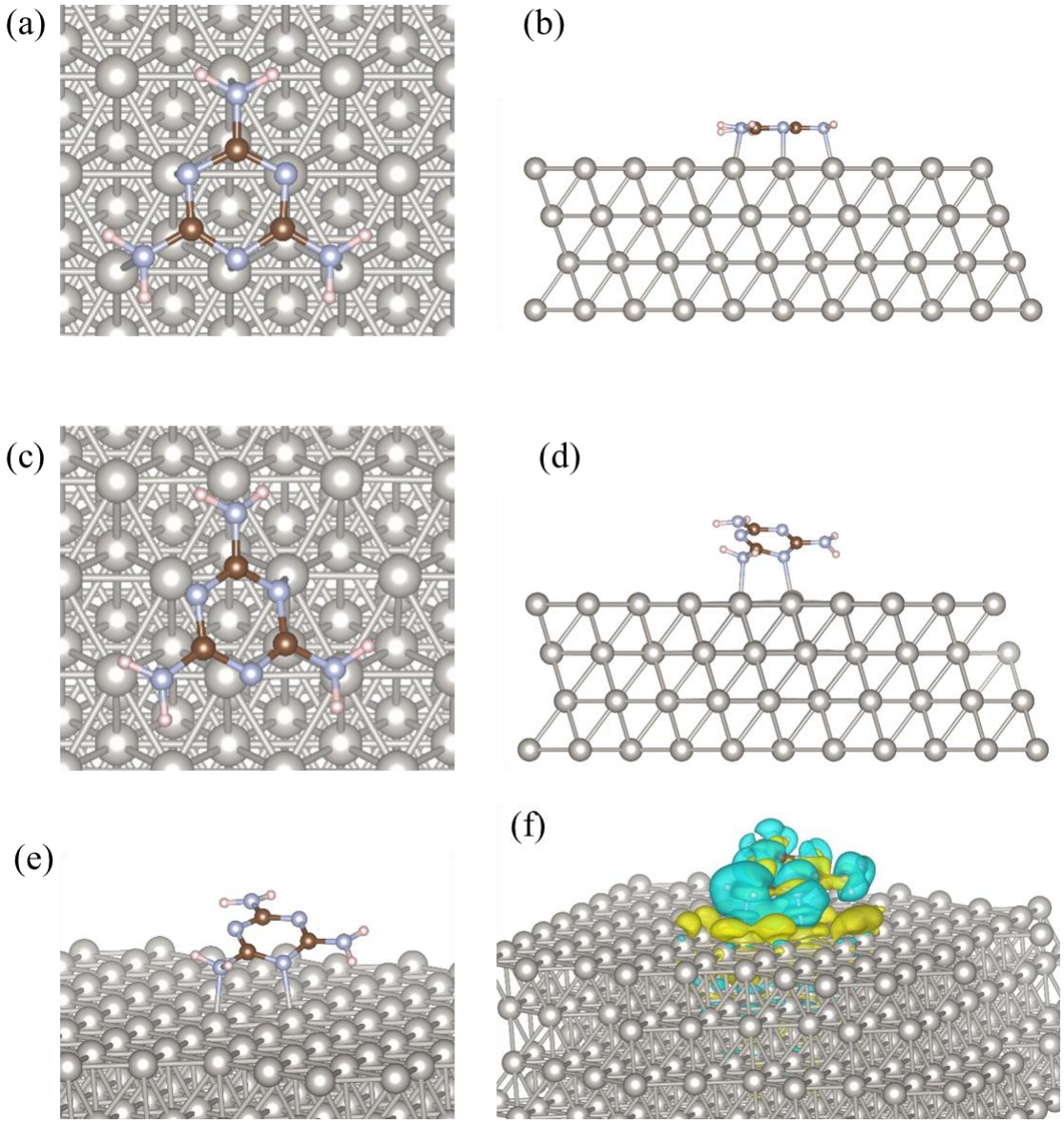

Figure S23. (a) Top and (b) side views of entry 1. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 1. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^3. Yellow and blue represent the decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

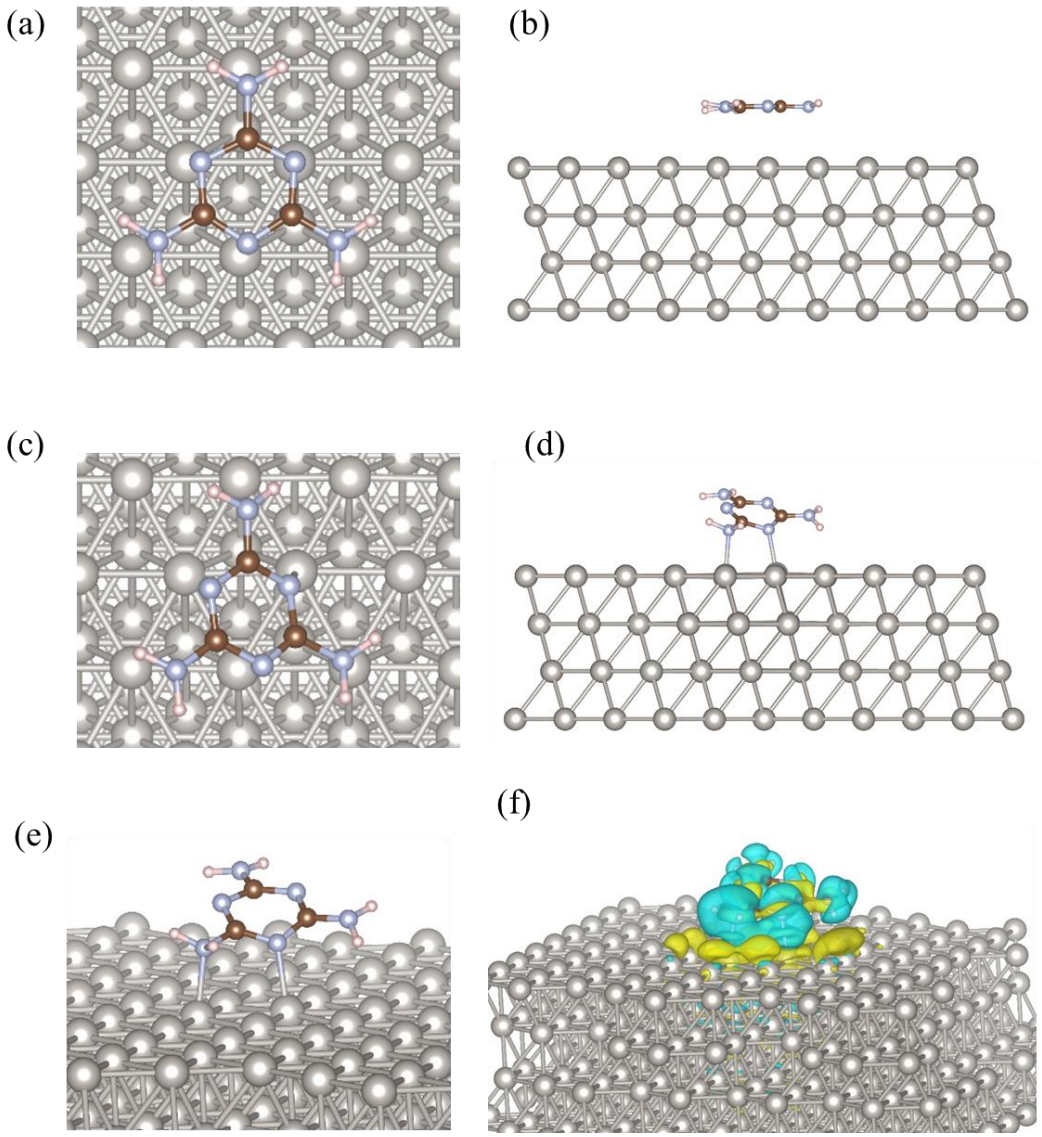

Figure S24. (a) Top and (b) side views of entry 2. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 2. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^3. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

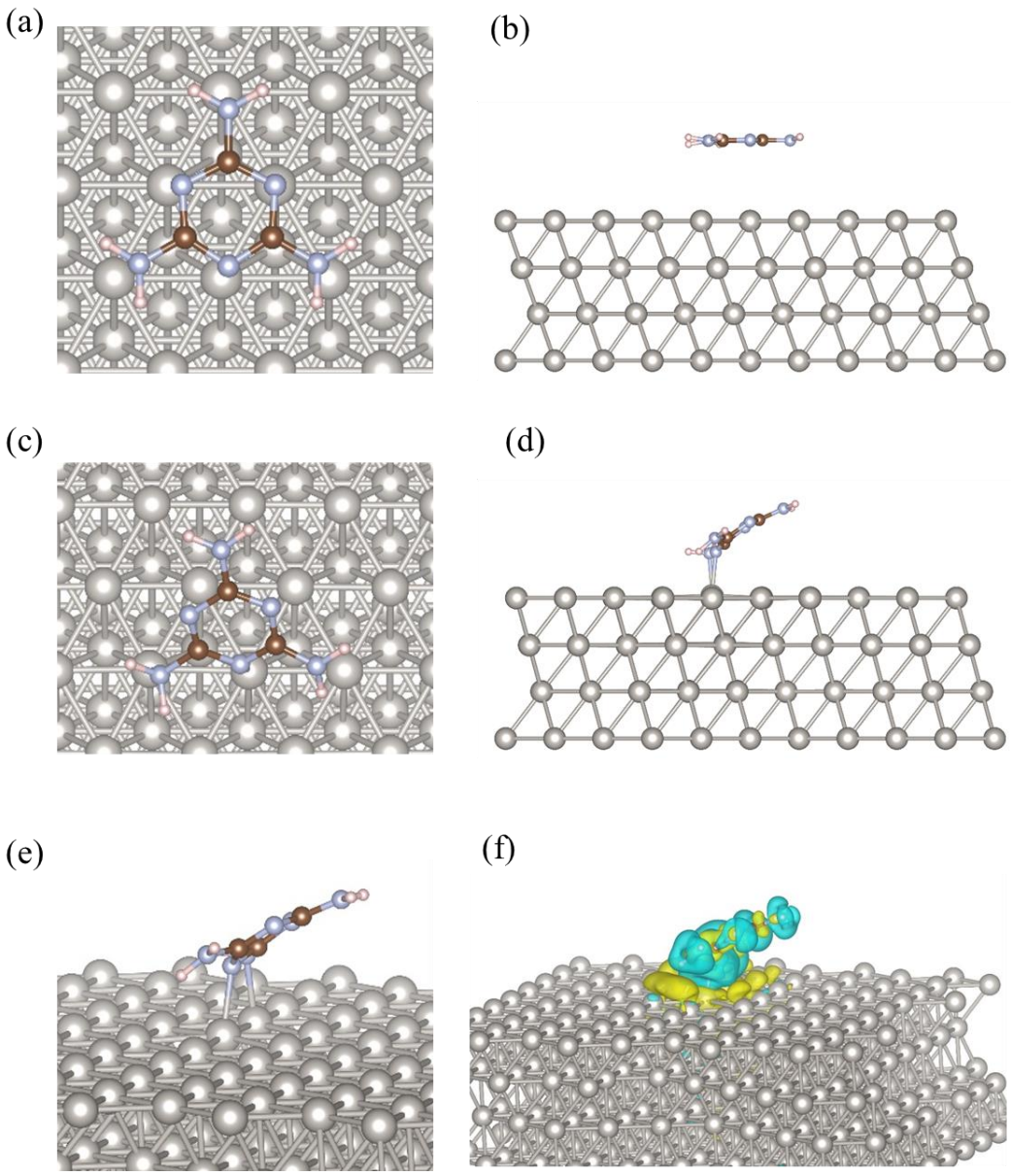

Figure S25. (a) Top and (b) side views of entry 3. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 3. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^3. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

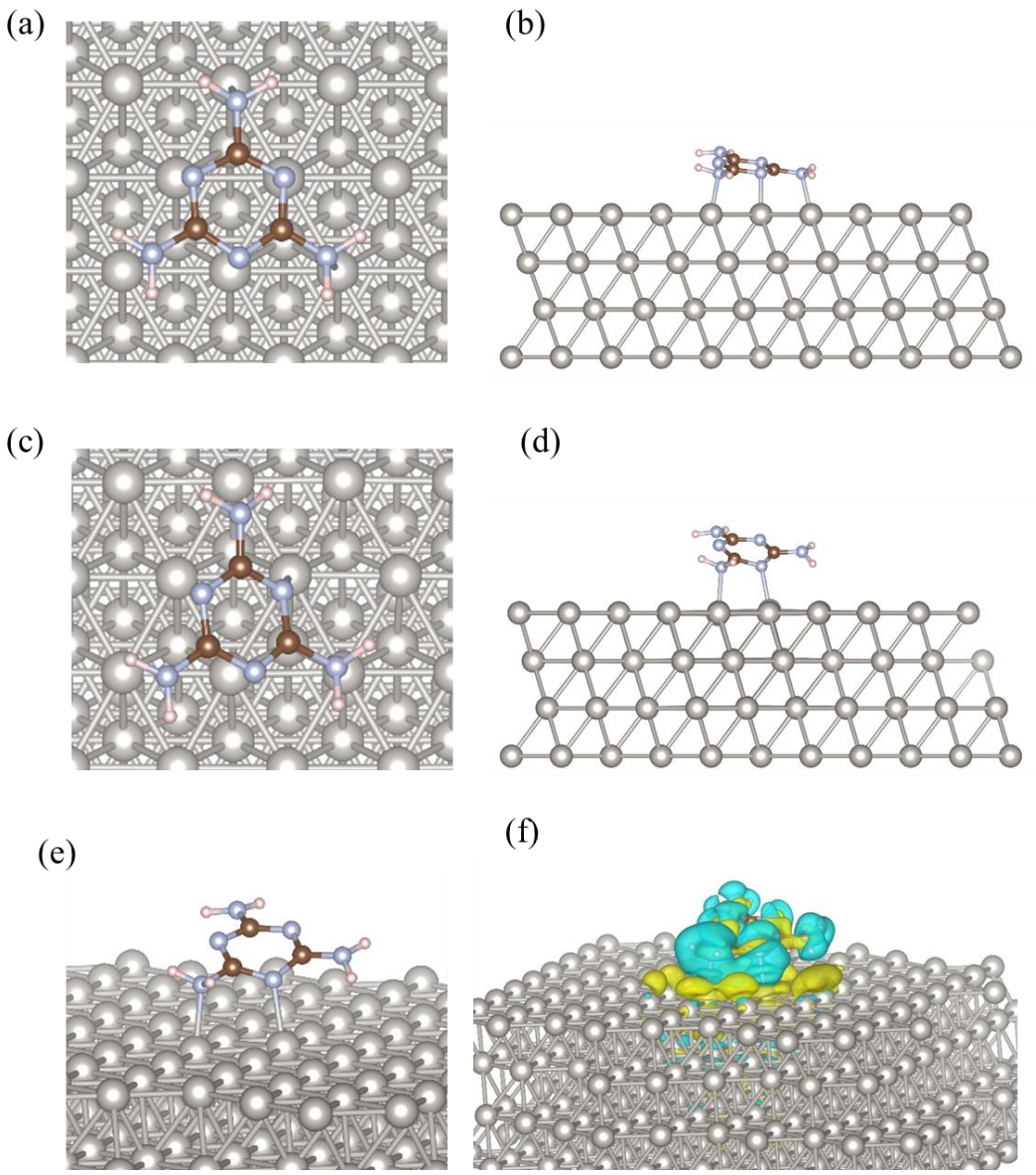

Figure S26. (a) Top and (b) side views of entry 4. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 4. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^3. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

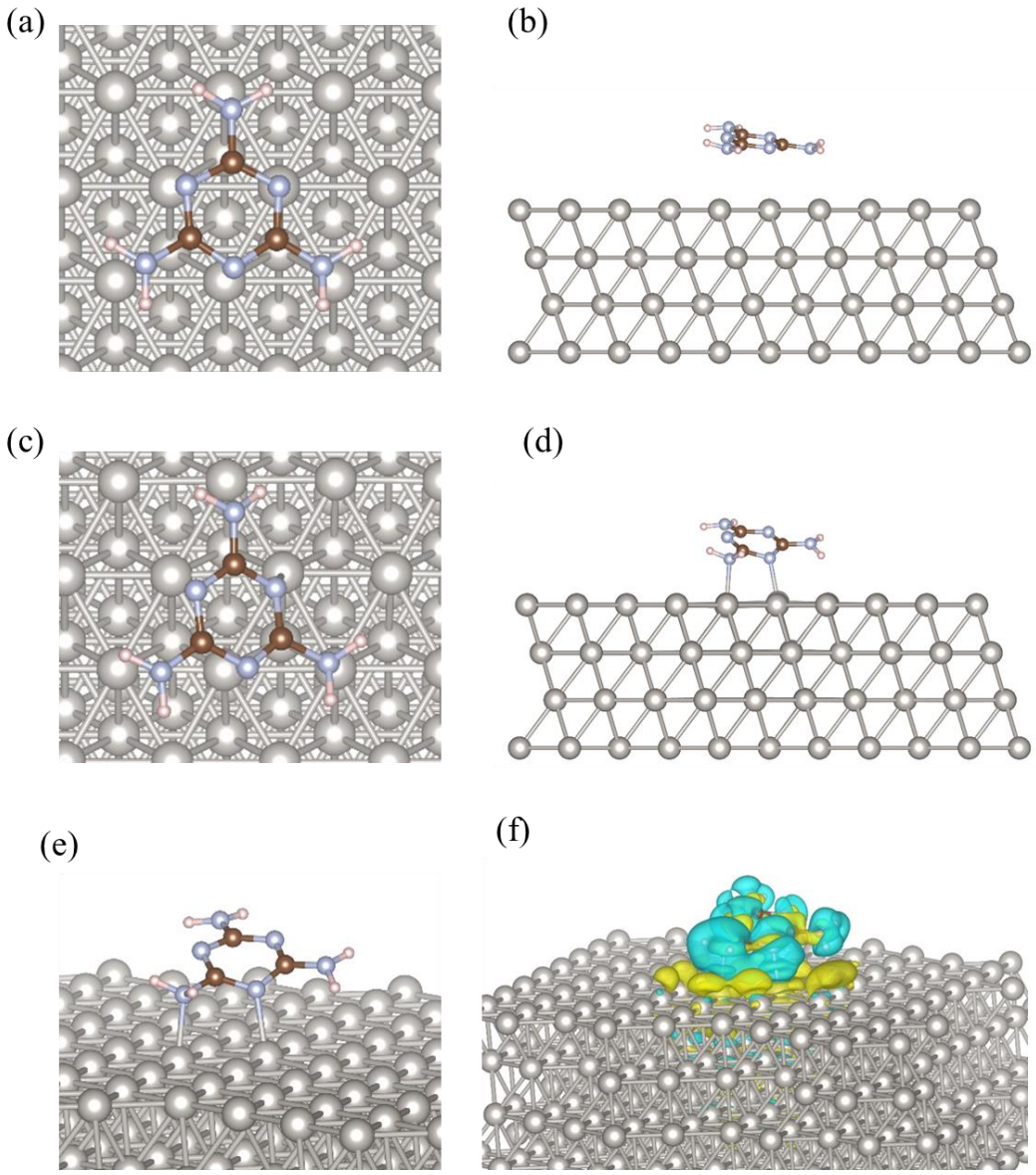

Figure S27. (a) Top and (b) side views of entry 5. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 5. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^3. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

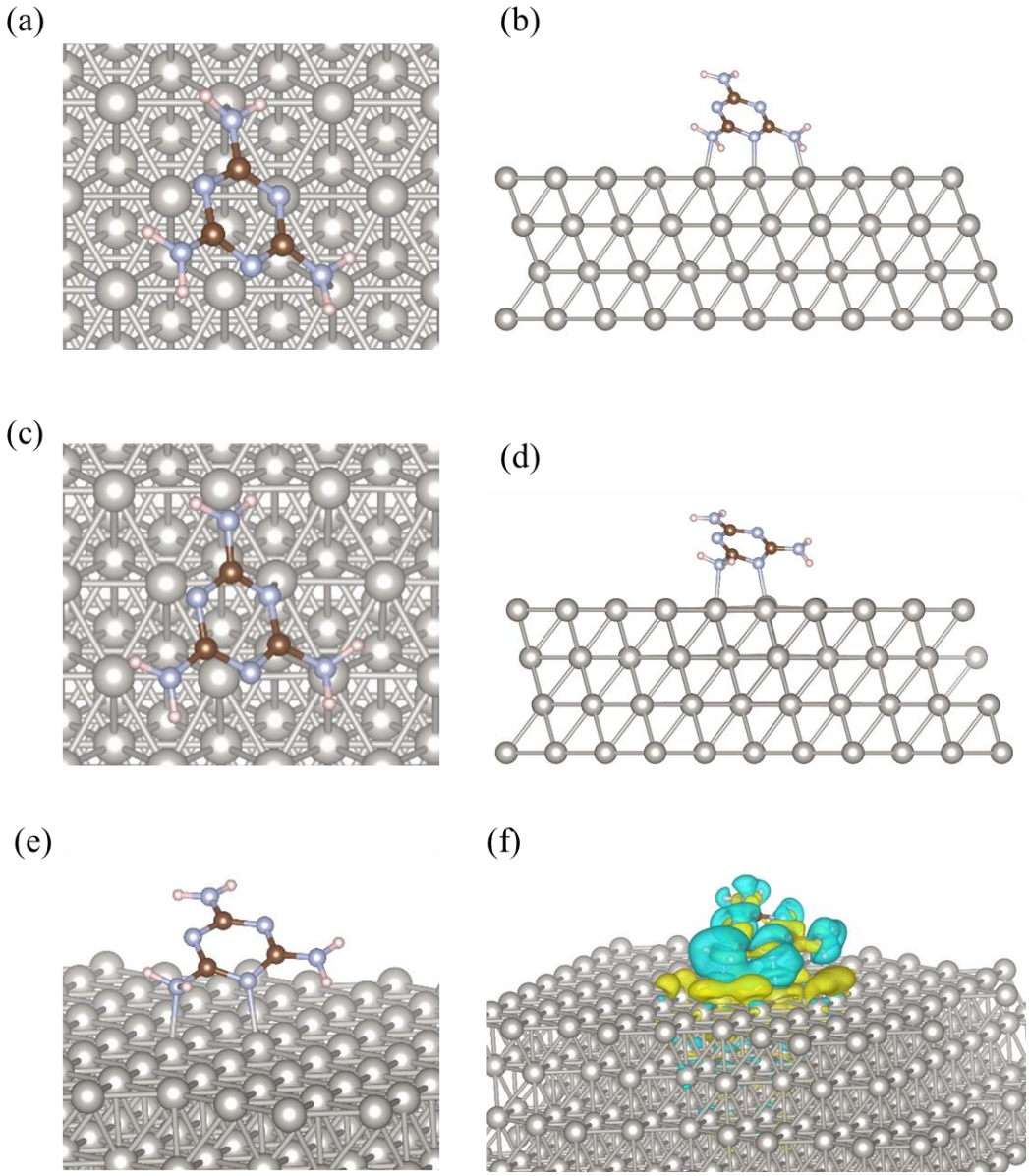

Figure S28. (a) Top and (b) side views of entry 6. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 6. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^3. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

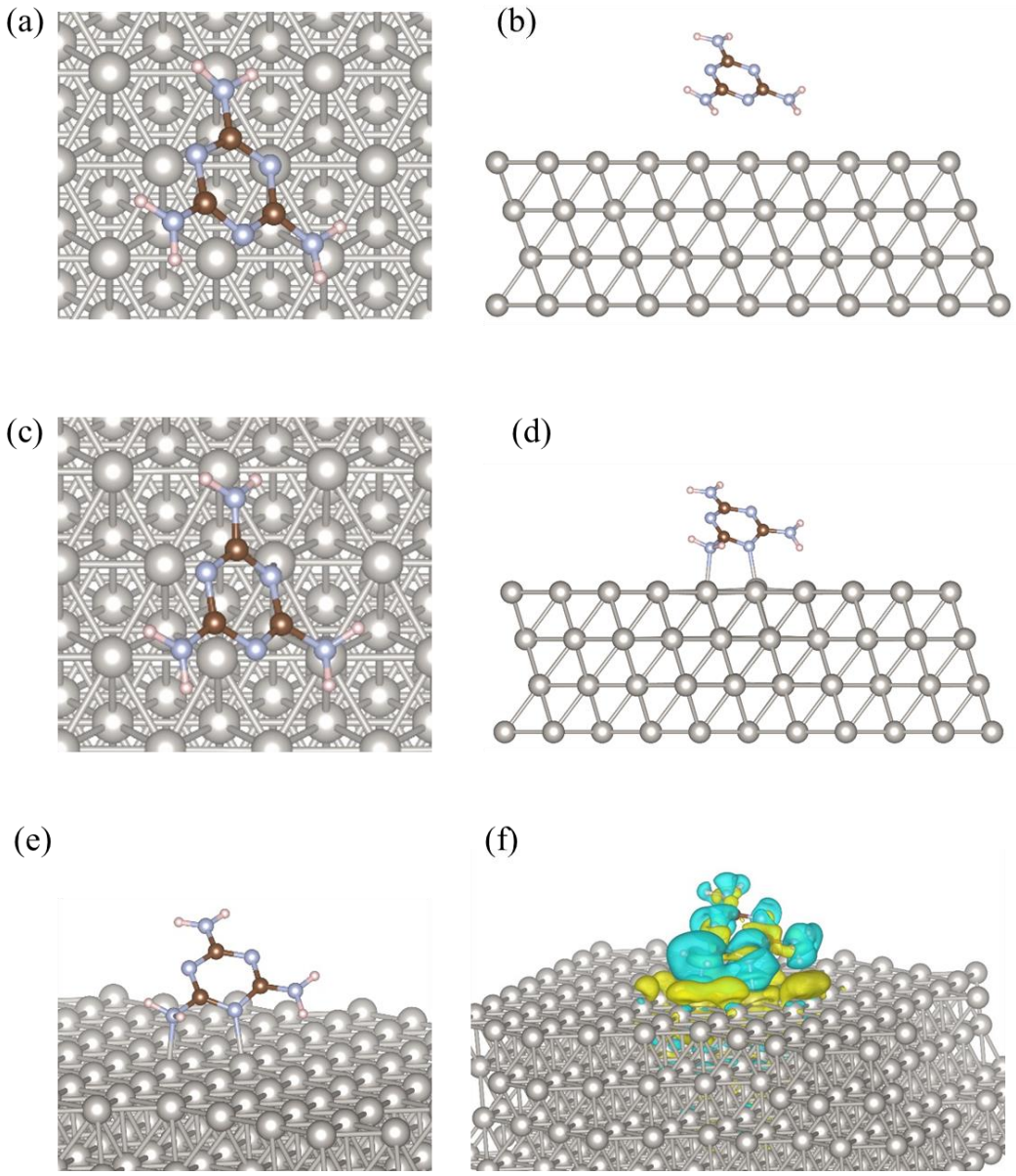

Figure S29. (a) Top and (b) side views of entry 7. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 7. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^3. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

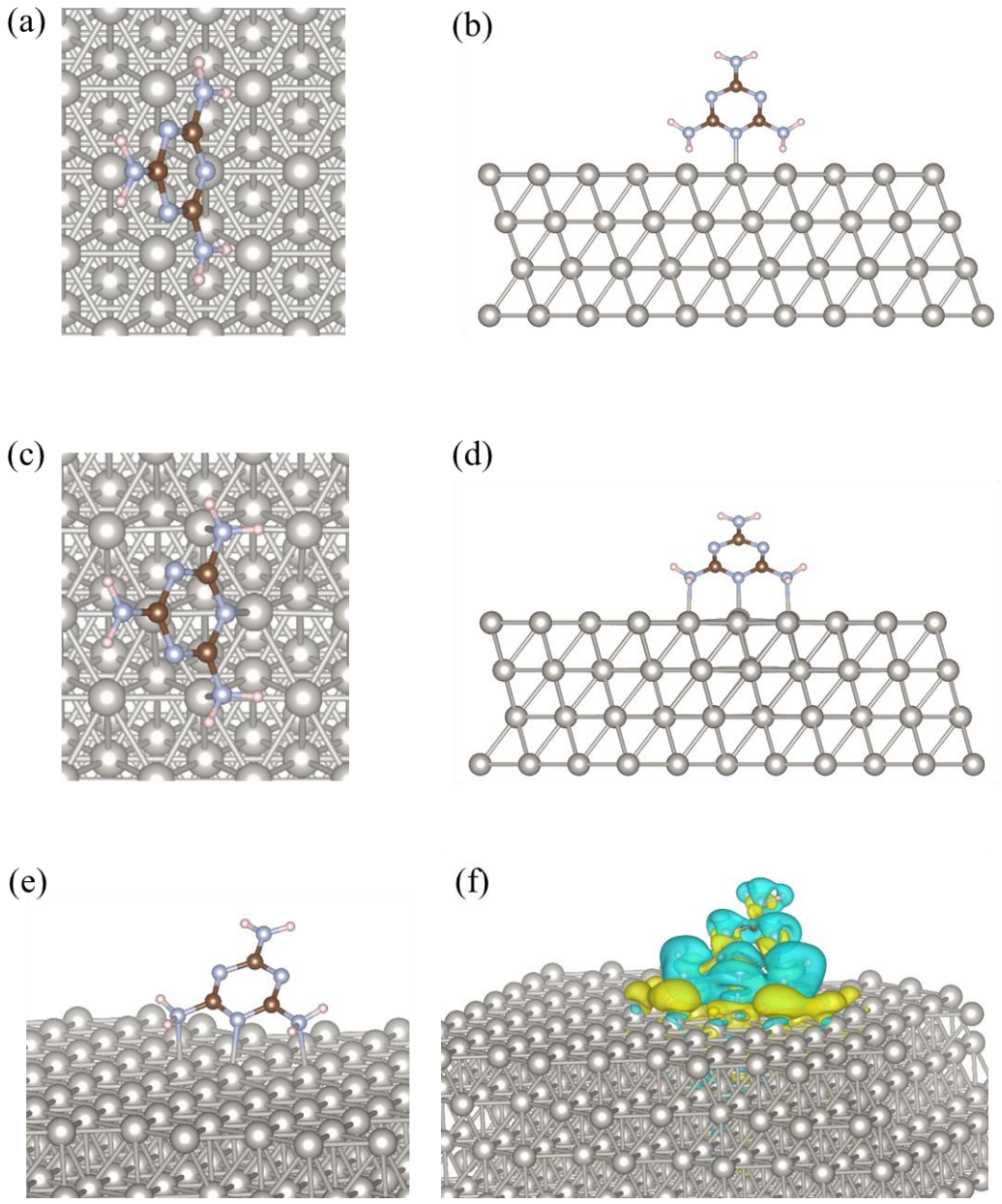

Figure S30. (a) Top and (b) side views of entry 8. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 8. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^3. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

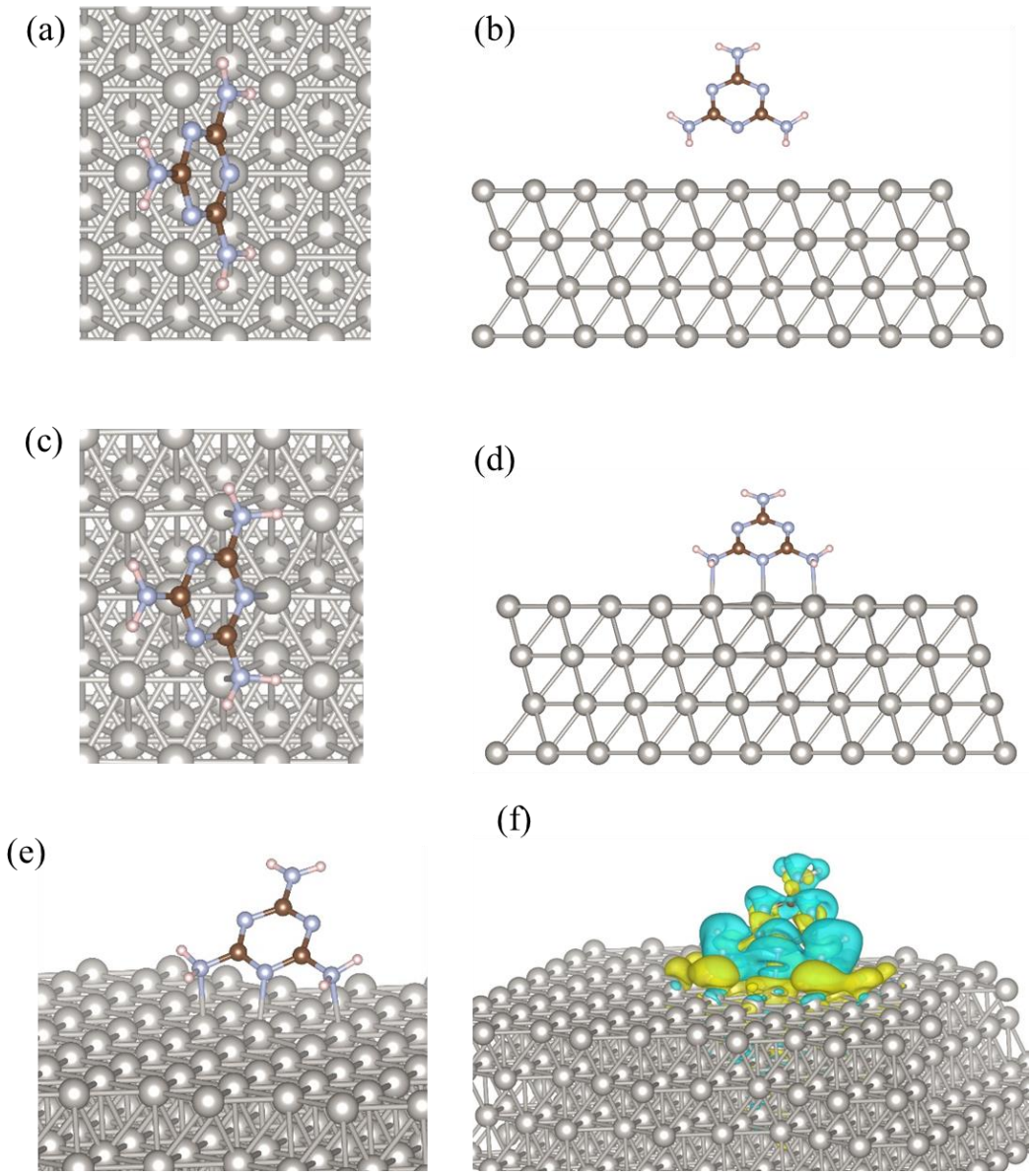

Figure S31. (a) Top and (b) side views of entry 9. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 9. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^3. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

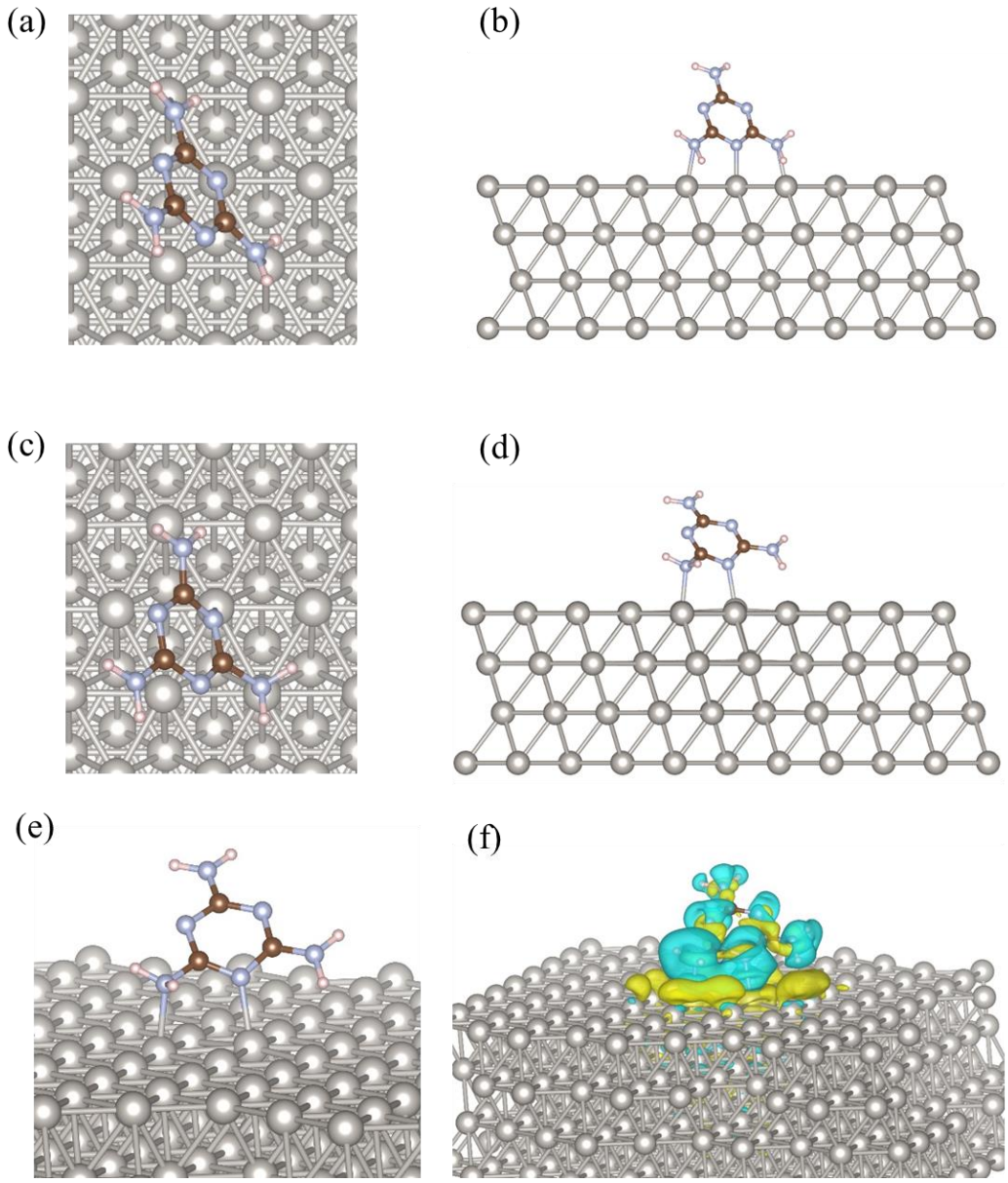

Figure S32. (a) Top and (b) side views of entry 10. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 10. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^3. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

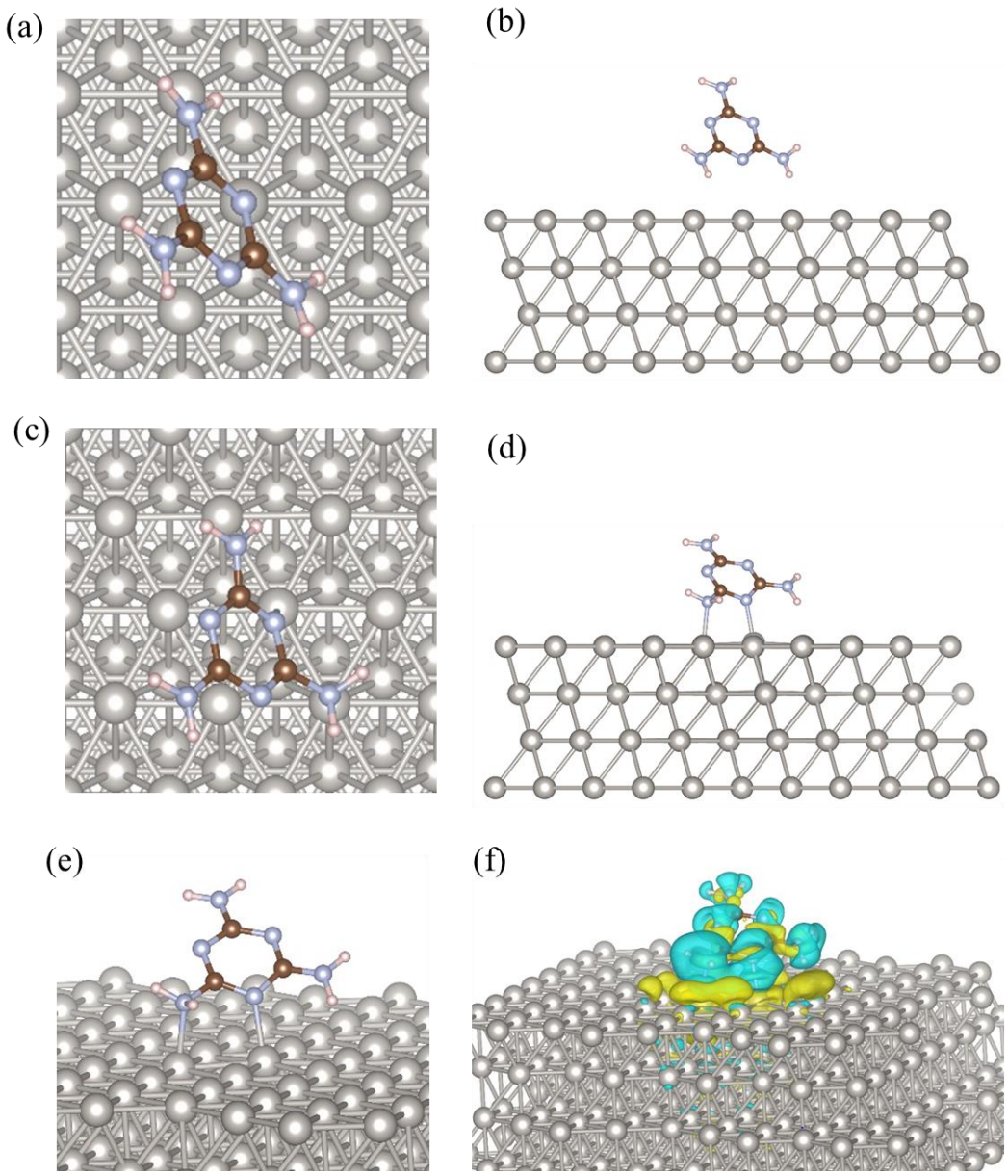

Figure S33. (a) Top and (b) side views of entry 11. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 11. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^3. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

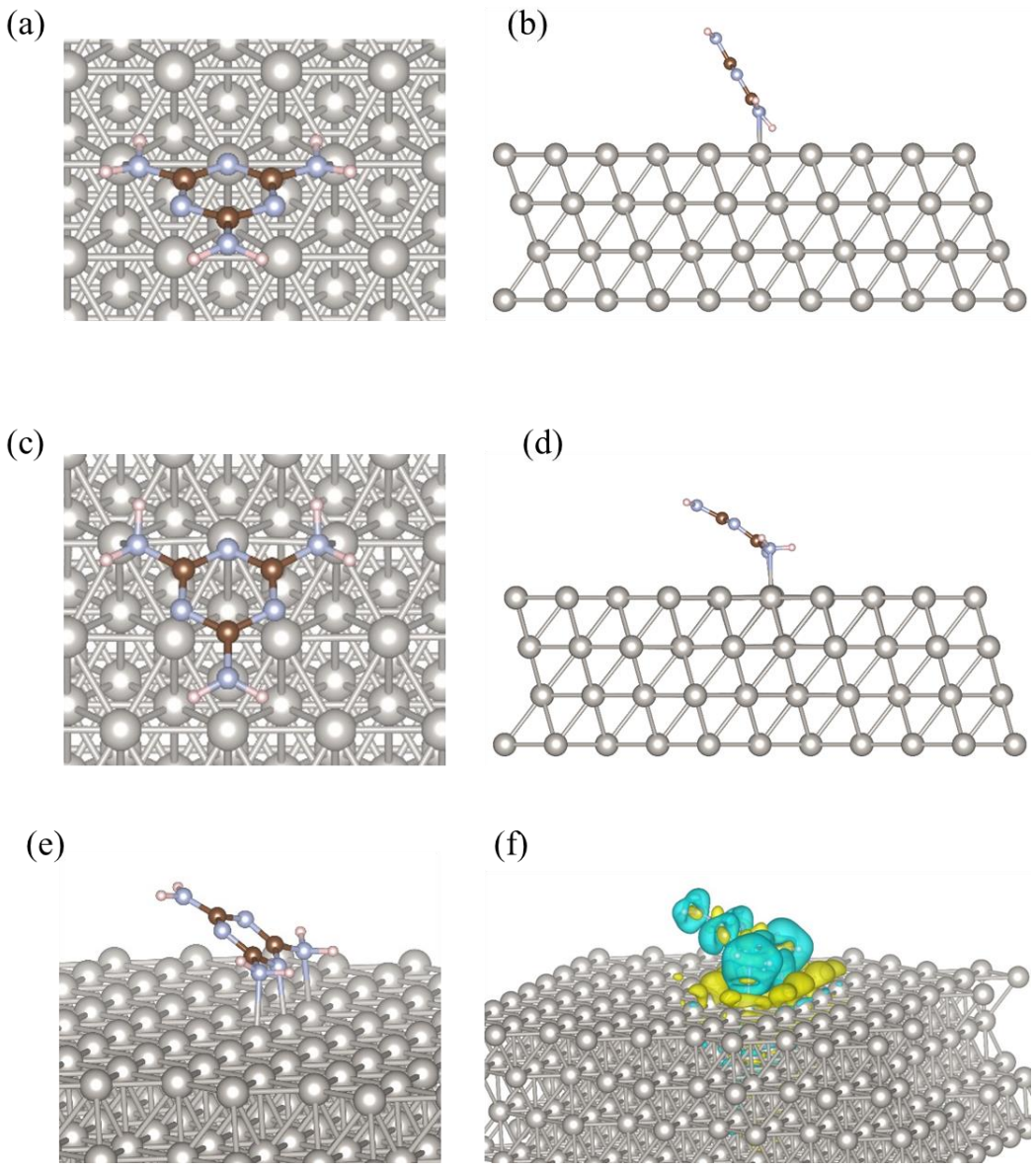

Figure S34. (a) Top and (b) side views of entry 12. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 12. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^{3}. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

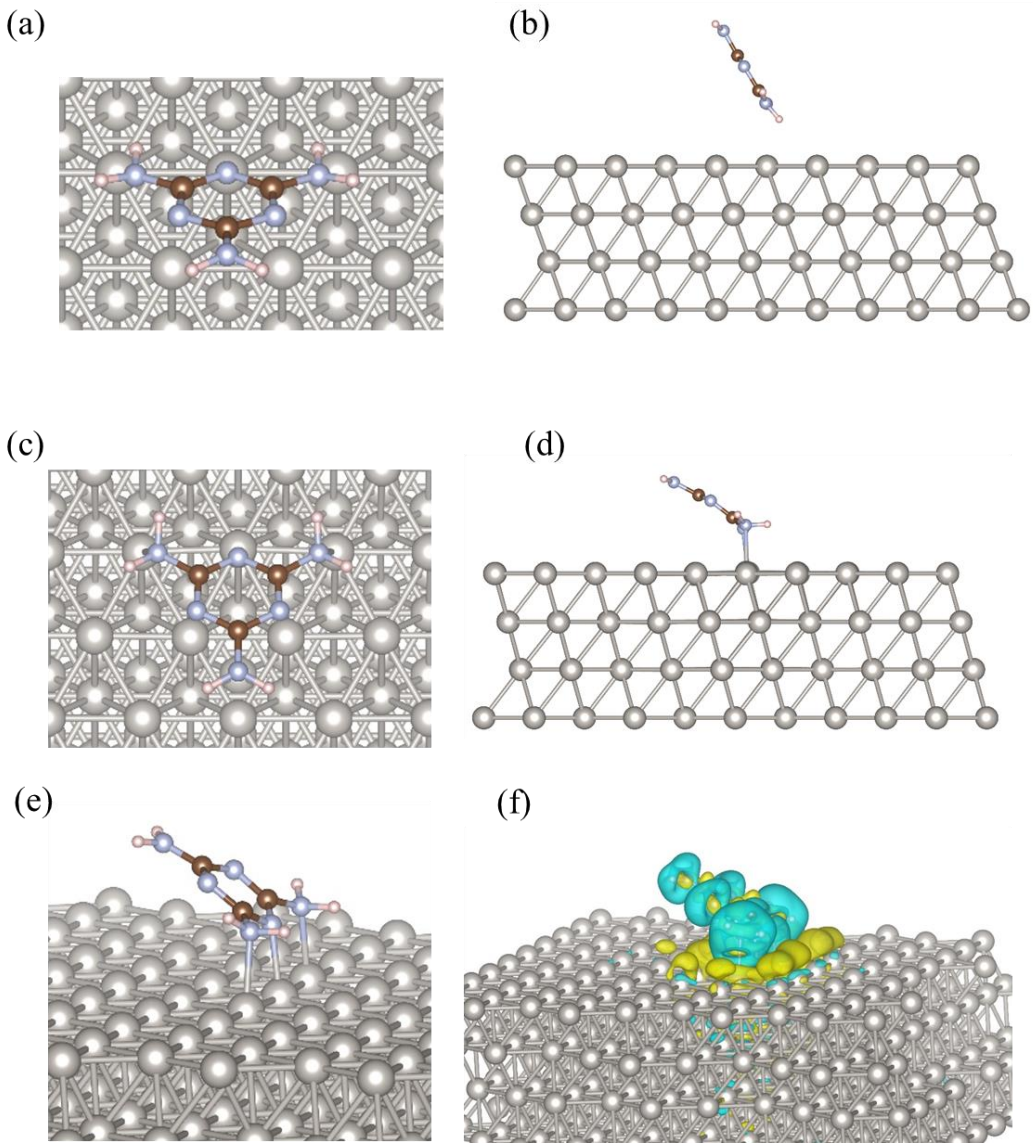

Figure S35. (a) Top and (b) side views of entry 13. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 13. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^{3}. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

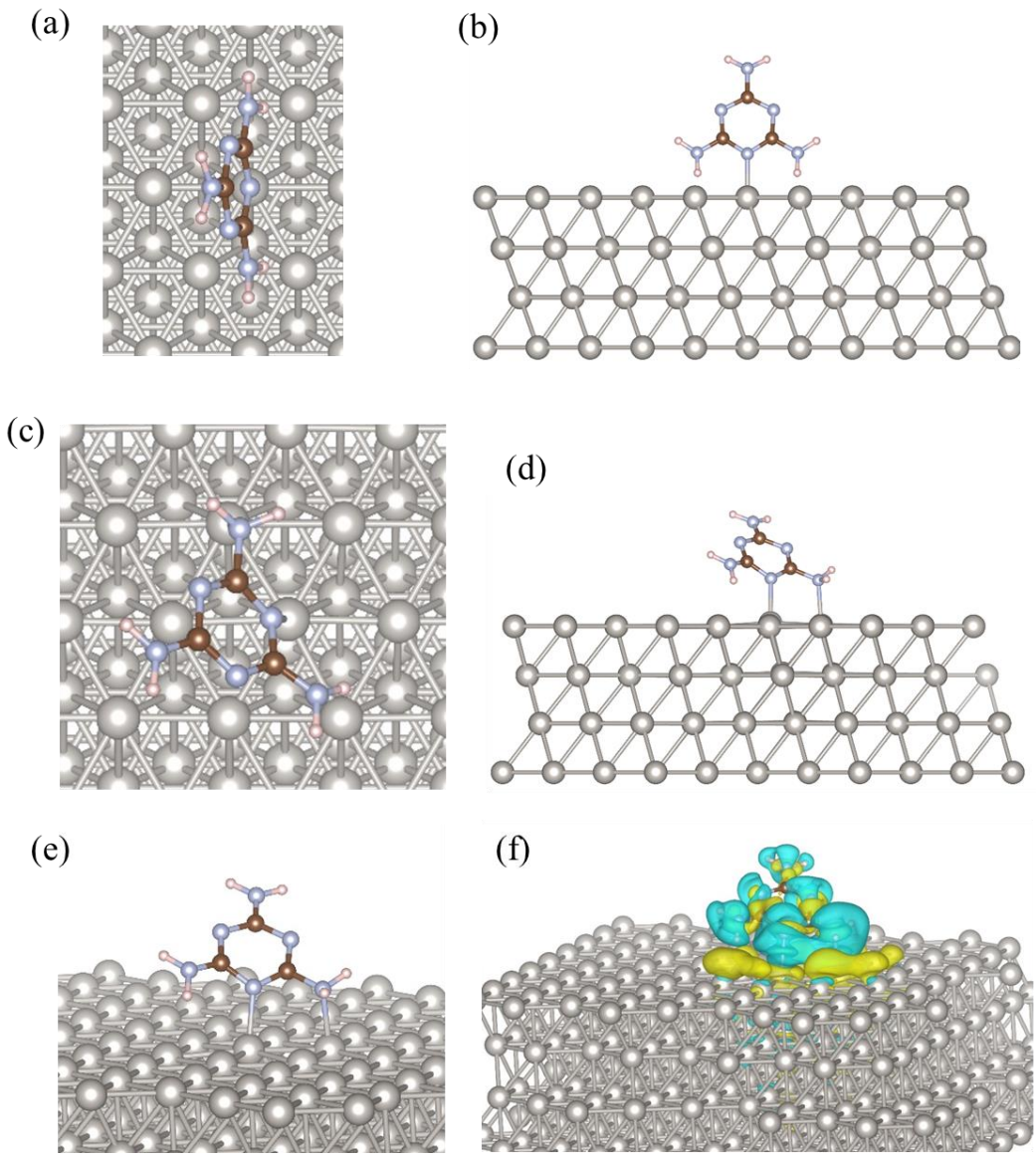

Figure S36. (a) Top and (b) side views of entry 14. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 14. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^3. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

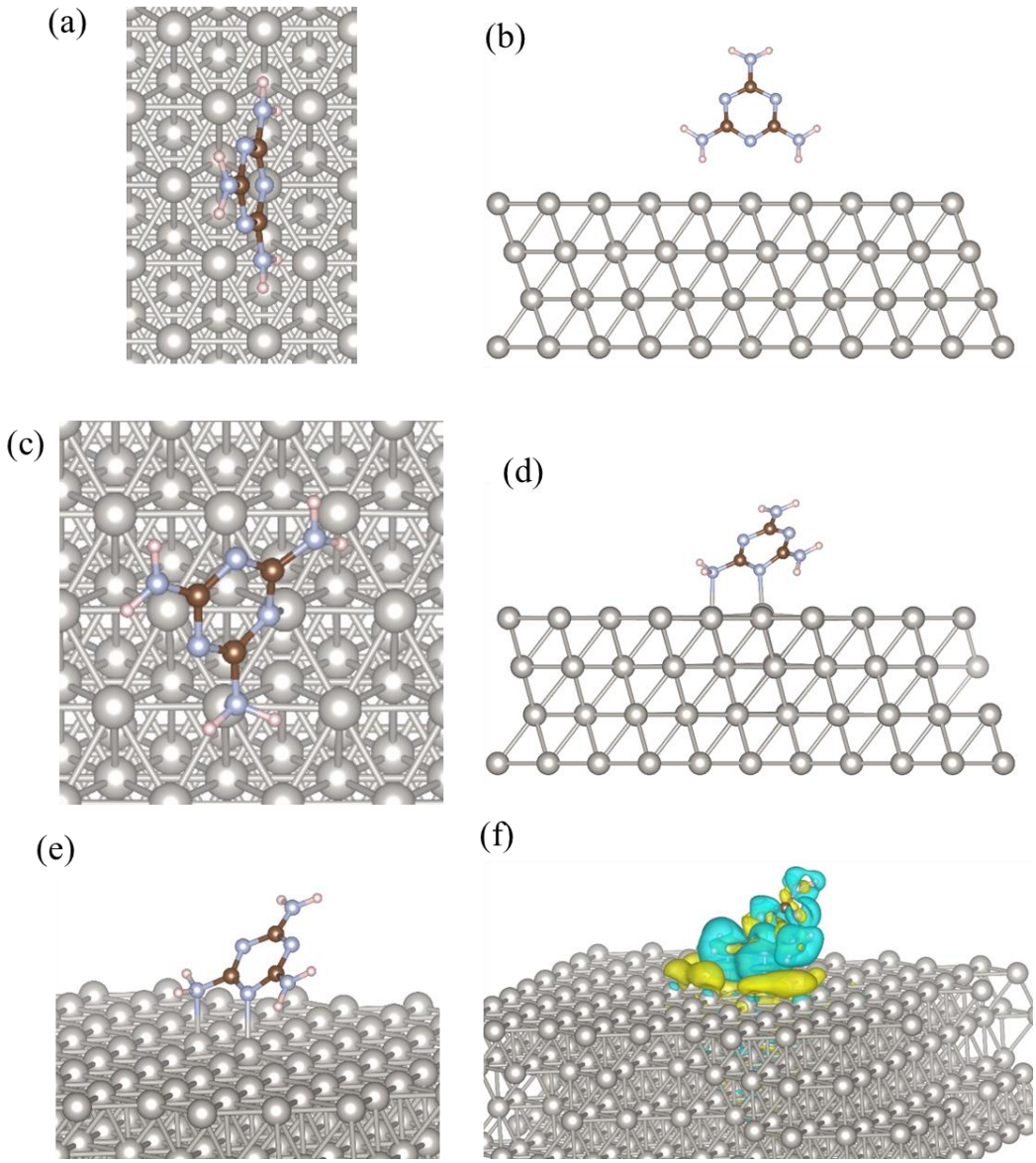

Figure S37. (a) Top and (b) side views of entry 15. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 15. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^{3}. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

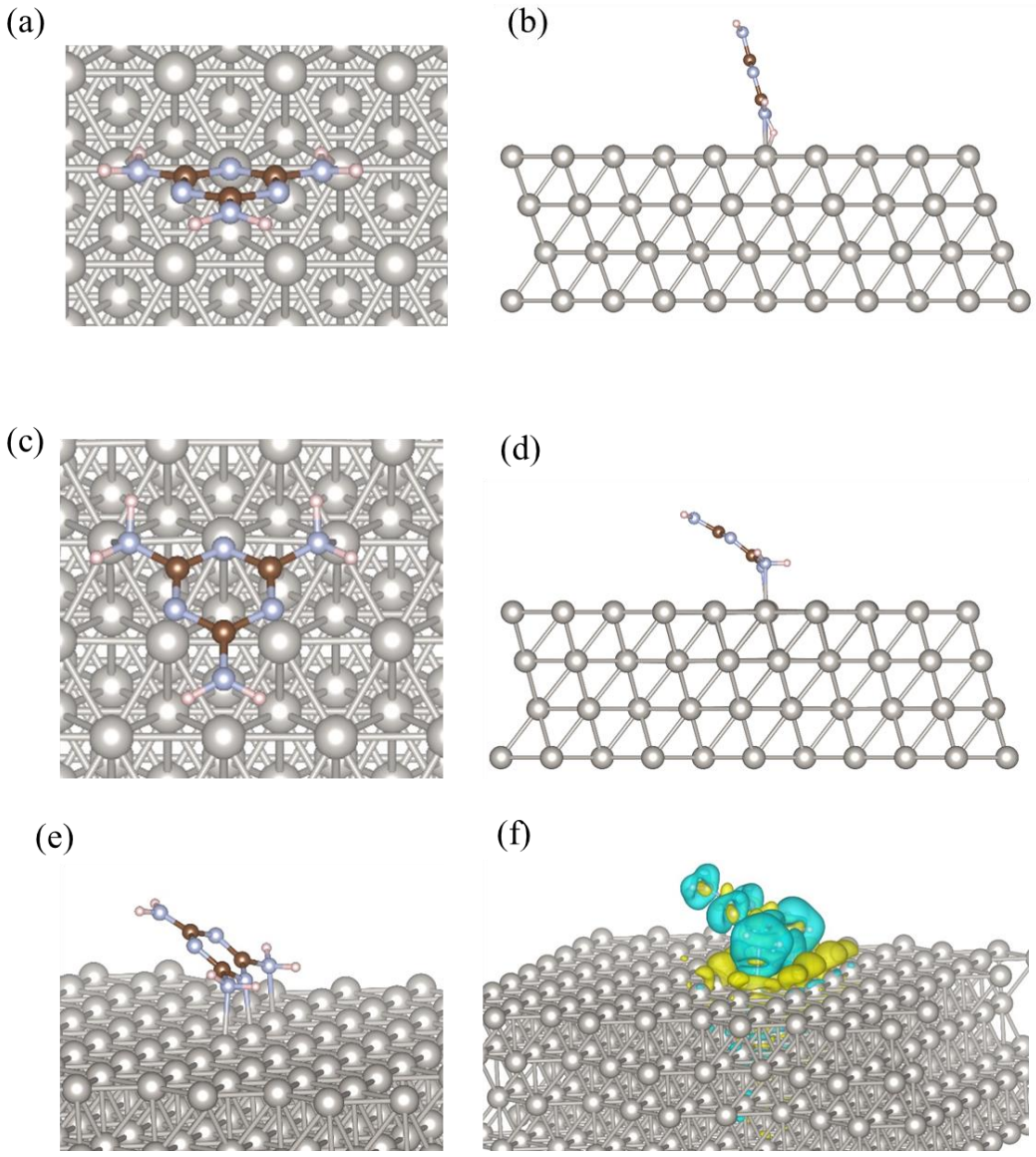

Figure S38. (a) Top and (b) side views of entry 16. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 16. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^3. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

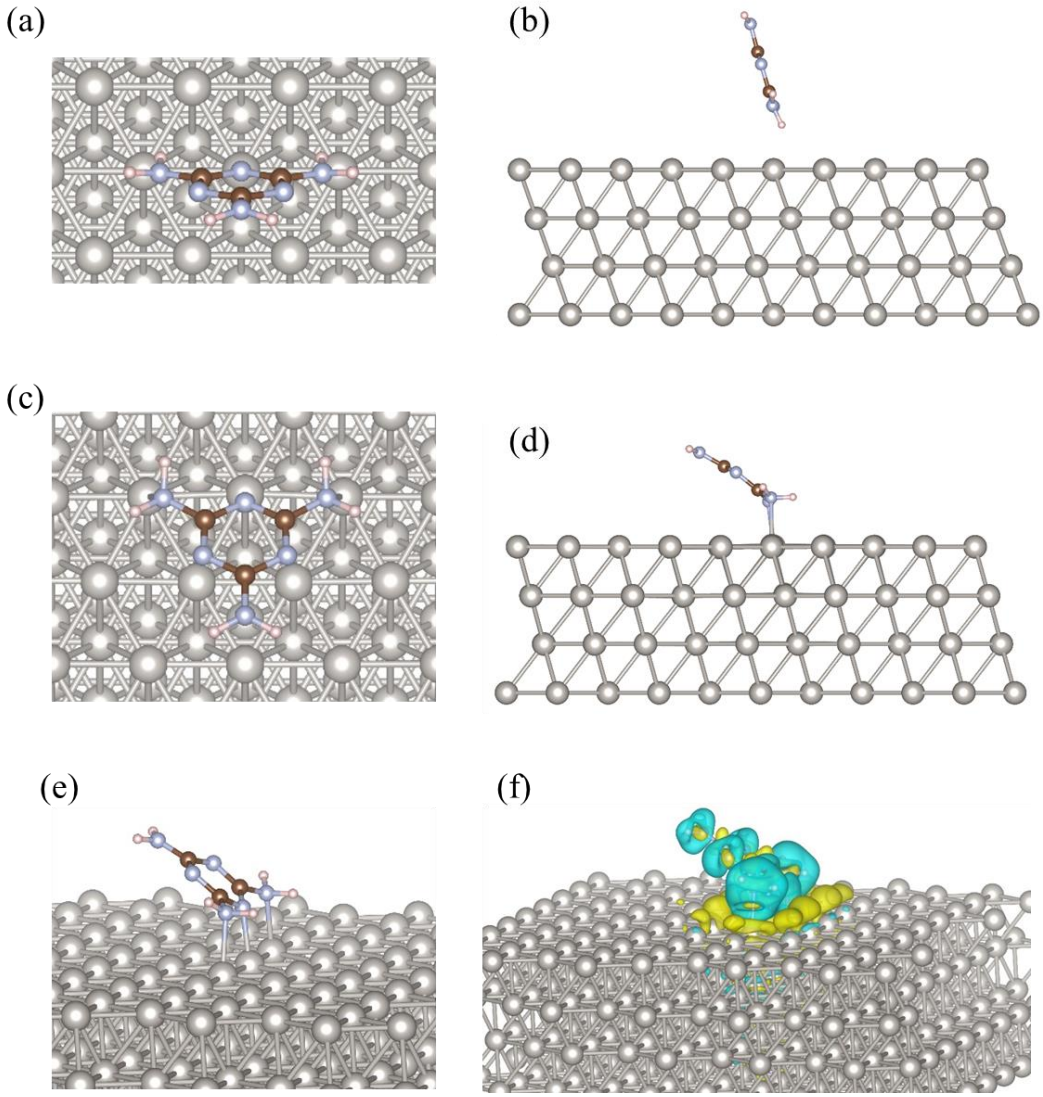

Figure S39. (a) Top and (b) side views of entry 17. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 17. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^3. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

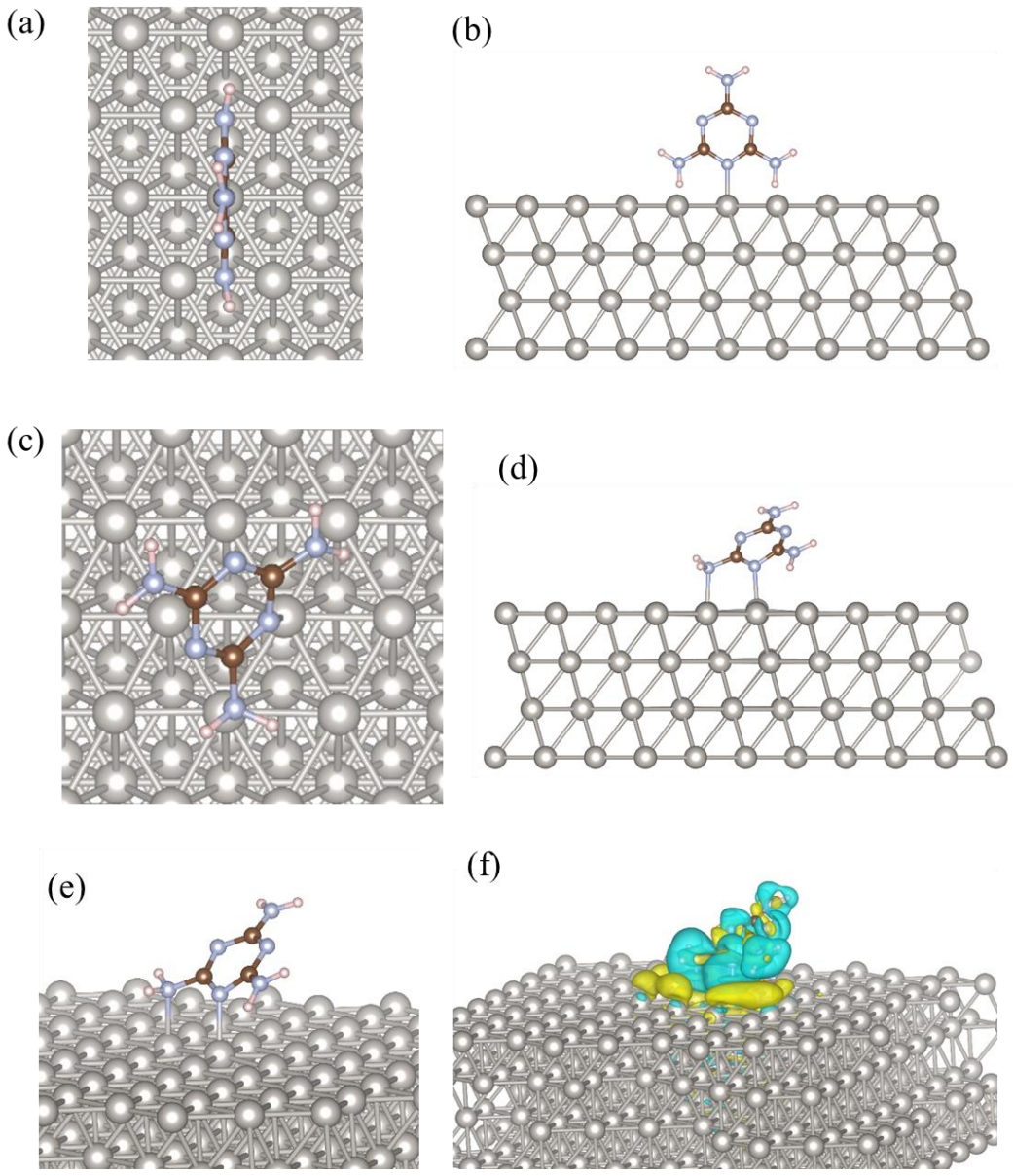

Figure S40. (a) Top and (b) side views of entry 18. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 18. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^3. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

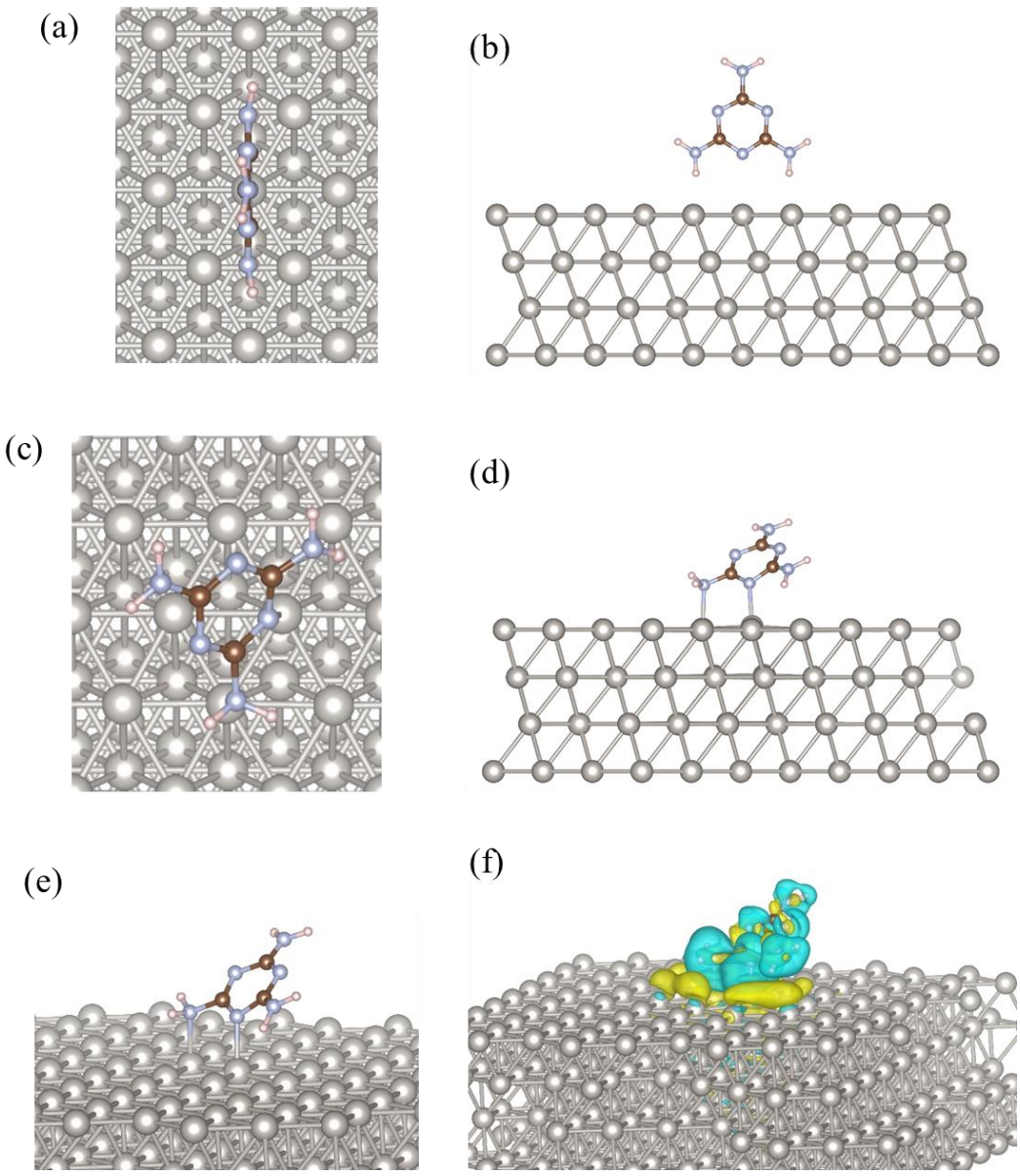

Figure S41. (a) Top and (b) side views of entry 19. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 19. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^3. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

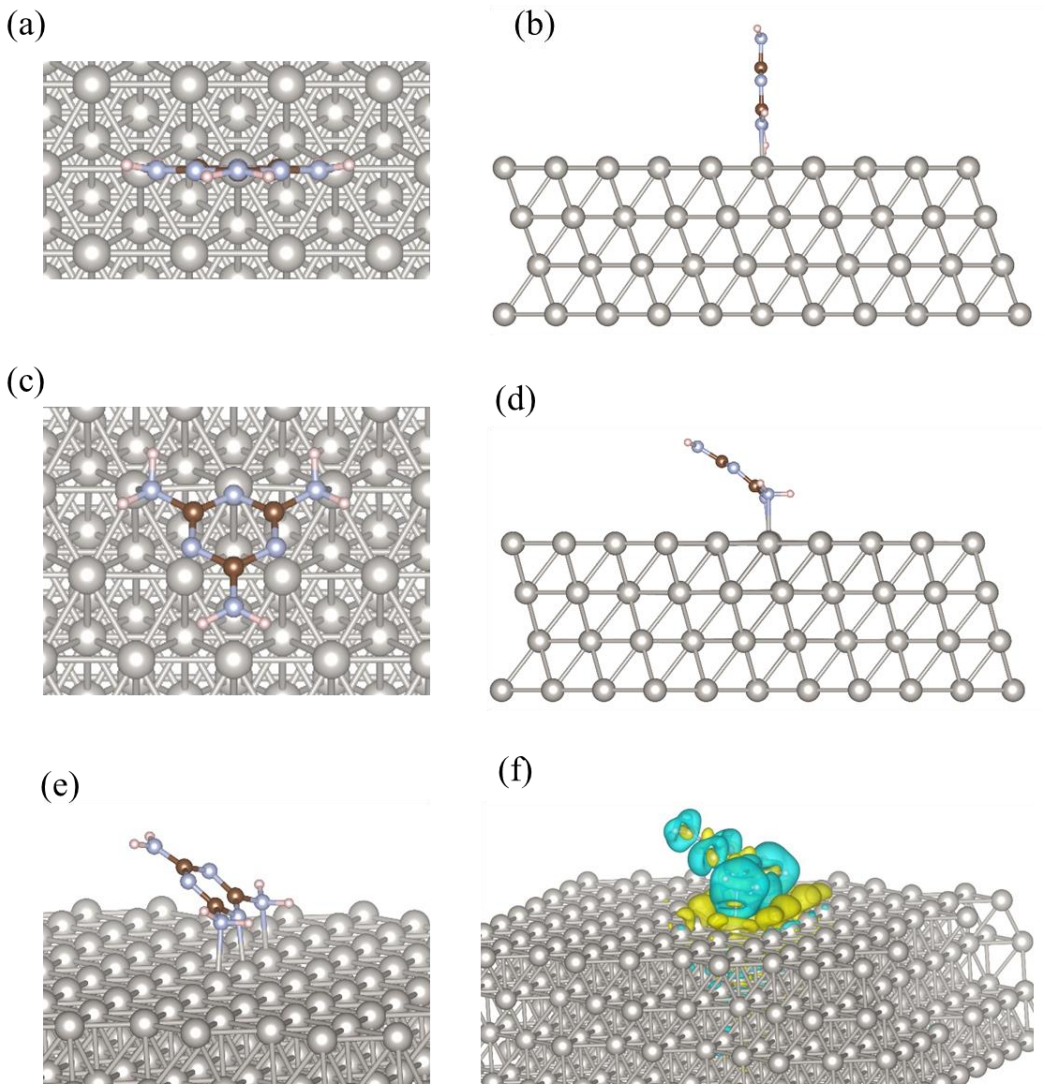

Figure S42. (a) Top and (b) side views of entry 20. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 20. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^3. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

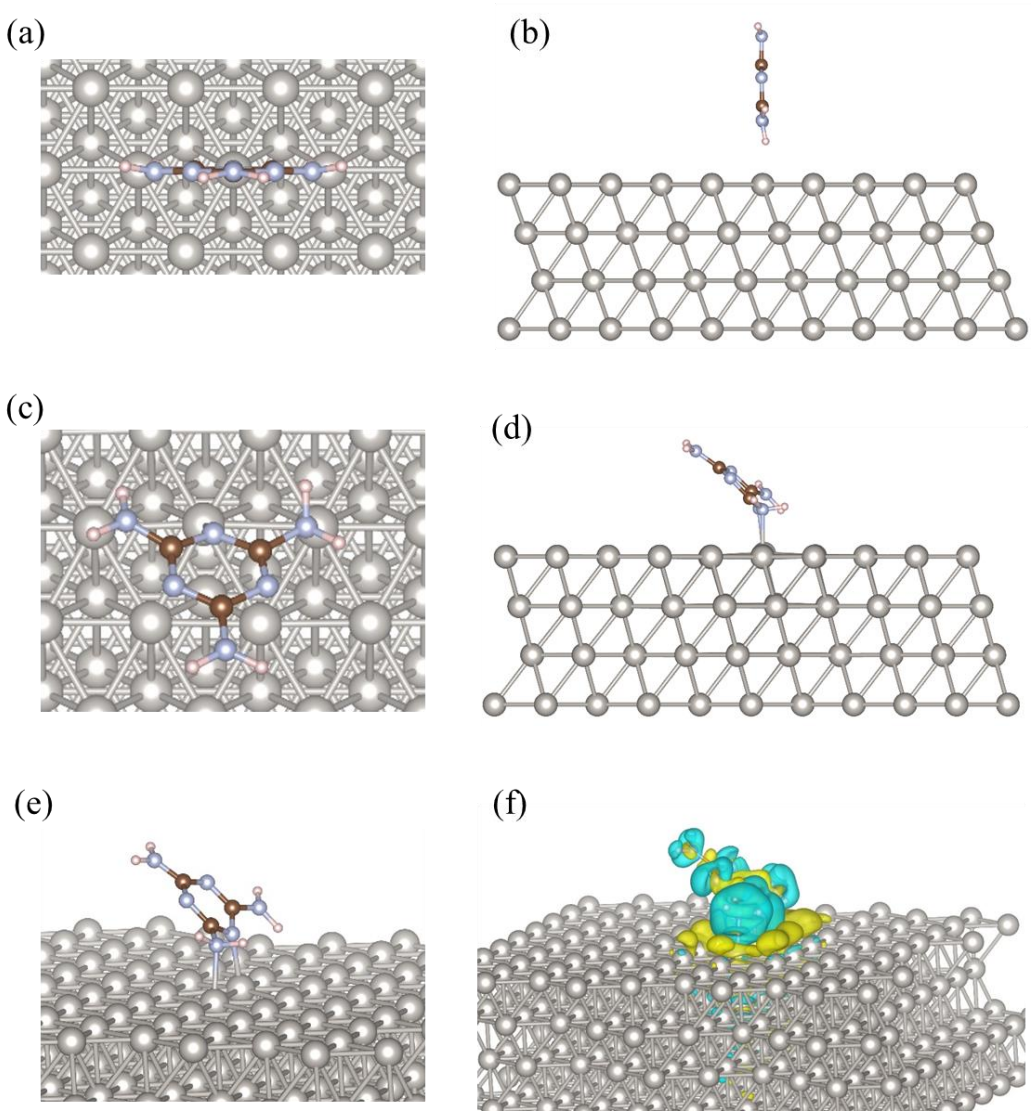

Figure S43. (a) Top and (b) side views of entry 21. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 21. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^3. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

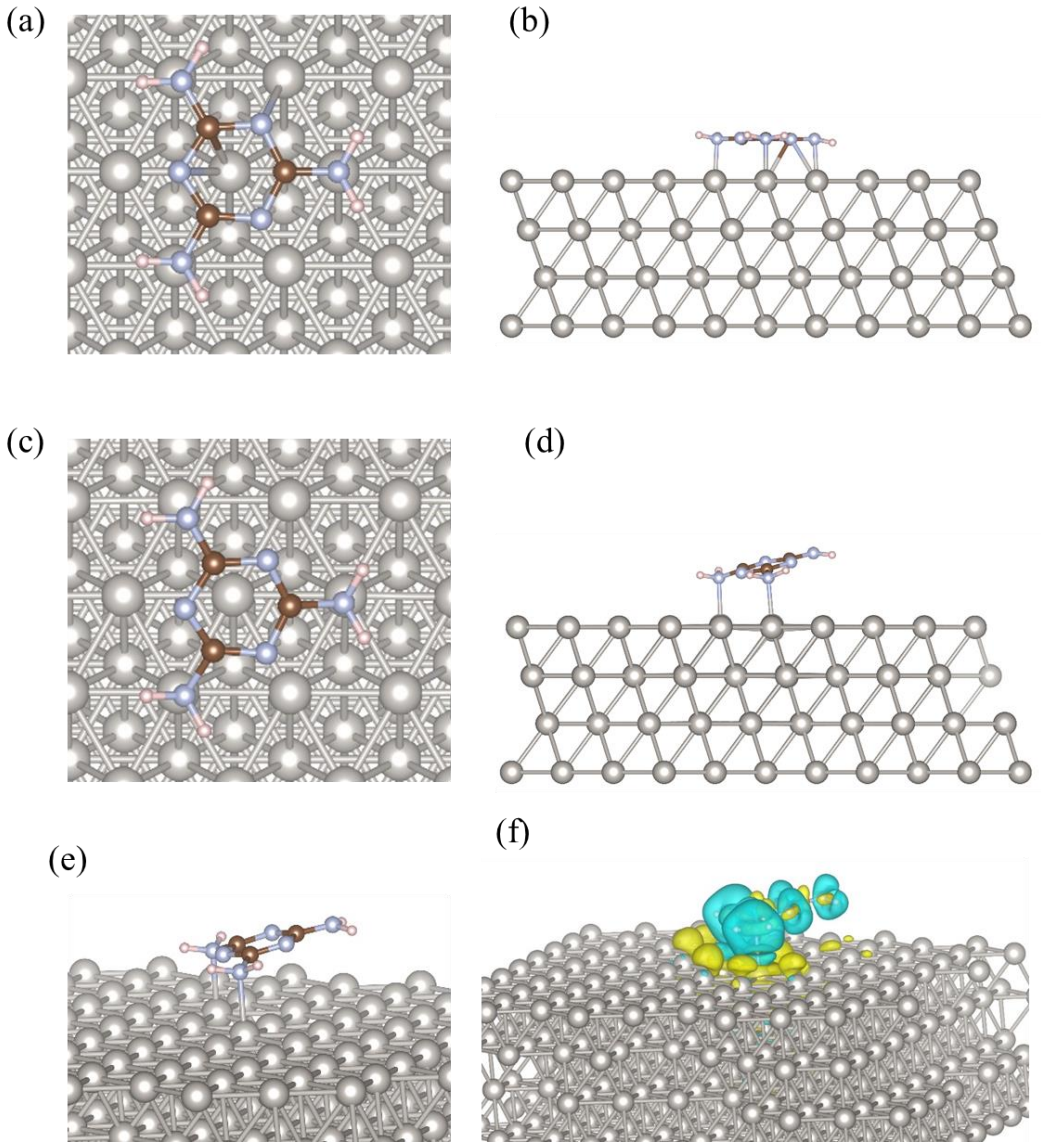

Figure S44. (a) Top and (b) side views of entry 22. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 22. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^3. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

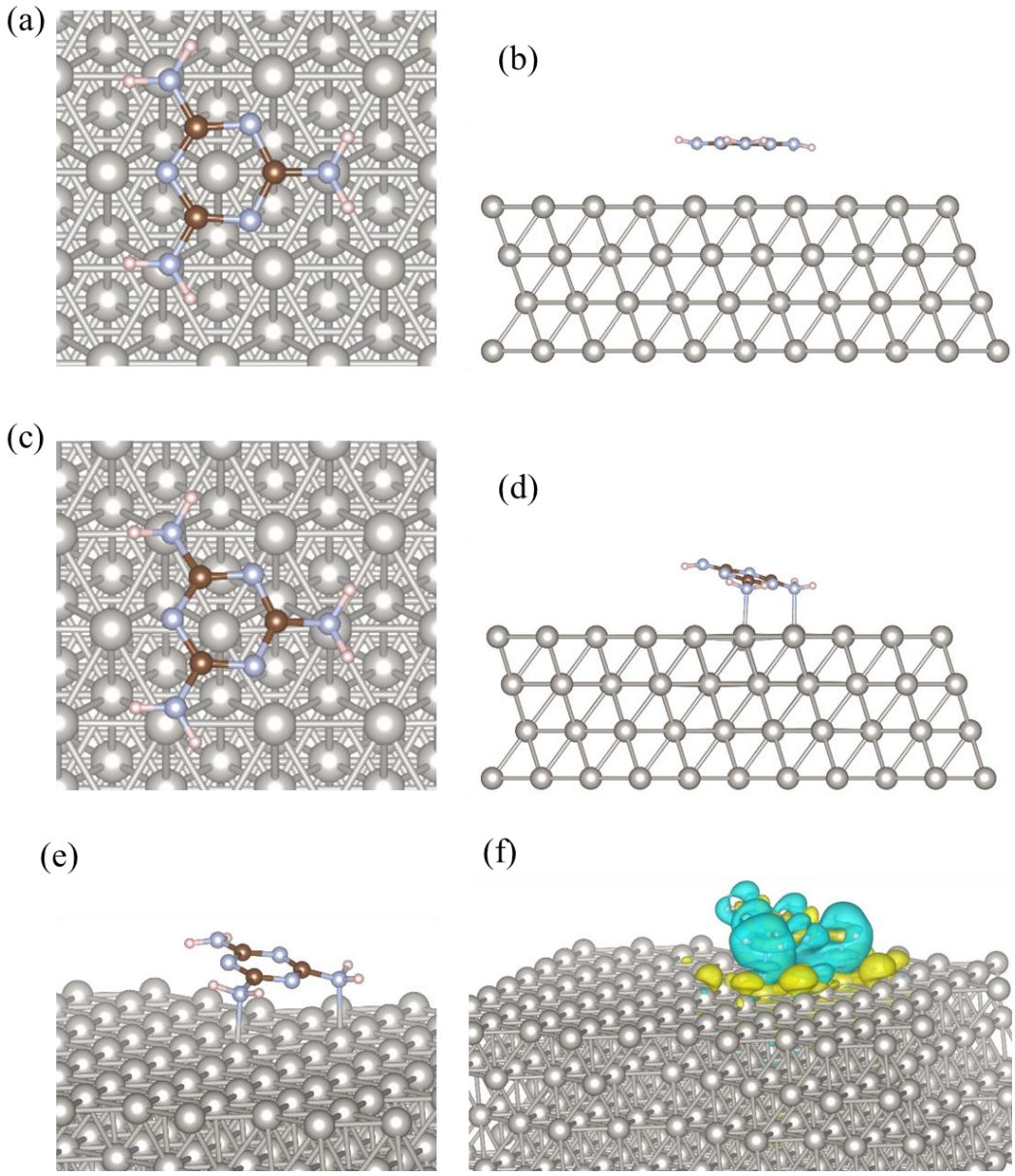

Figure S45. (a) Top and (b) side views of entry 23. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 23. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^3. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

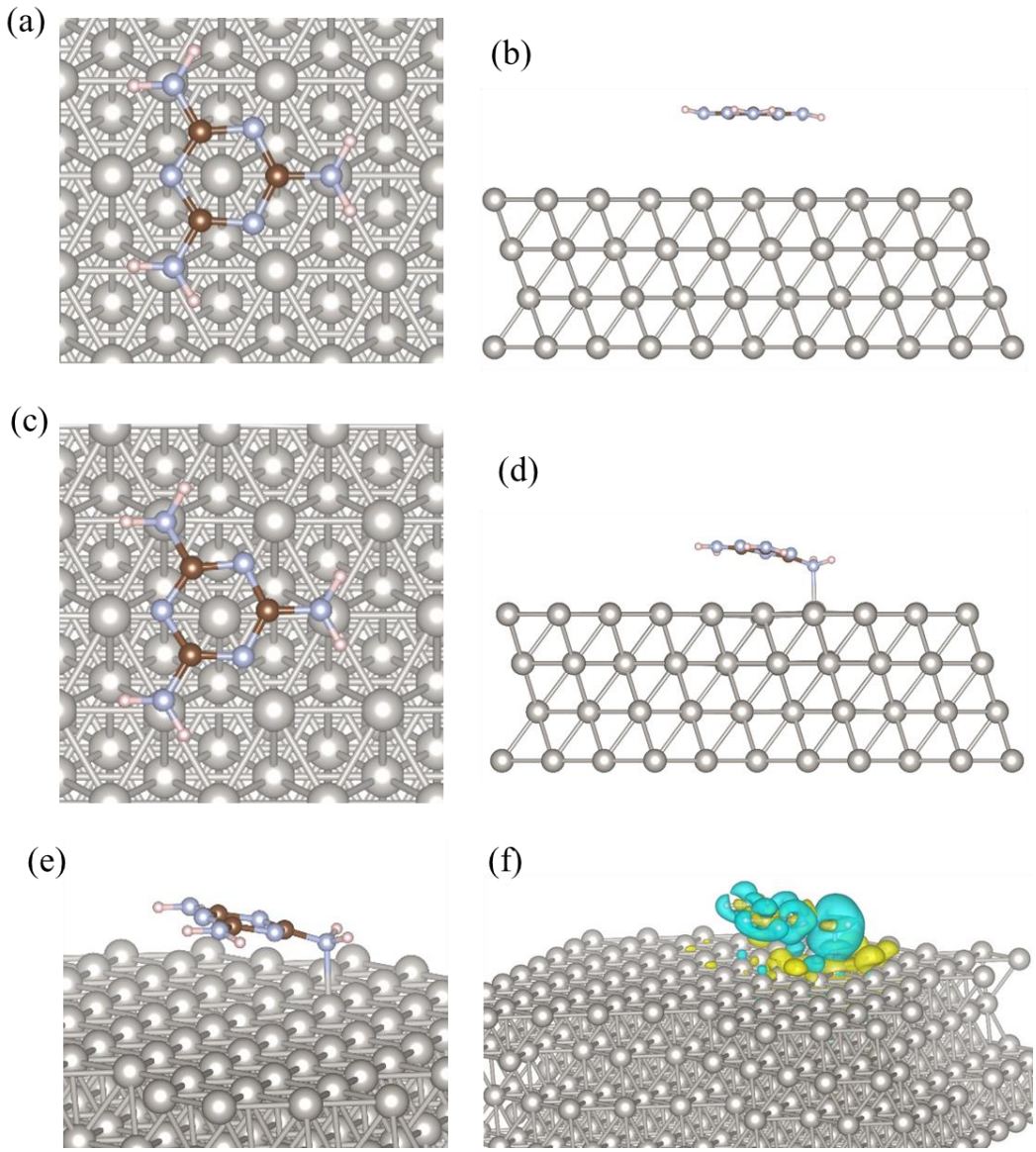

Figure S46. (a) Top and (b) side views of entry 24. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 24. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^3. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

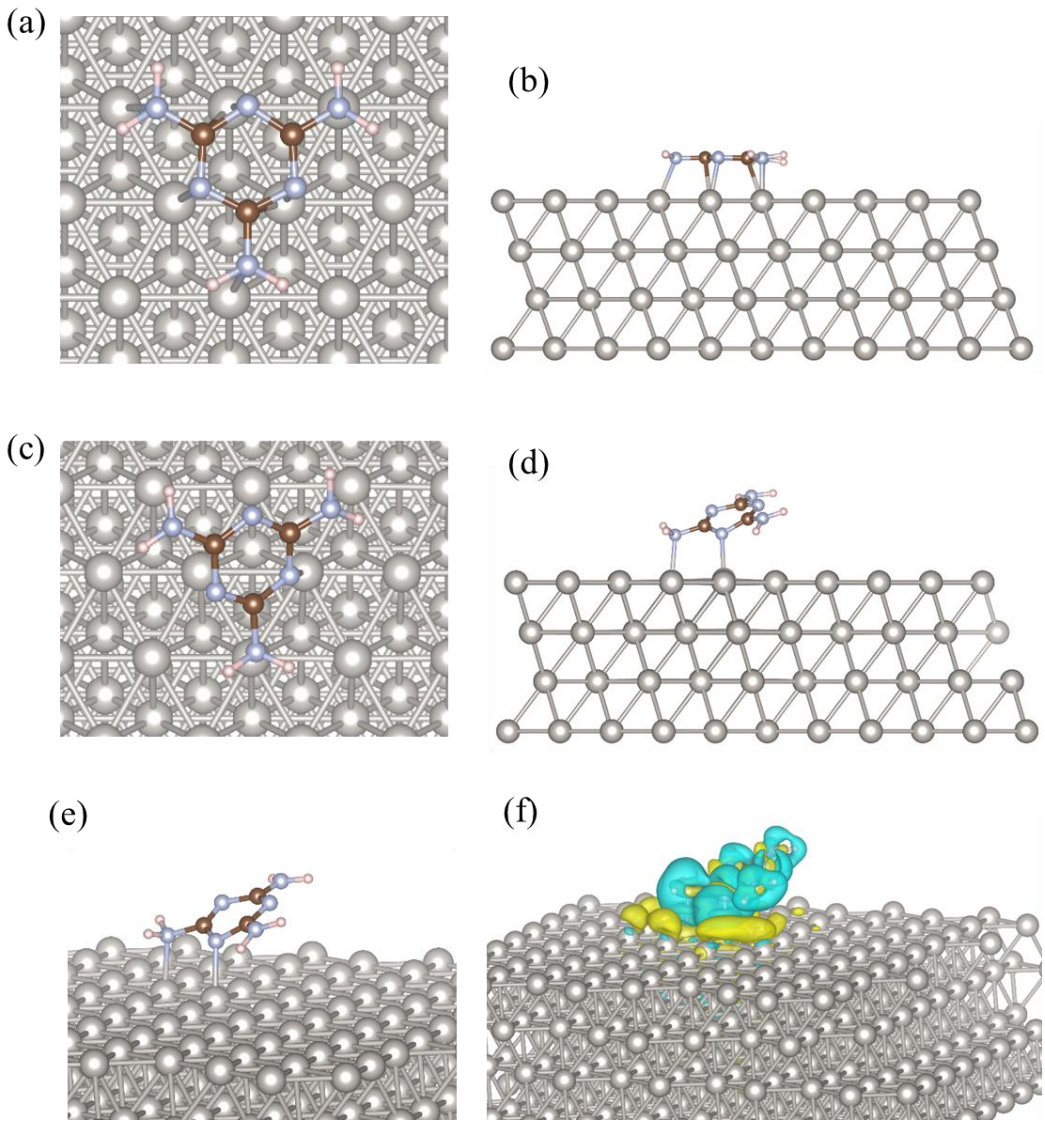

Figure S47. (a) Top and (b) side views of entry 25. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 25. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^3. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

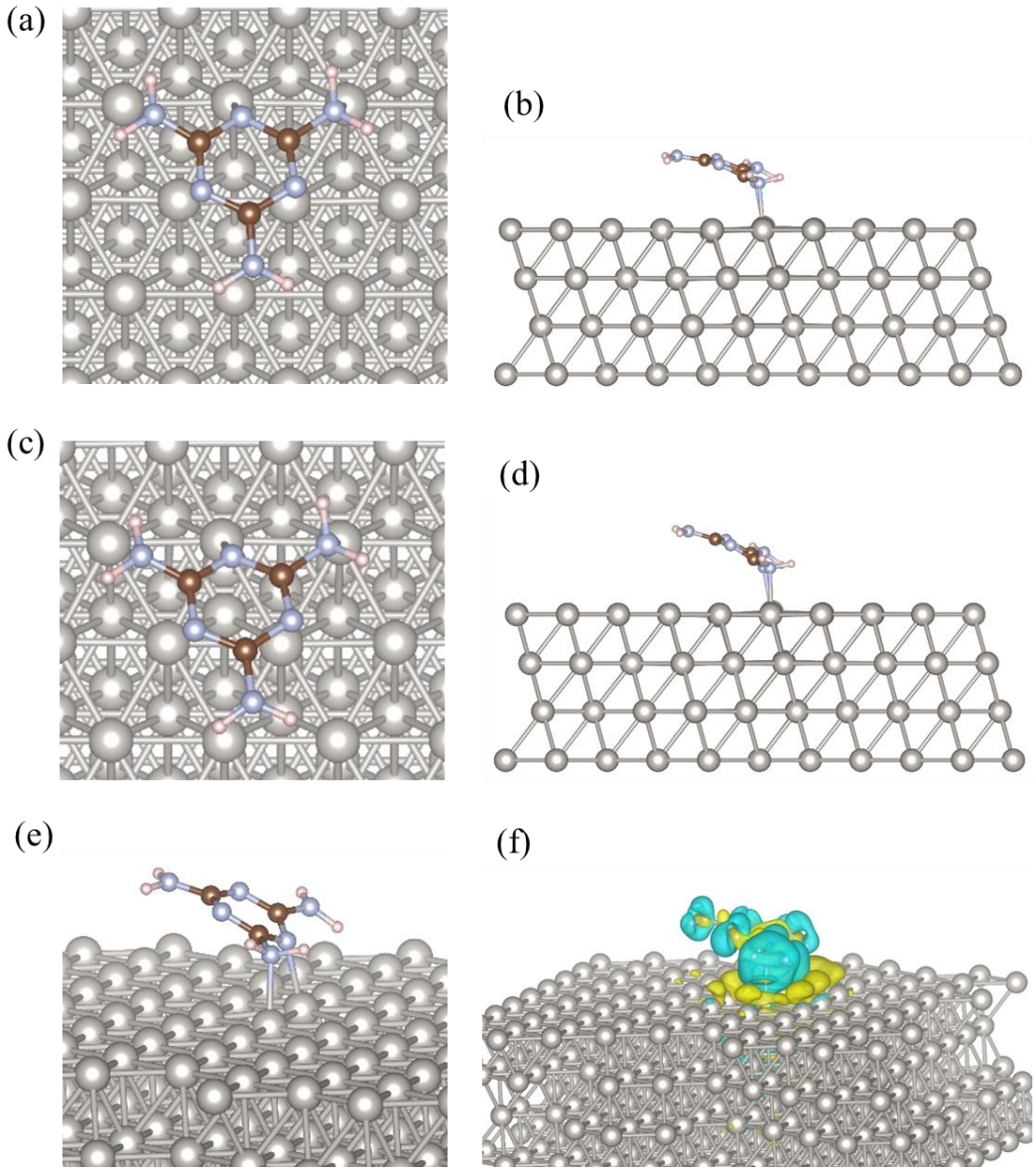

Figure S48. (a) Top and (b) side views of entry 26. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 26. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^{3}. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

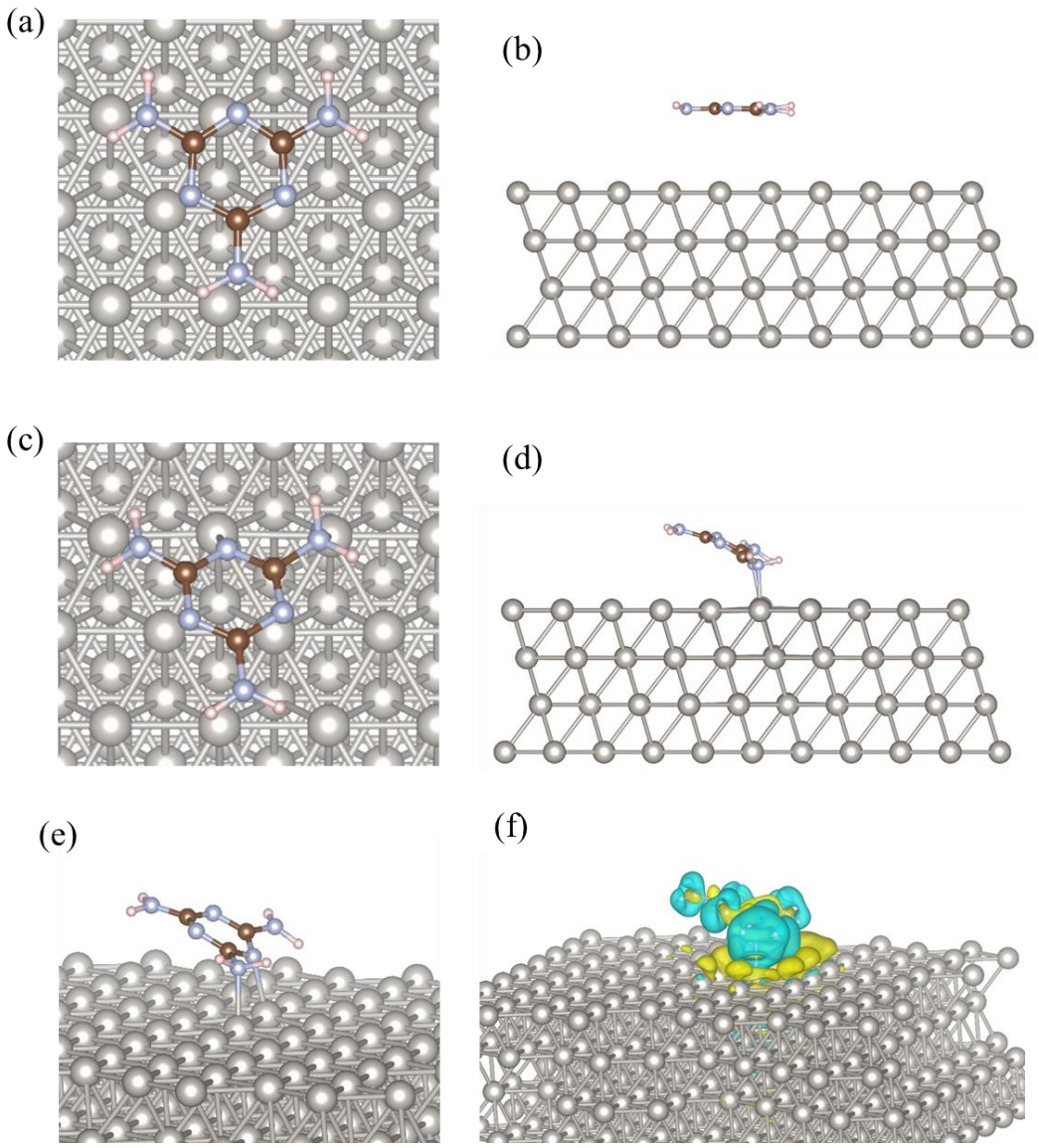

Figure S49. (a) Top and (b) side views of entry 27. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 27. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^3. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

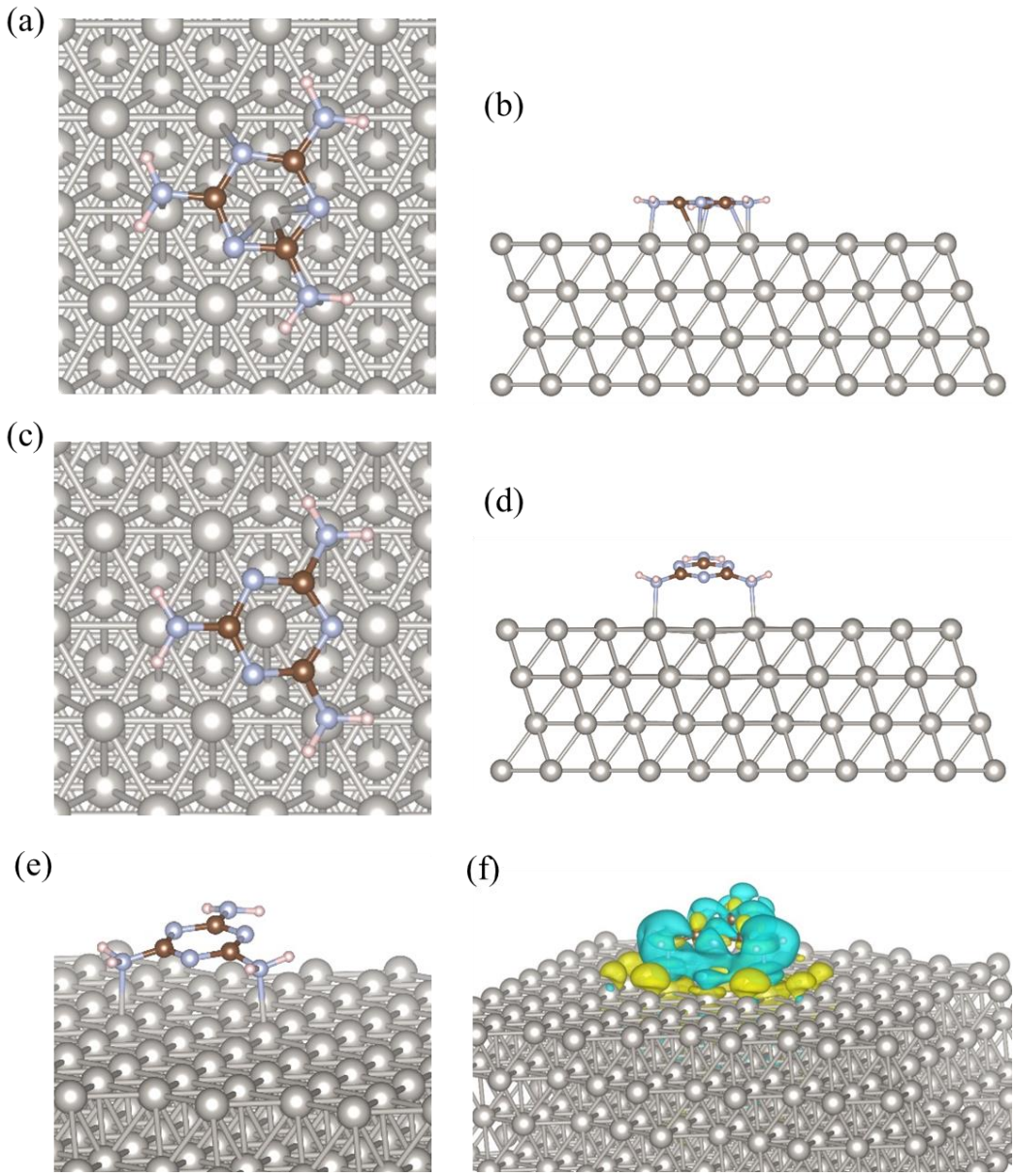

Figure S50. (a) Top and (b) side views of entry 28. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 28. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^3. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

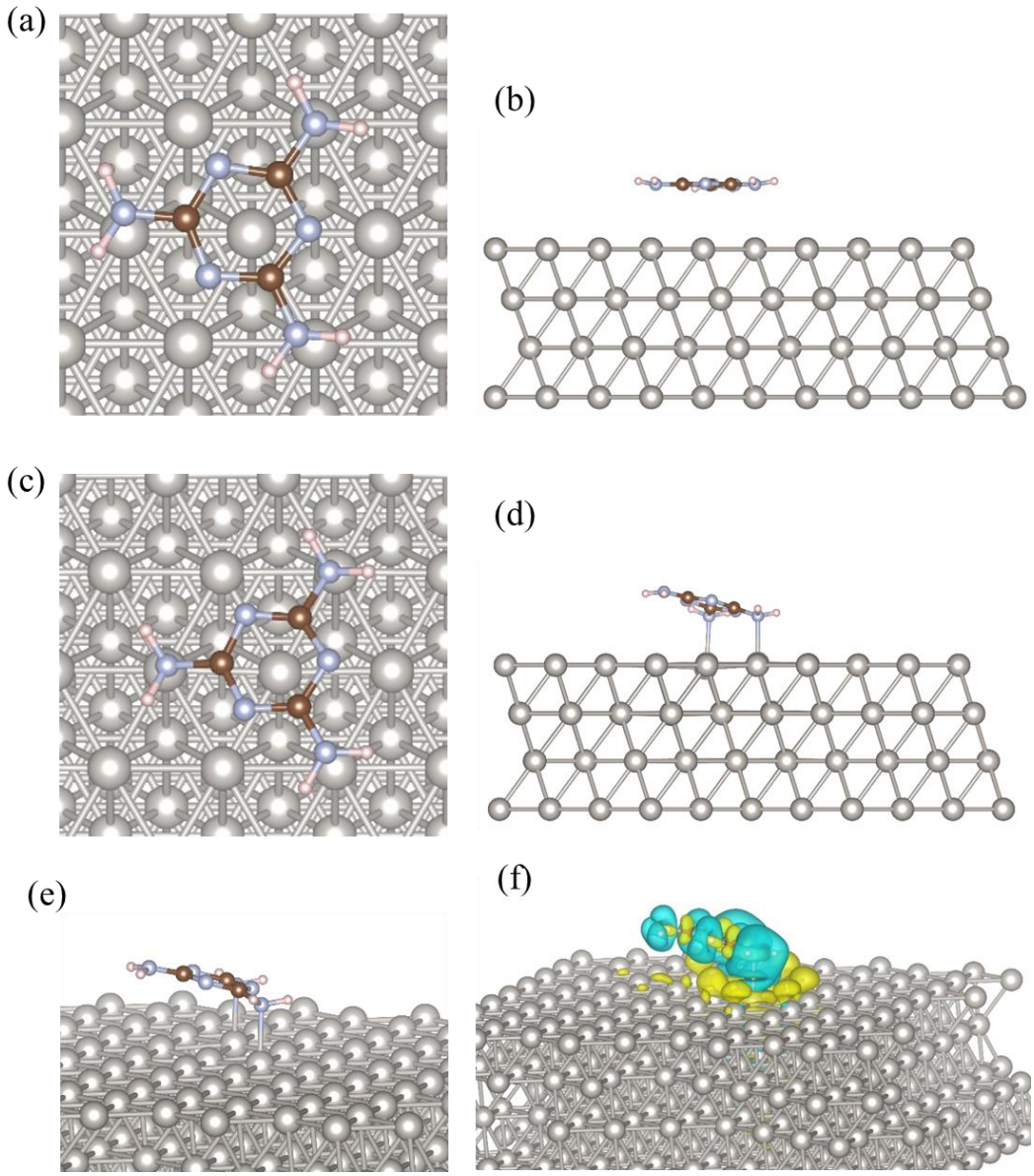

Figure S51. (a) Top and (b) side views of entry 29. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 29. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^3. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

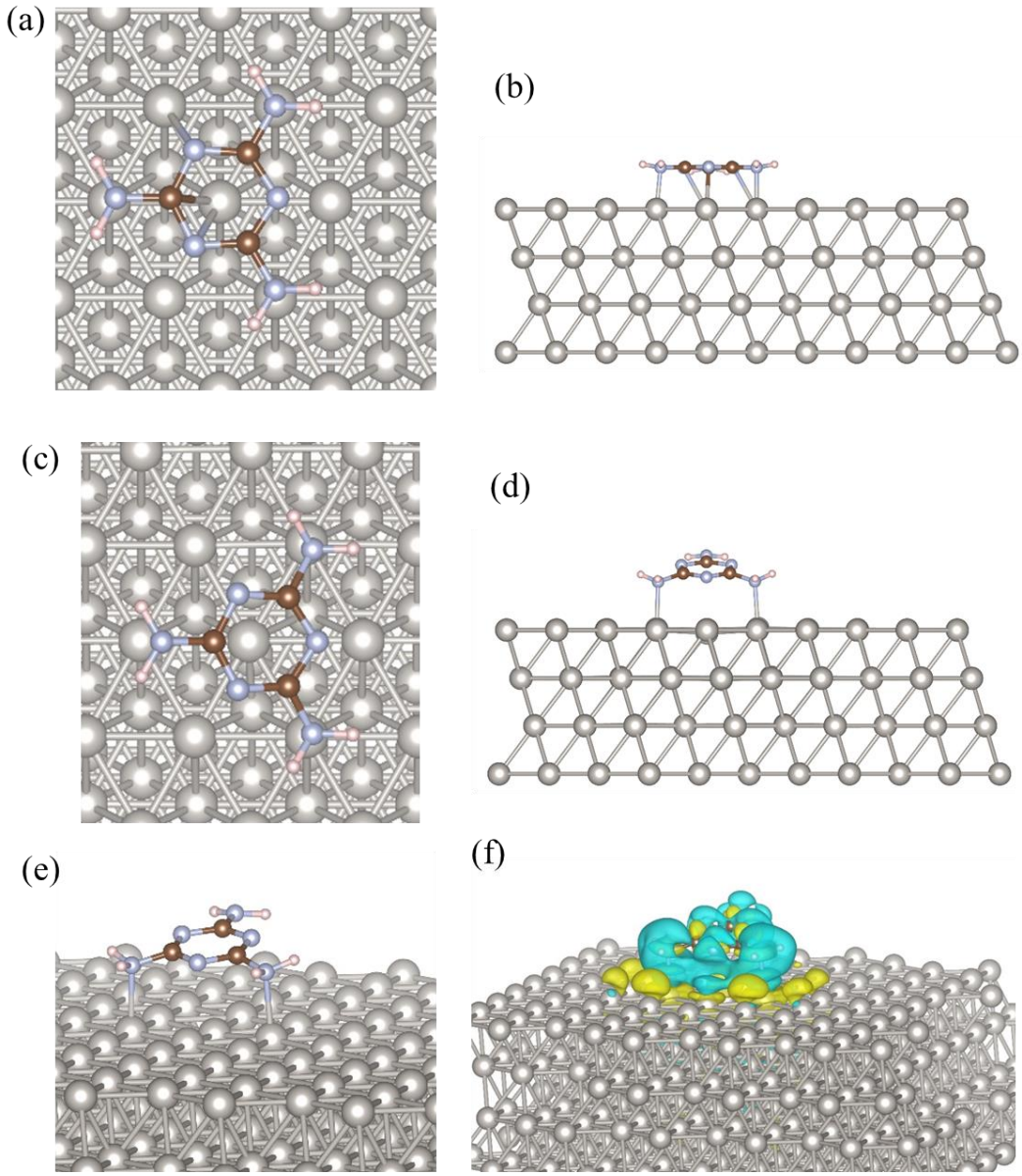

Figure S52. (a) Top and (b) side views of entry 30. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 30. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^3. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

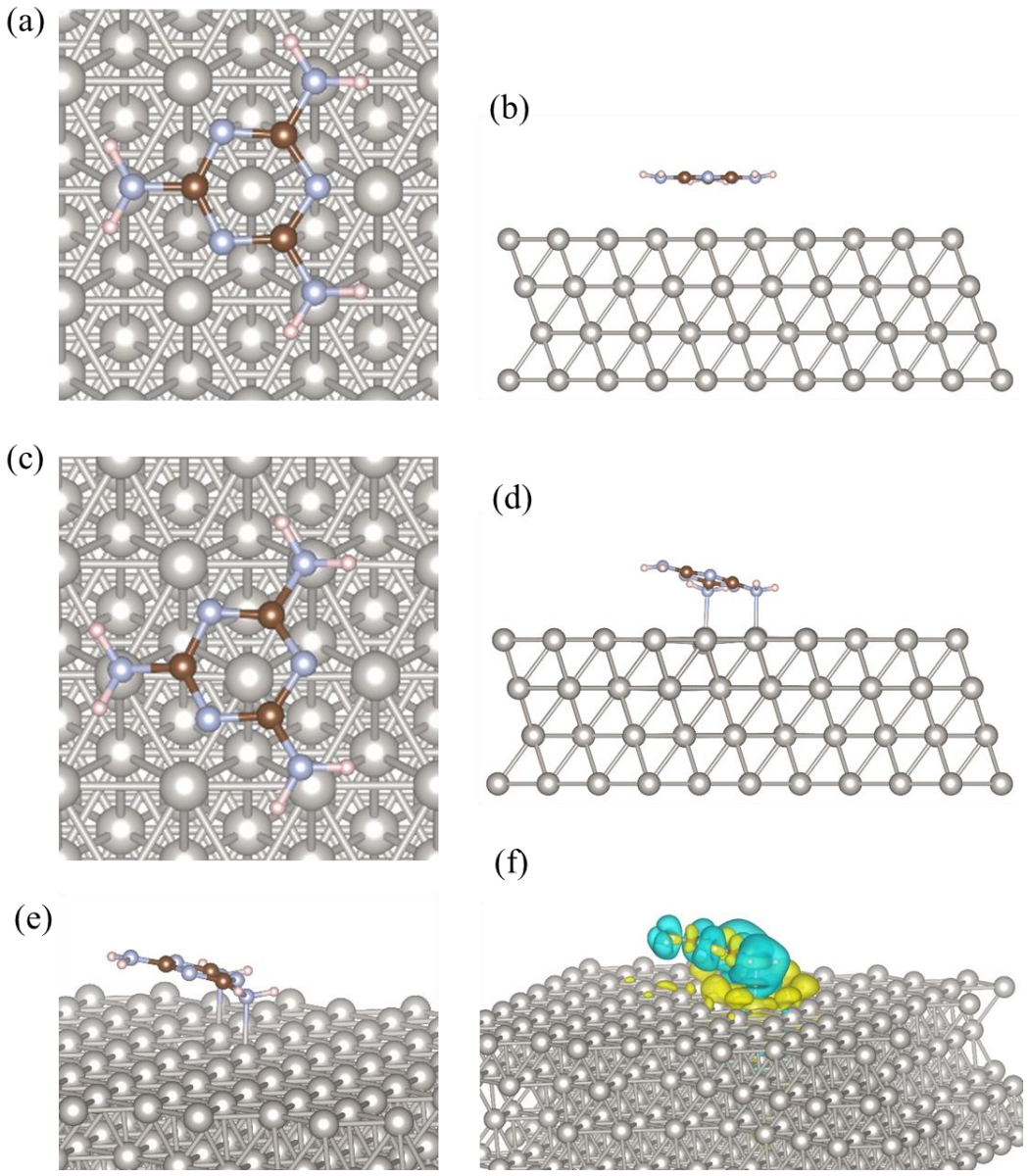

Figure S53. (a) Top and (b) side views of entry 31. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 31. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^3. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

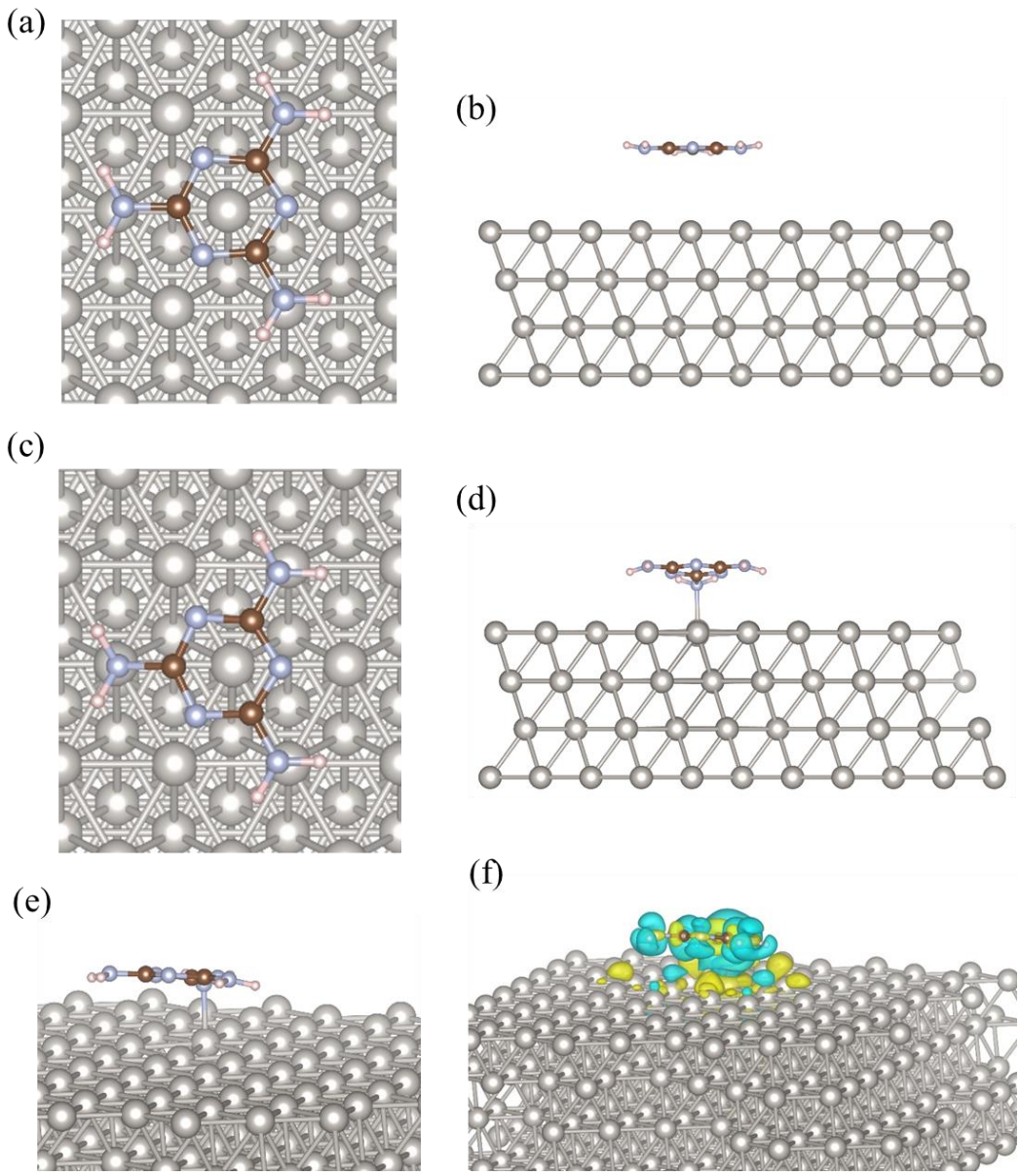

Figure S54. (a) Top and (b) side views of entry 32. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 32. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e–/Bohr3. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

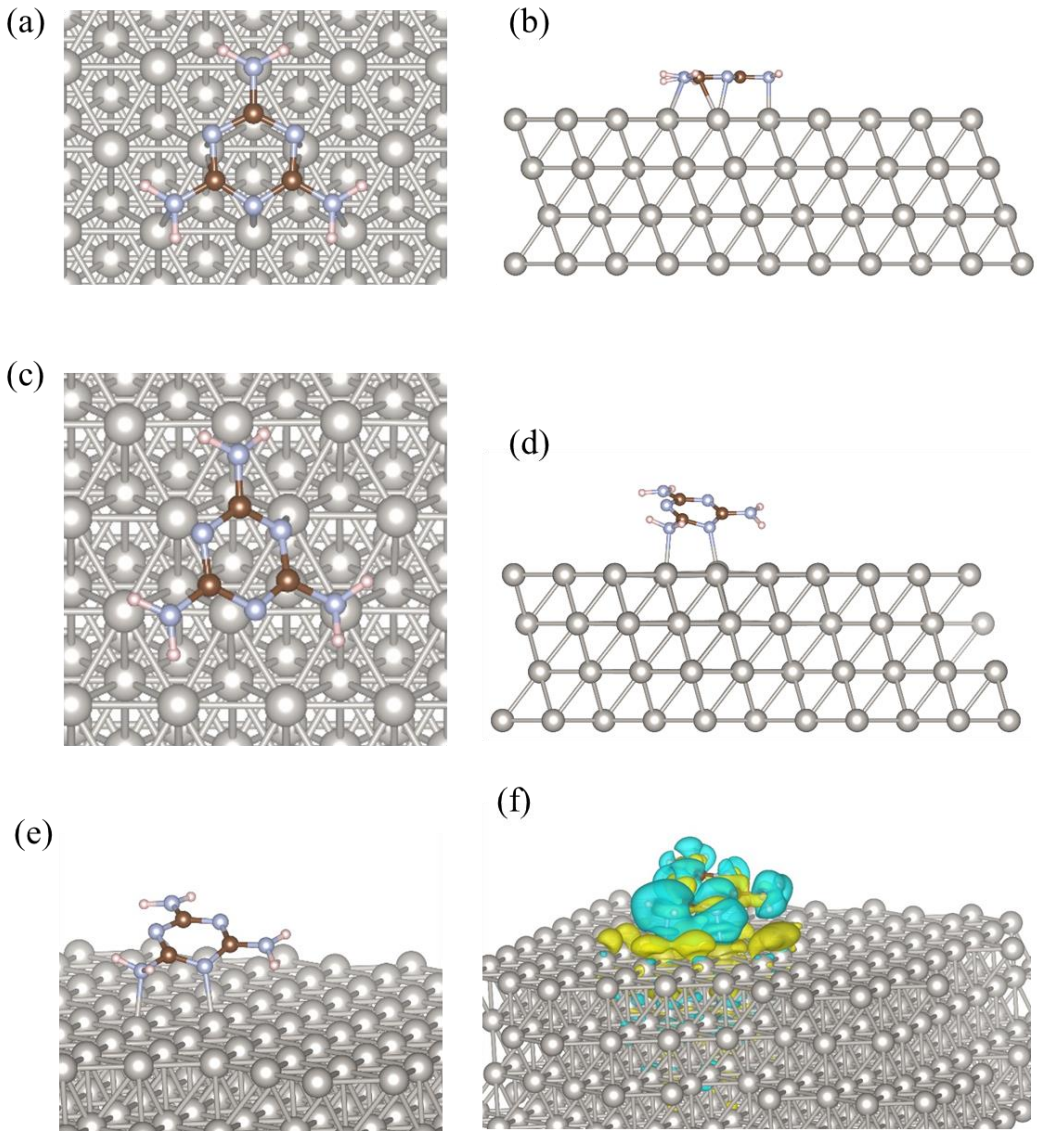

Figure S55. (a) Top and (b) side views of entry 33. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 33. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^{3}. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

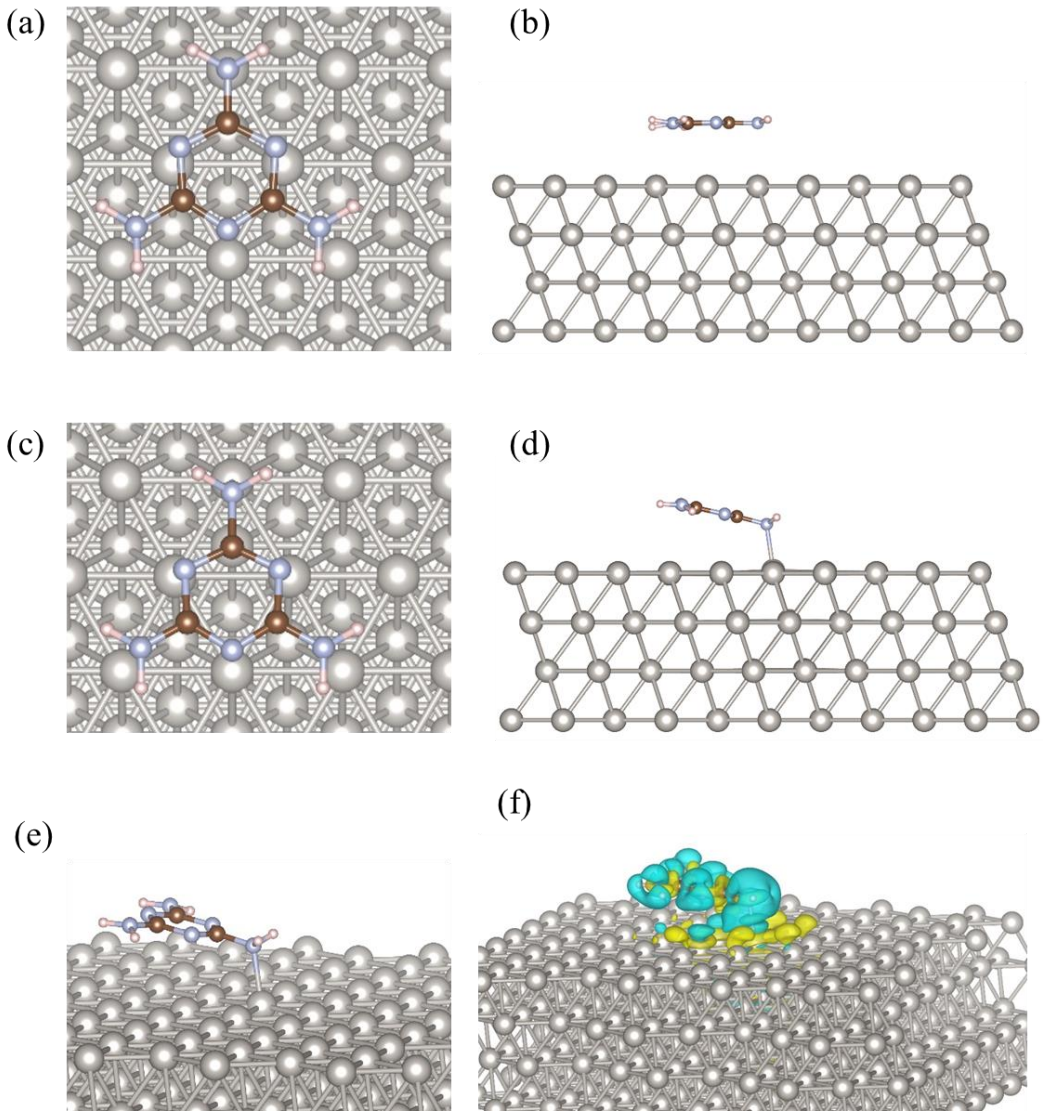

Figure S56. (a) Top and (b) side views of entry 34. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 34. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^3. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

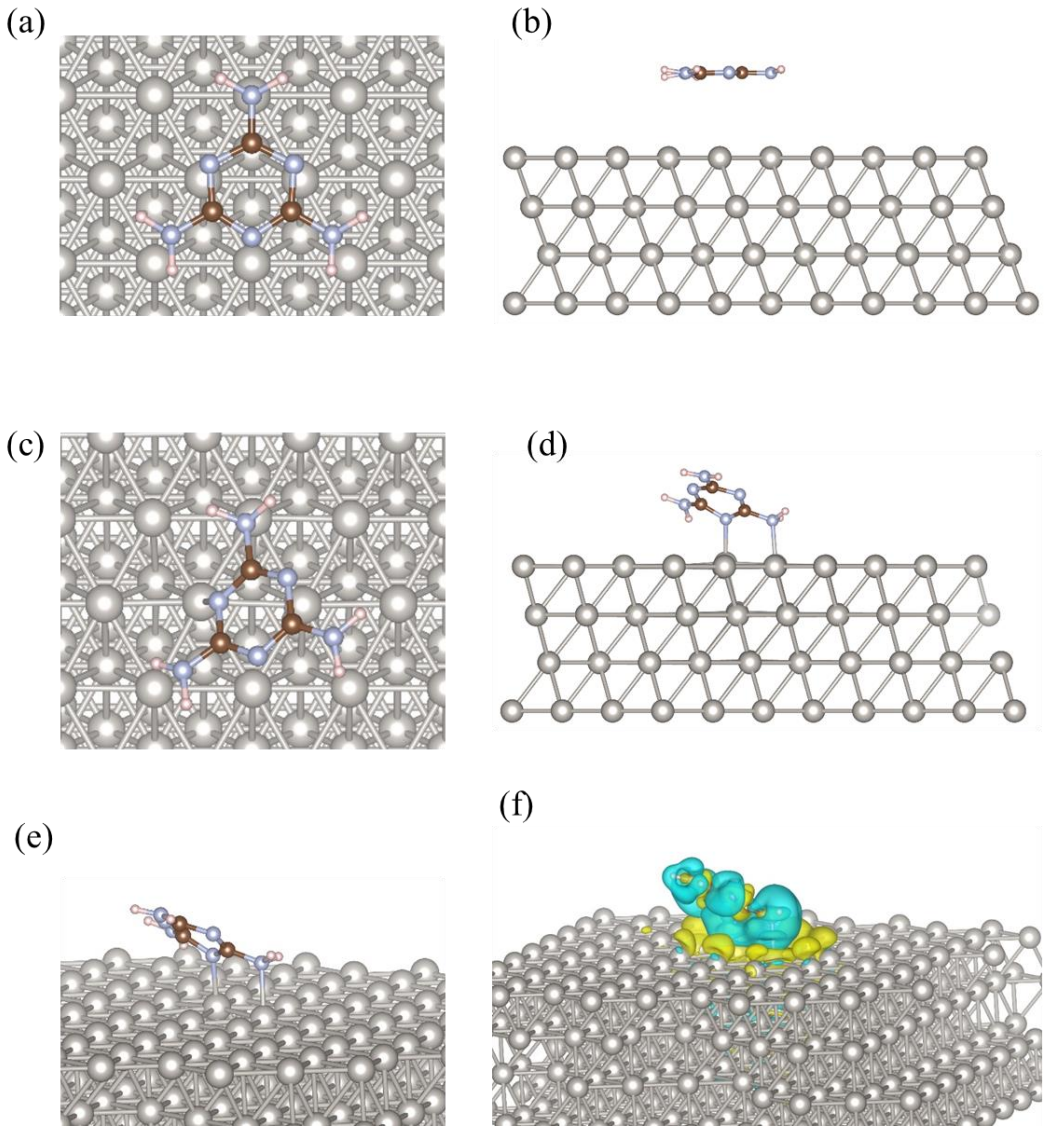

Figure S57. (a) Top and (b) side views of entry 35. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 35. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^3. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

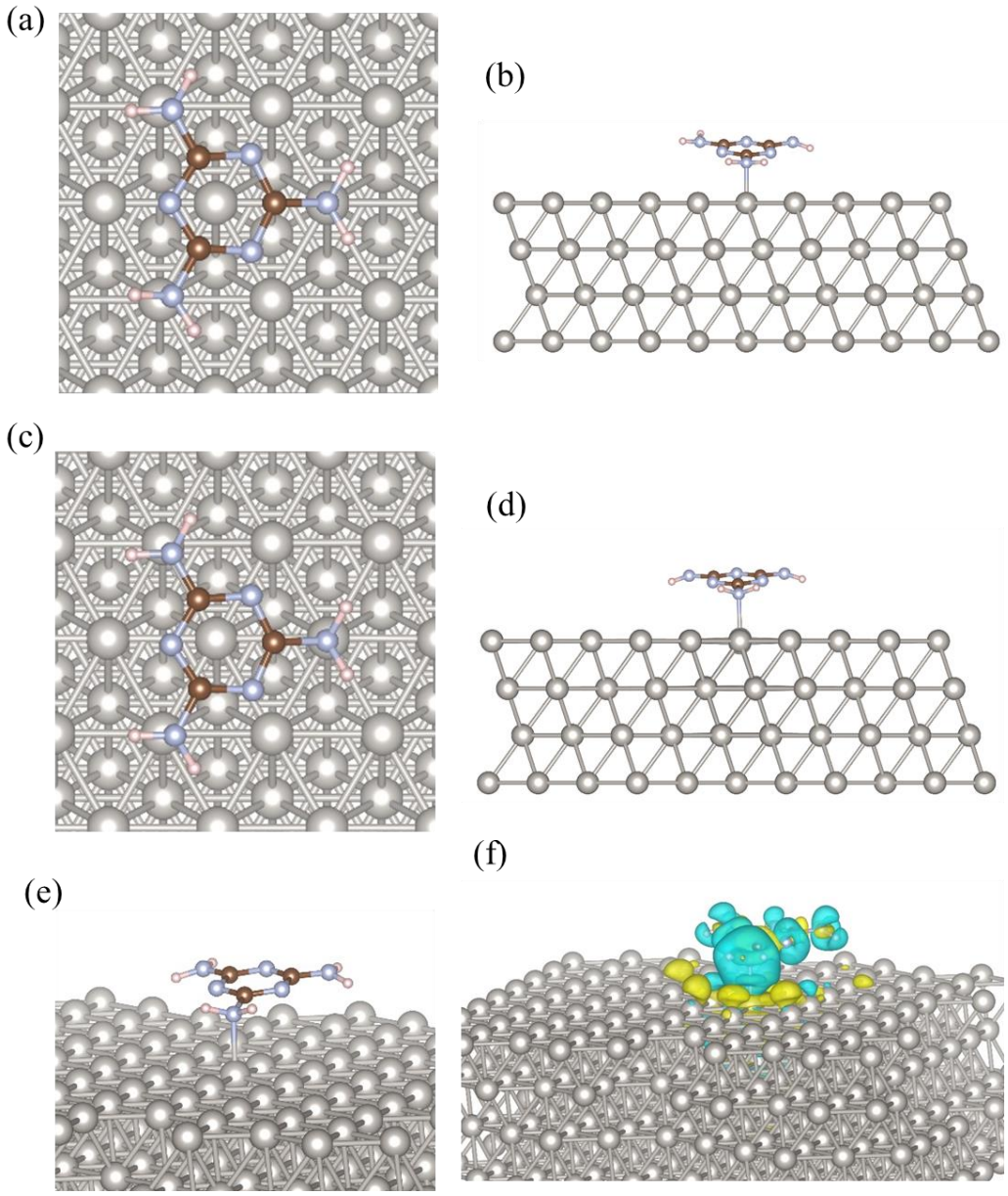

Figure S58. (a) Top and (b) side views of entry 36. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 36. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^3. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

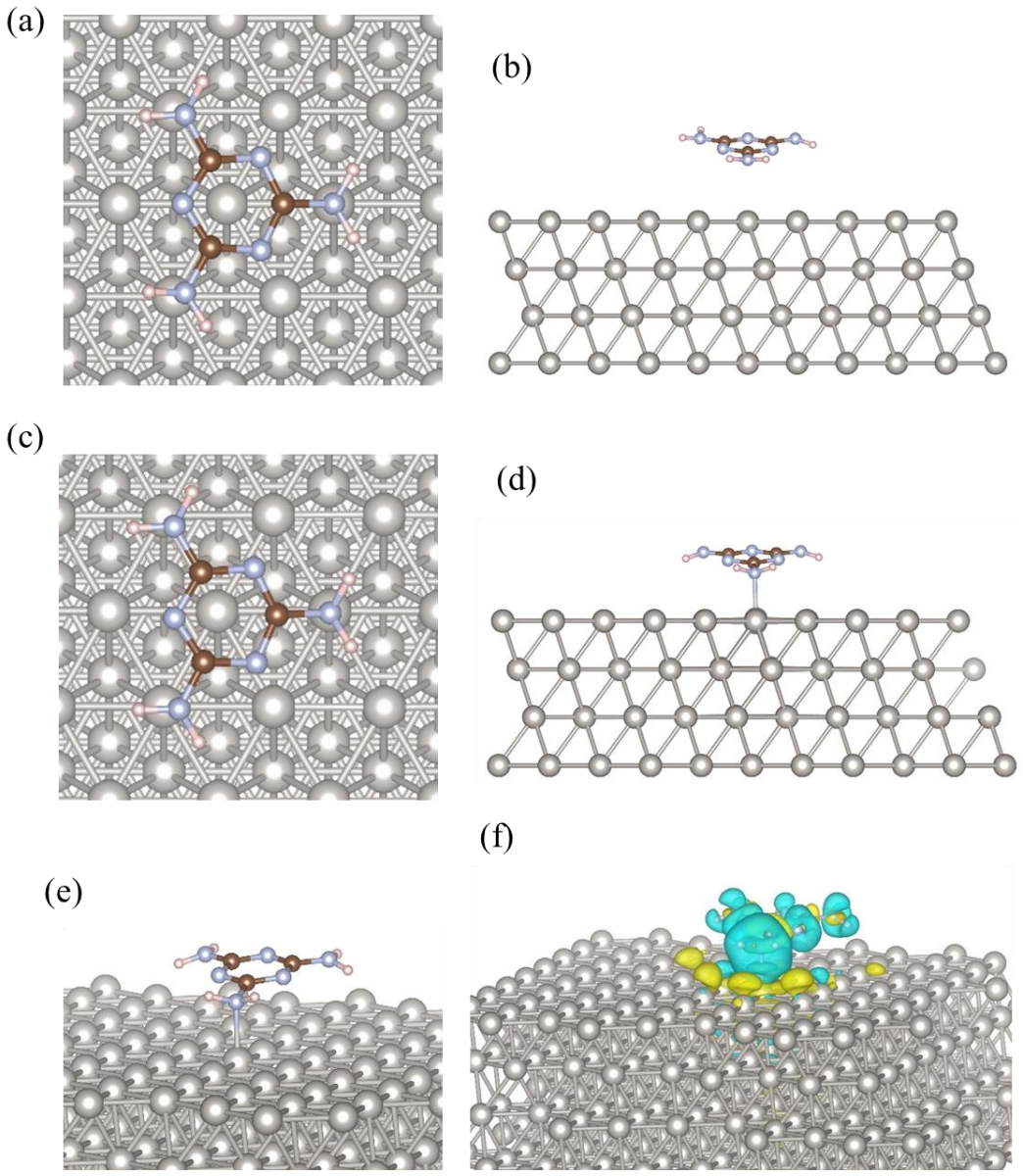

Figure S59. (a) Top and (b) side views of entry 37. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 37. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^3. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

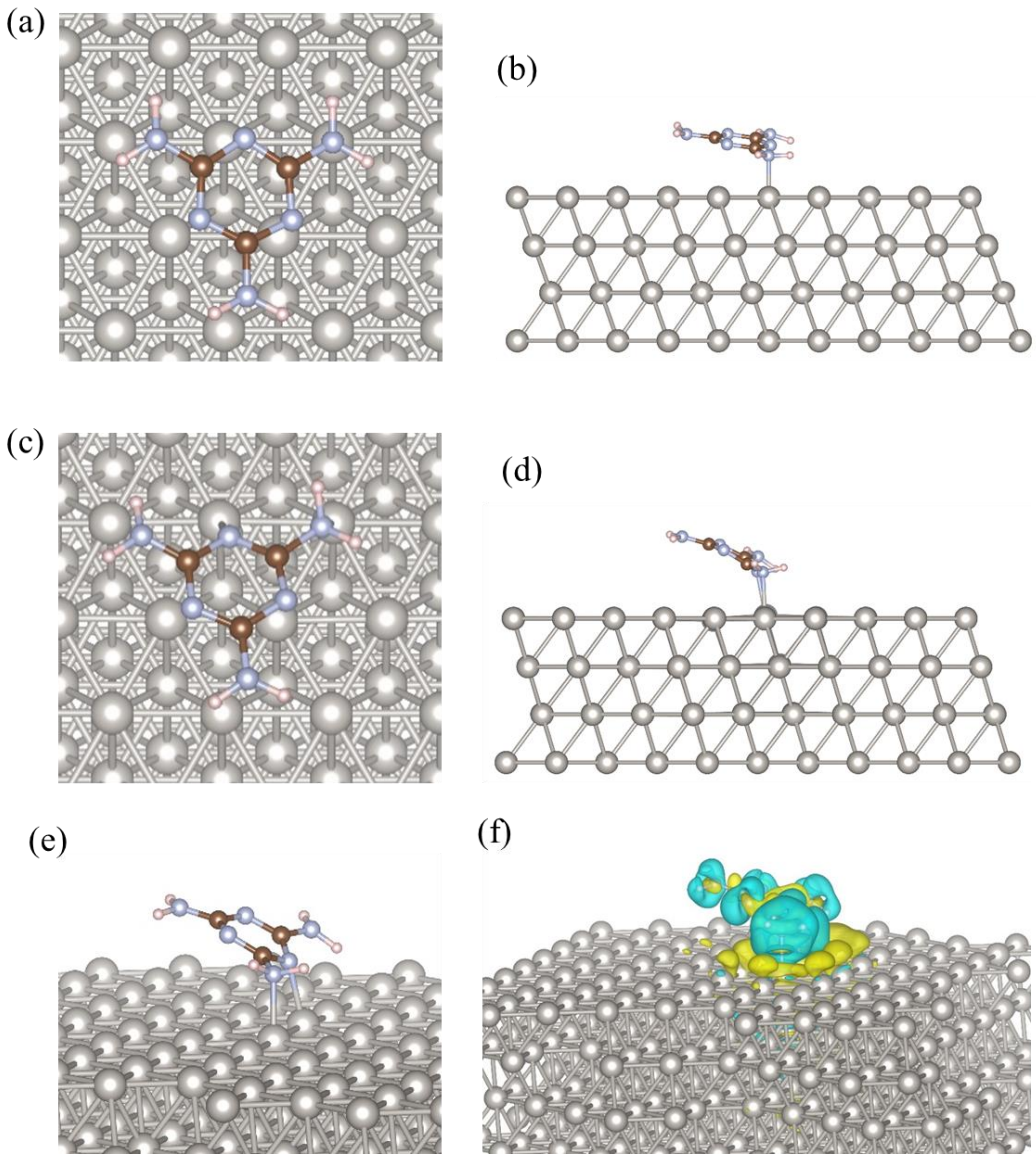

Figure S60. (a) Top and (b) side views of entry 38. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 38. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^3. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

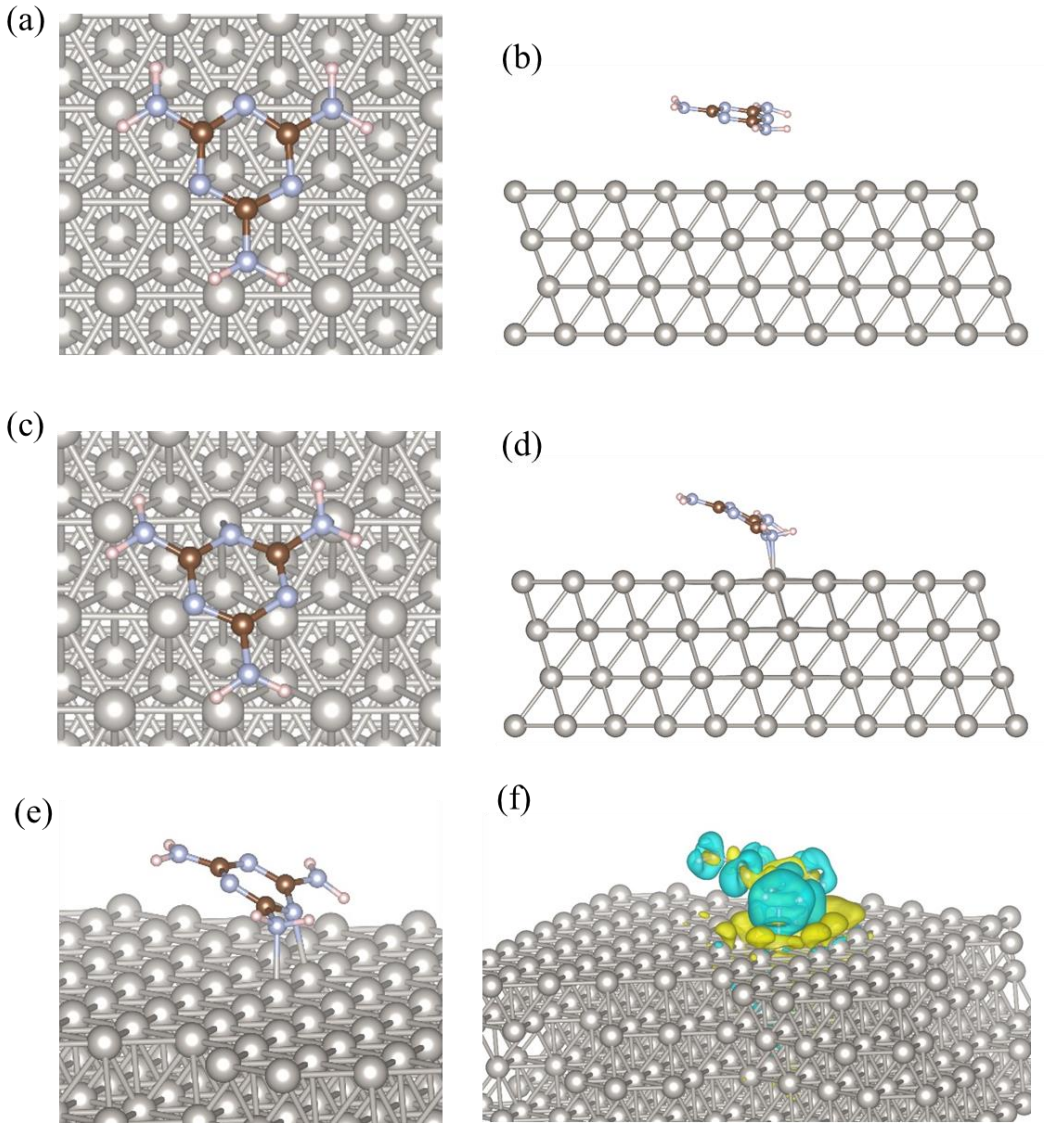

Figure S61. (a) Top and (b) side views of entry 39. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 39. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^3. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

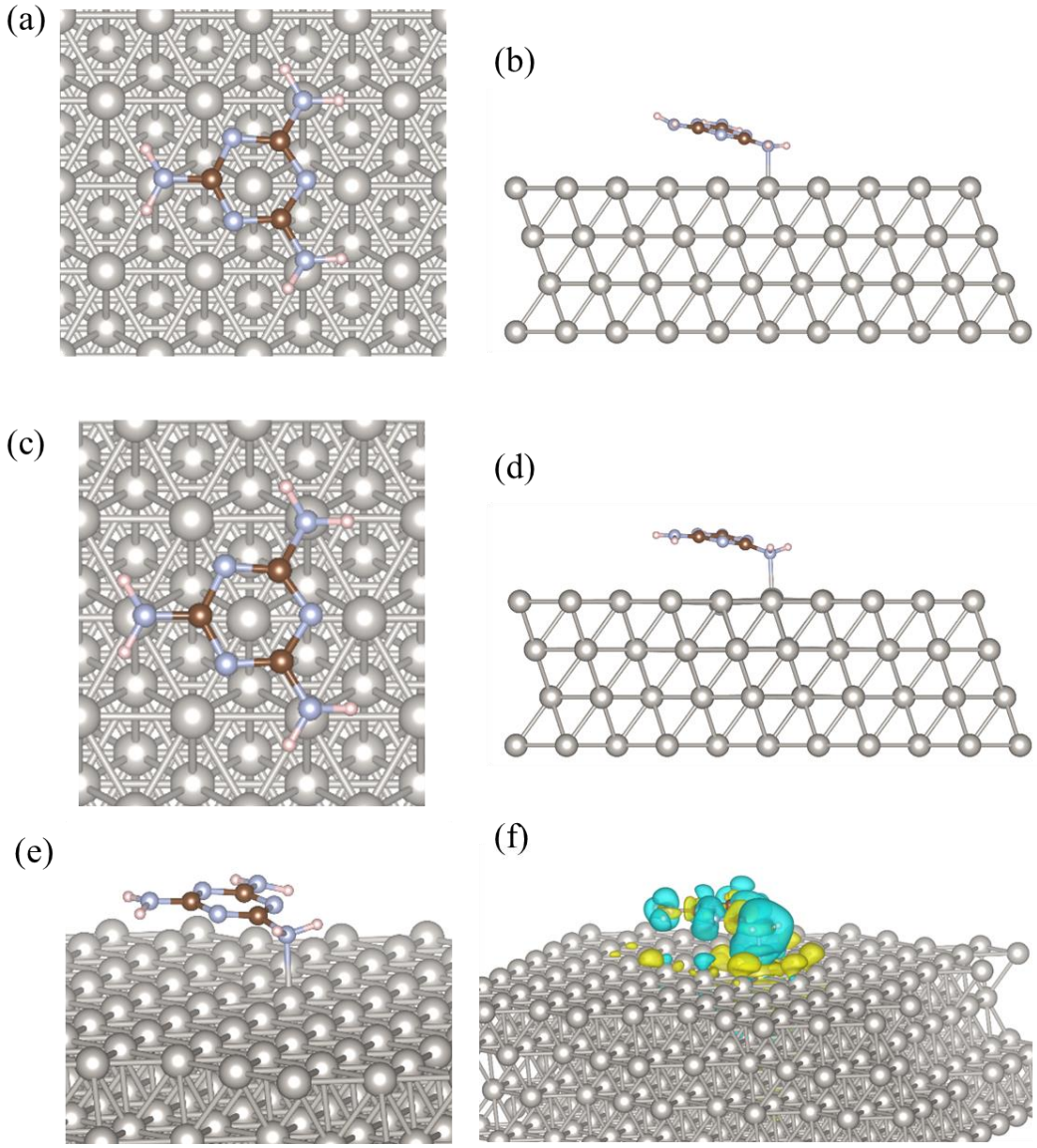

Figure S62. (a) Top and (b) side views of entry 40. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 40. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^{3}. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

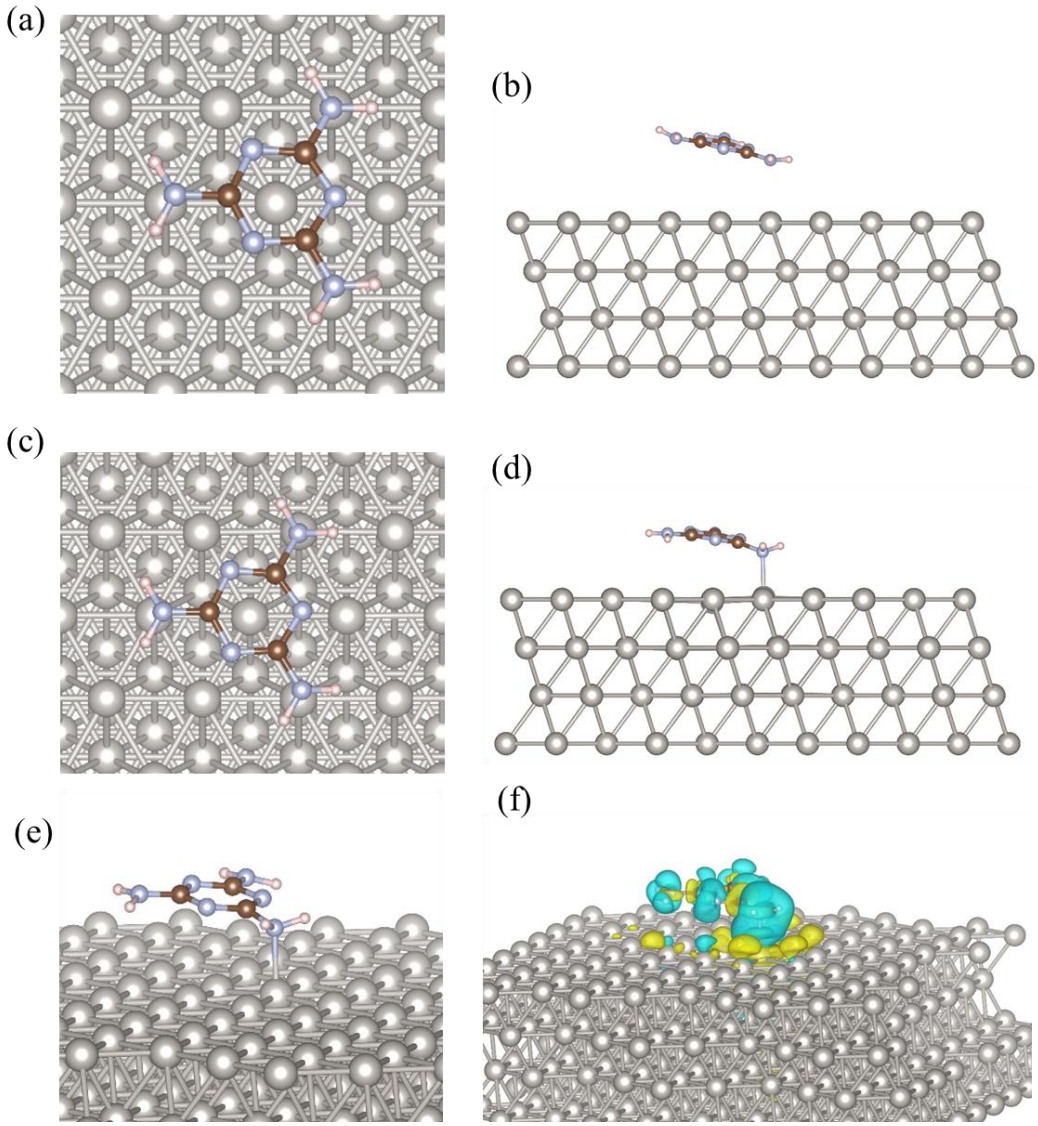

Figure S63. (a) Top and (b) side views of entry 41. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 41. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^3. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

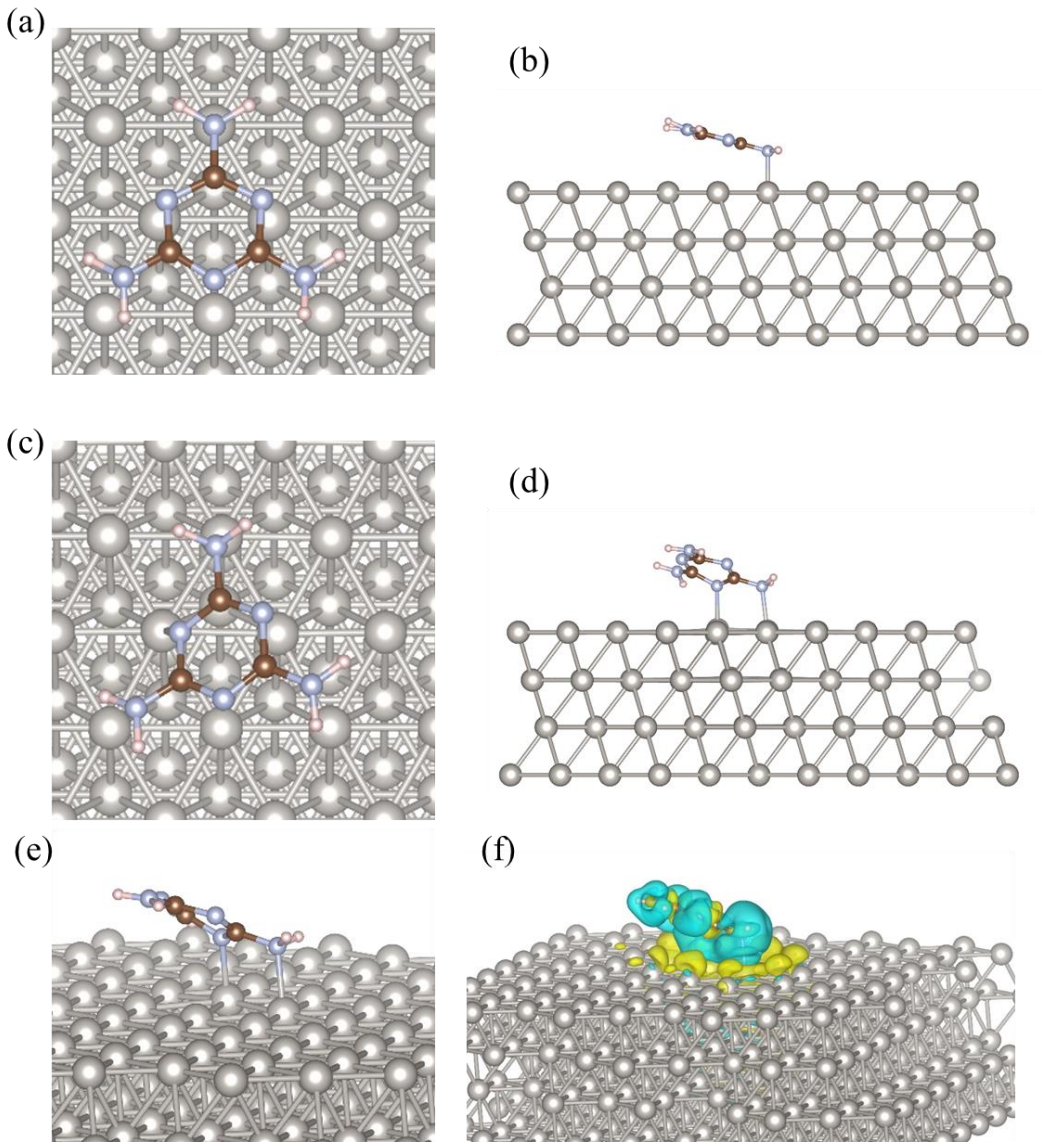

Figure S64. (a) Top and (b) side views of entry 42. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 42. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^{3}. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

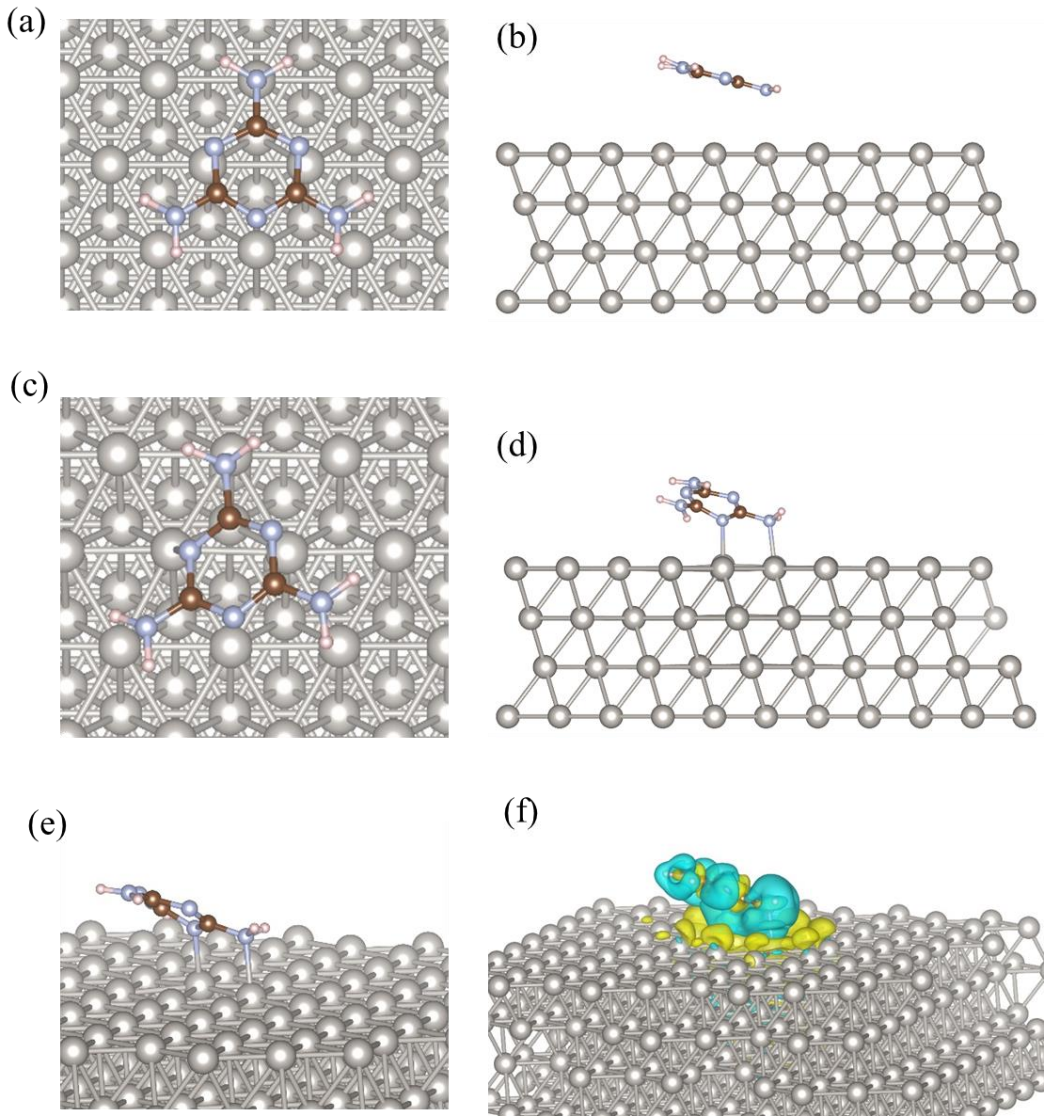

Figure S65. (a) Top and (b) side views of entry 43. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 43. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^3. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

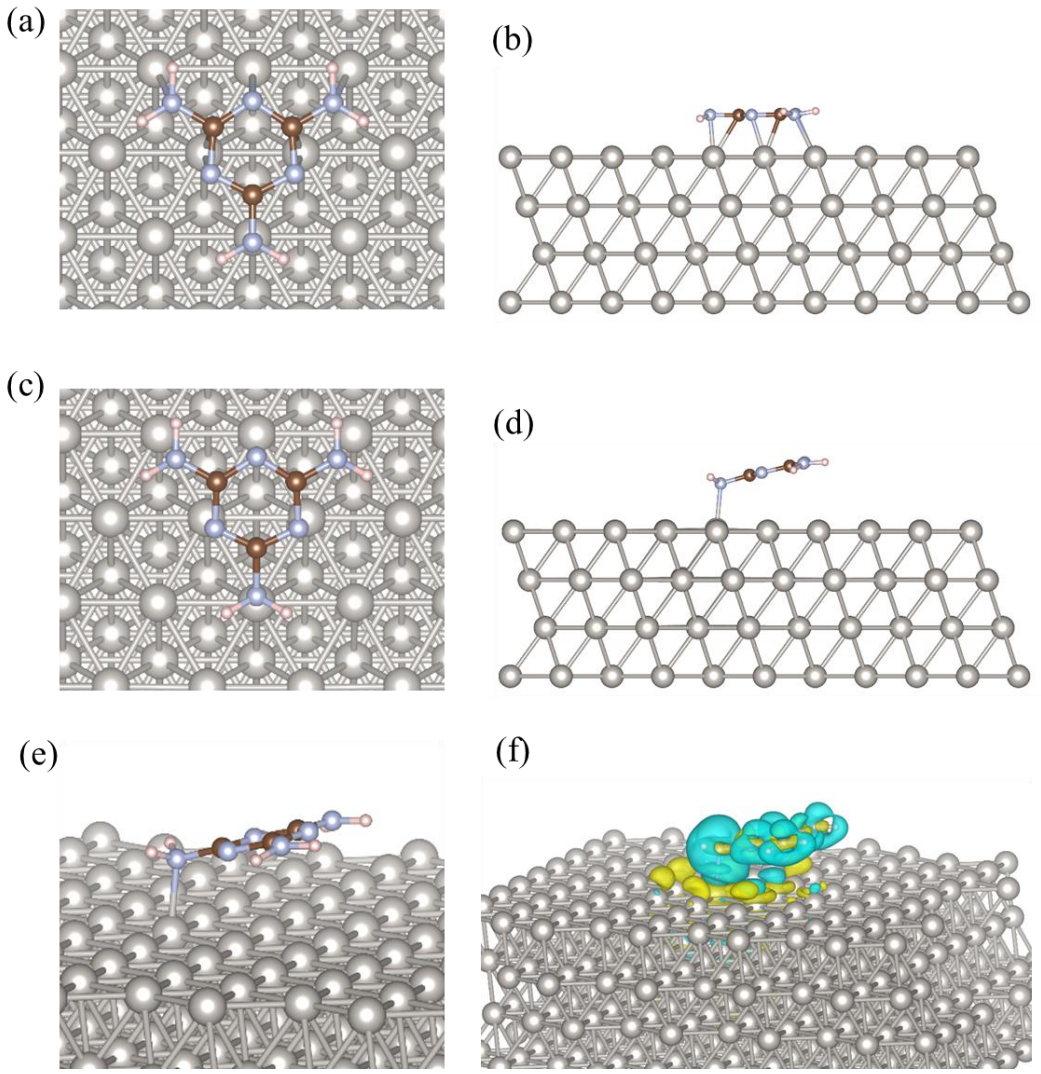

Figure S66. (a) Top and (b) side views of entry 44. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 44. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^3. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

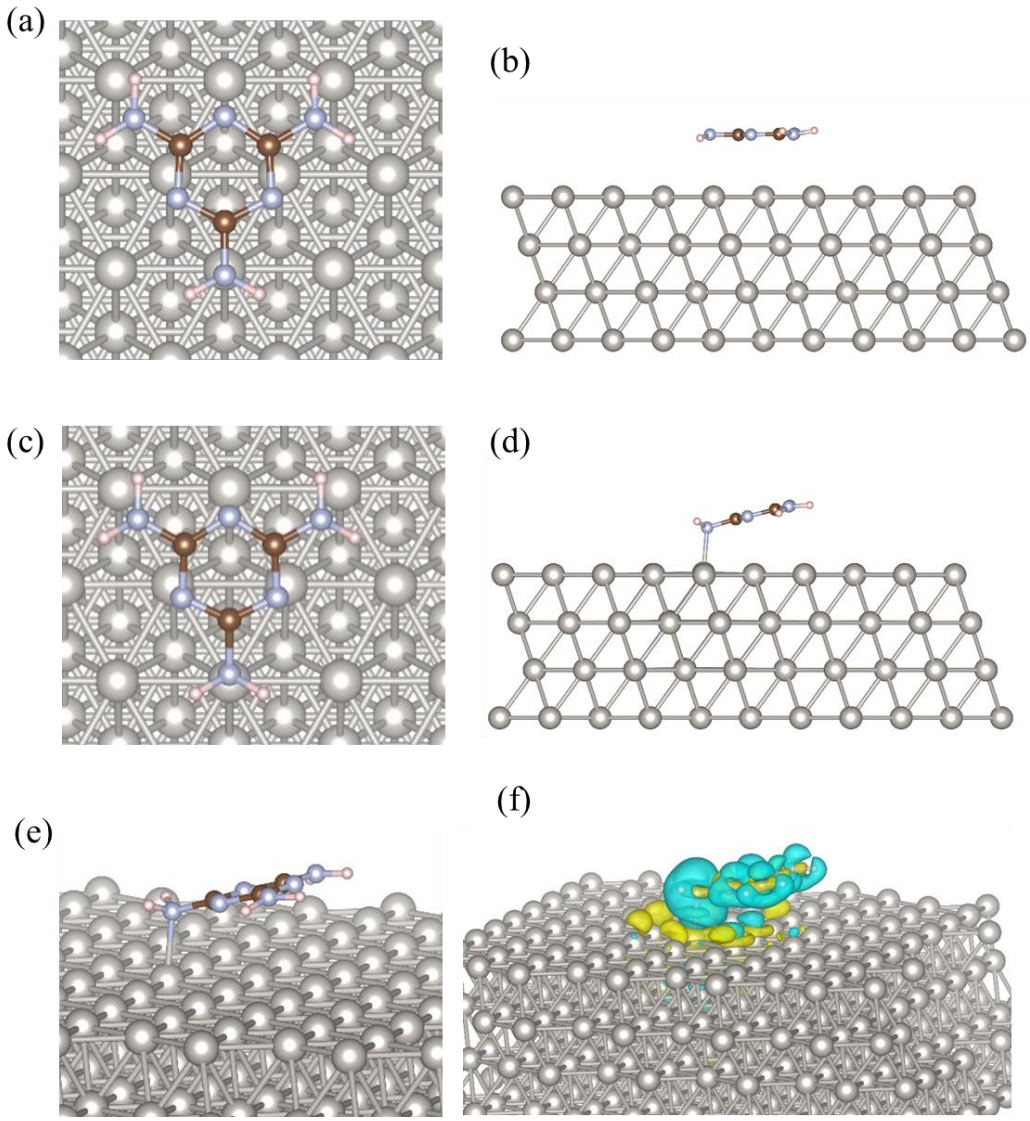

Figure S67. (a) Top and (b) side views of entry 45. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 45. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e–/Bohr^3. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

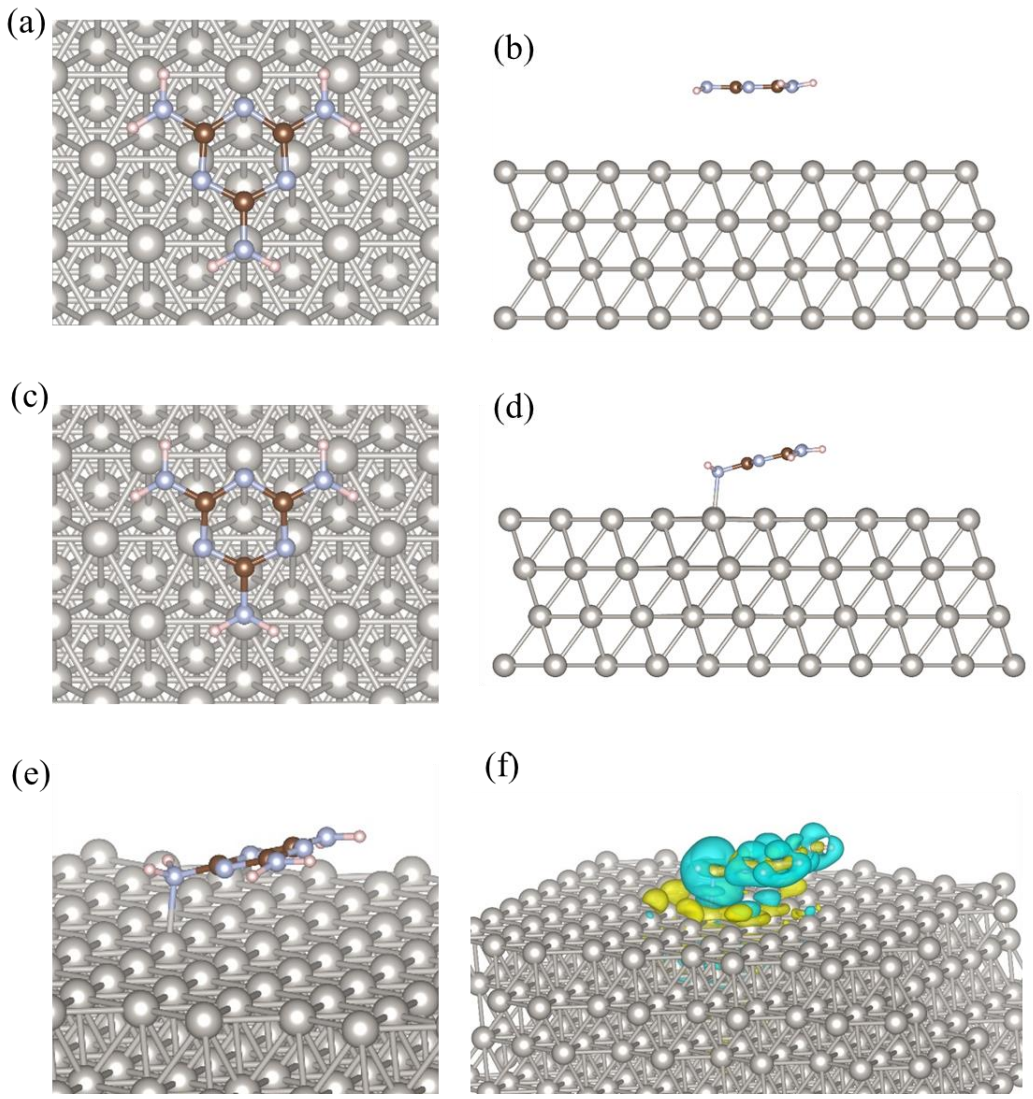

Figure S68. (a) Top and (b) side views of entry 46. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 46. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^3. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

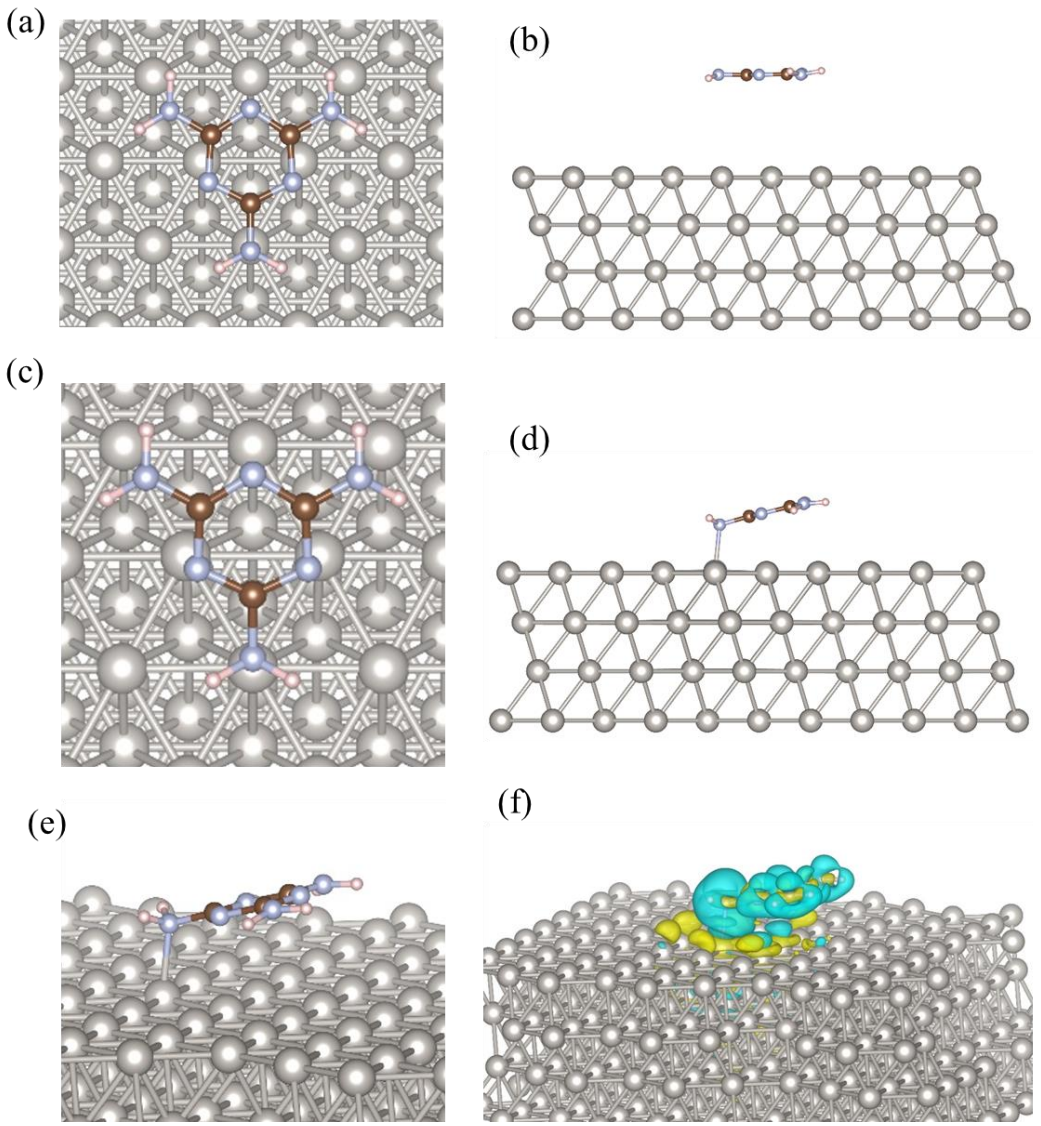

Figure S69. (a) Top and (b) side views of entry 47. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 47. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^3. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

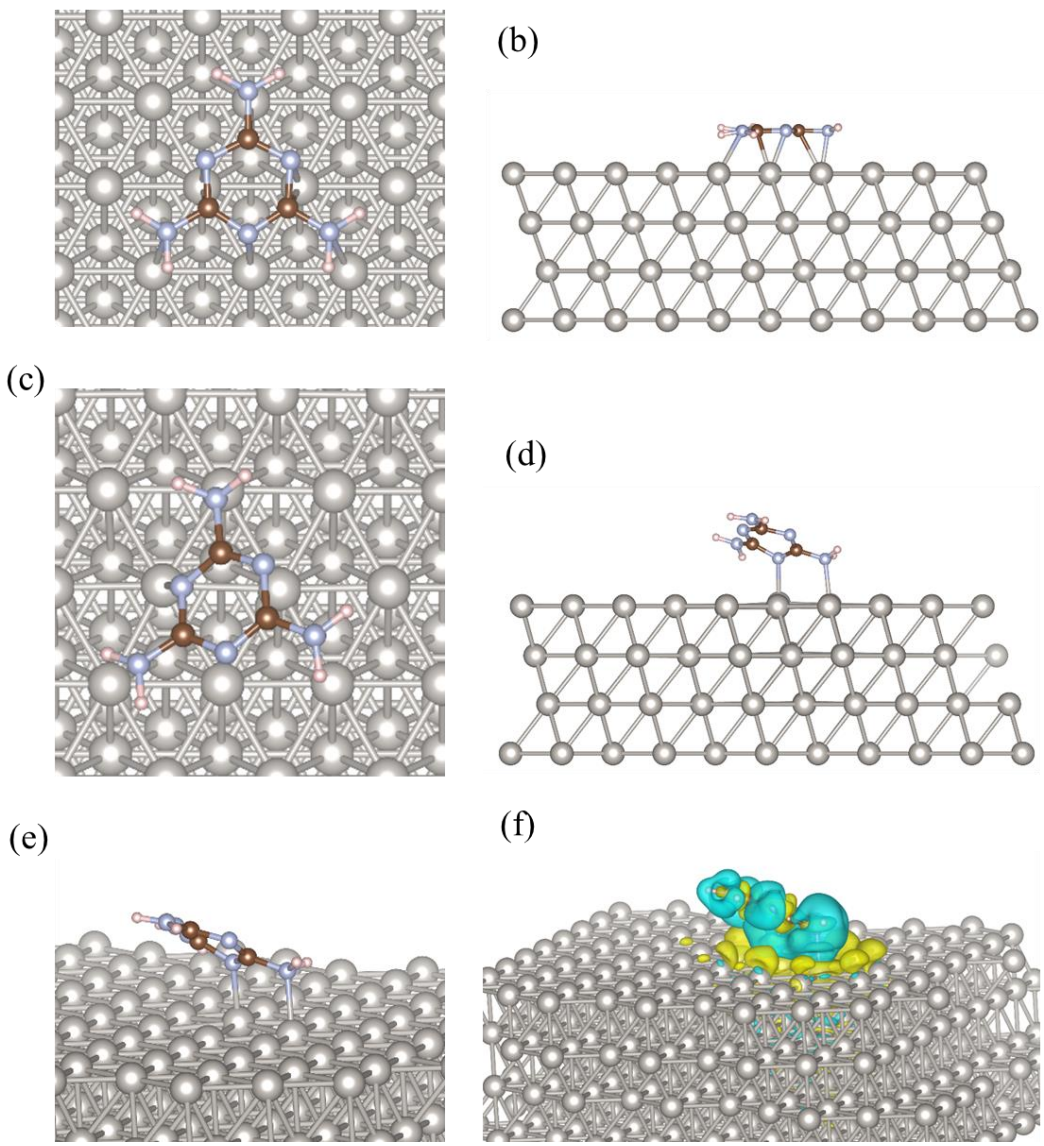

Figure S70. (a) Top and (b) side views of entry 48. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 48. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^3. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

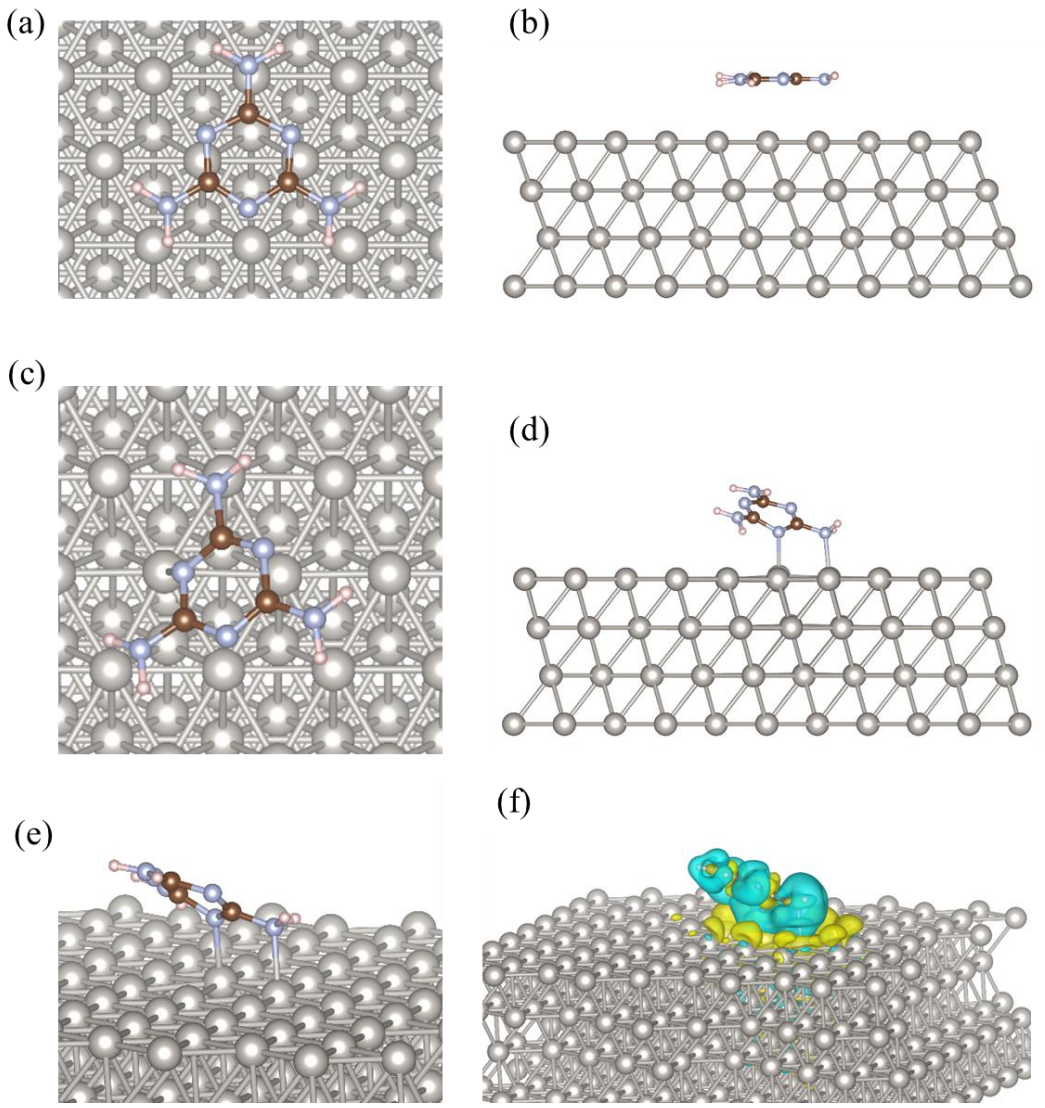

Figure S71. (a) Top and (b) side views of entry 49. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 49. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^3. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

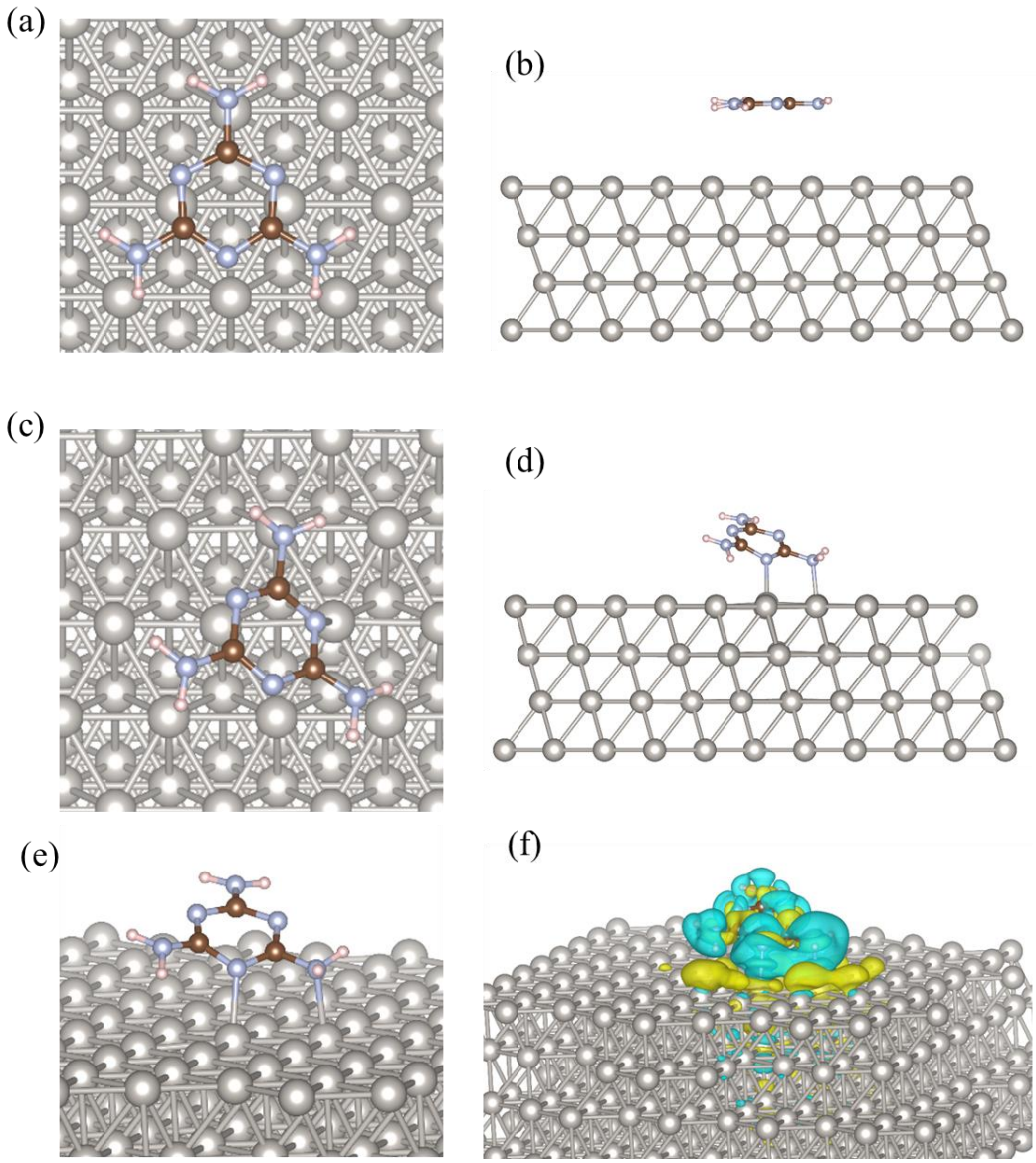

Figure S72. (a) Top and (b) side views of entry 50. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 50. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^3. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

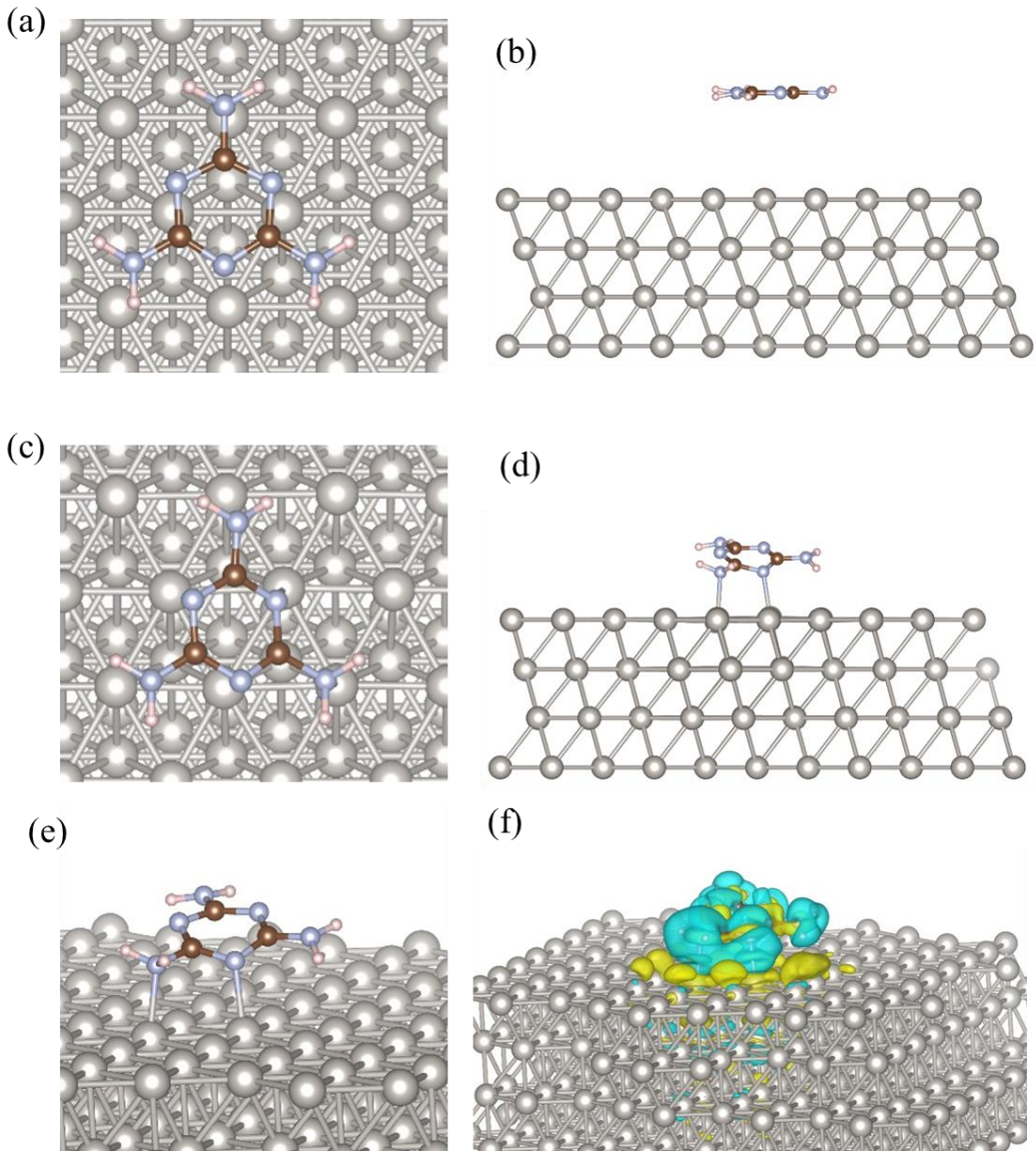

Figure S73. (a) Top and (b) side views of entry 51. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 51. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^{3}. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

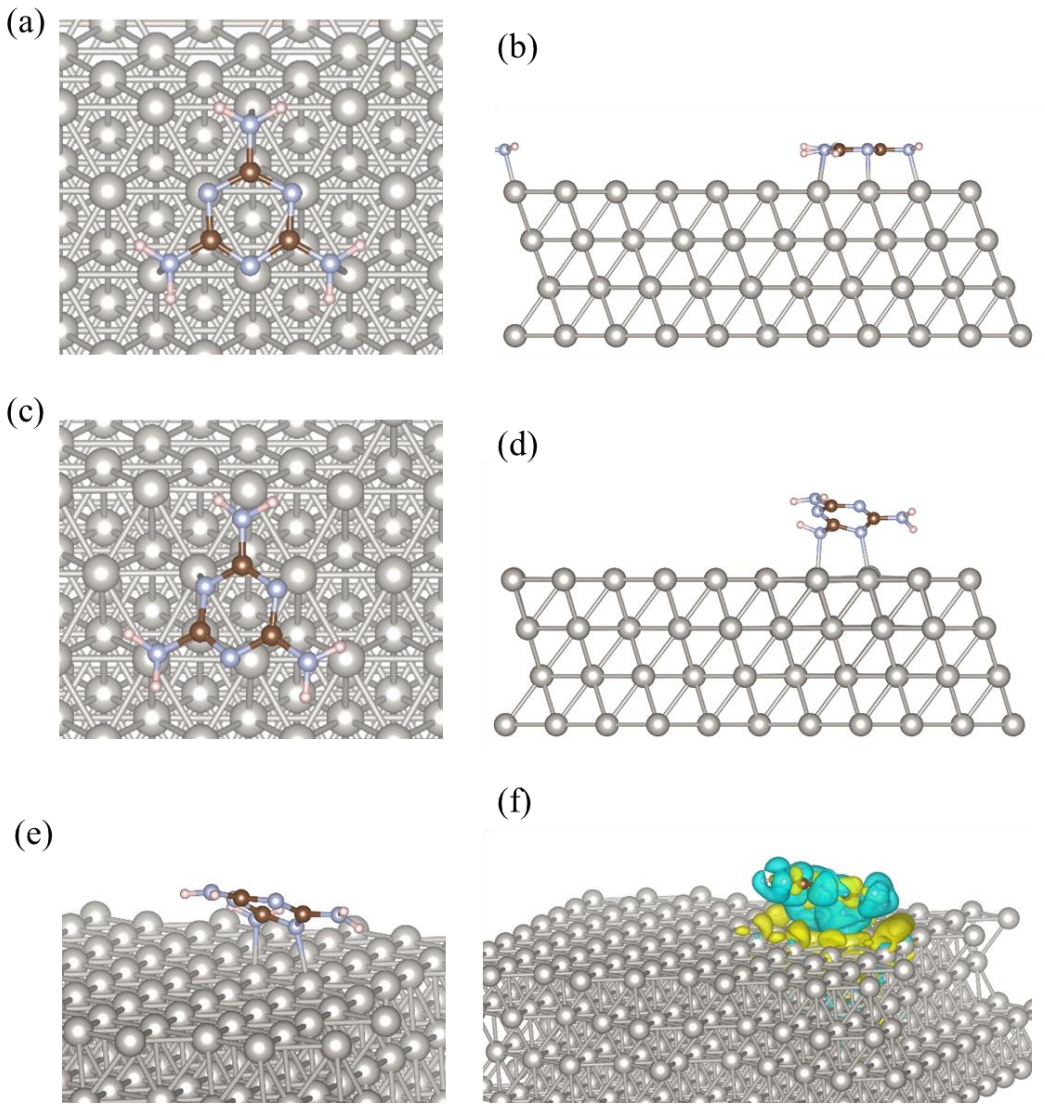

Figure S74. (a) Top and (b) side views of entry 52. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 52. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^3. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

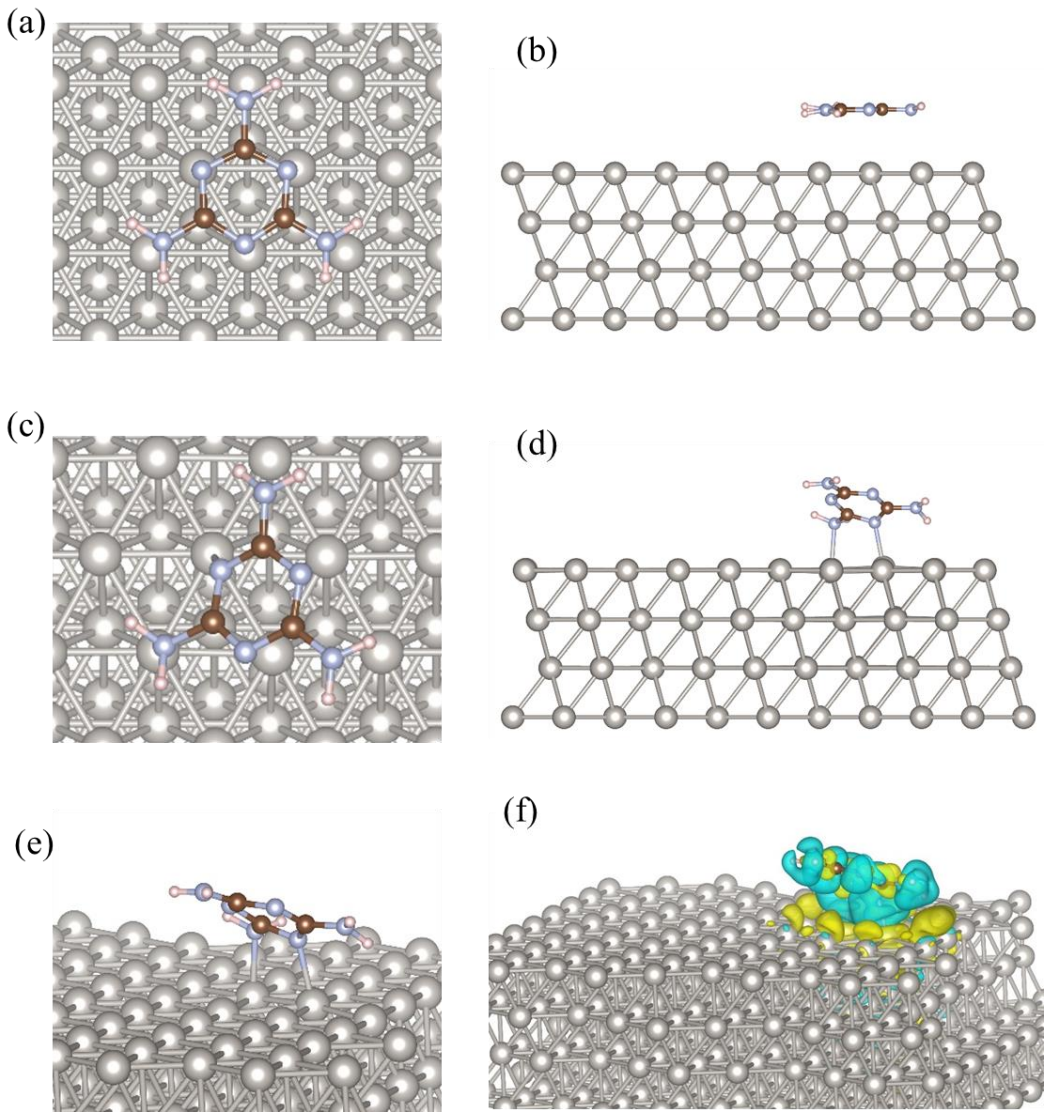

Figure S75. (a) Top and (b) side views of entry 53. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 53. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^3. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

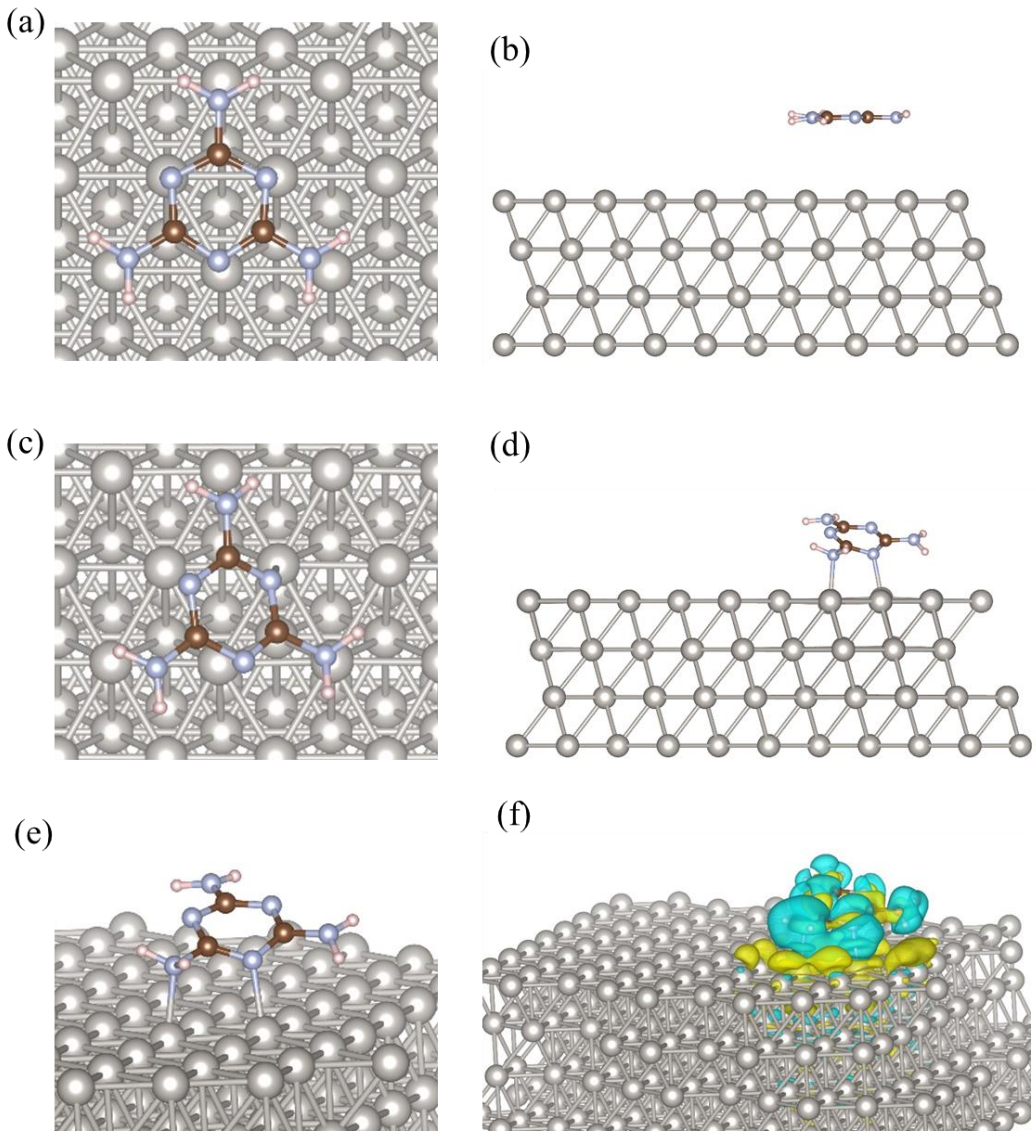

Figure S76. (a) Top and (b) side views of entry 54. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 54. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^3. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

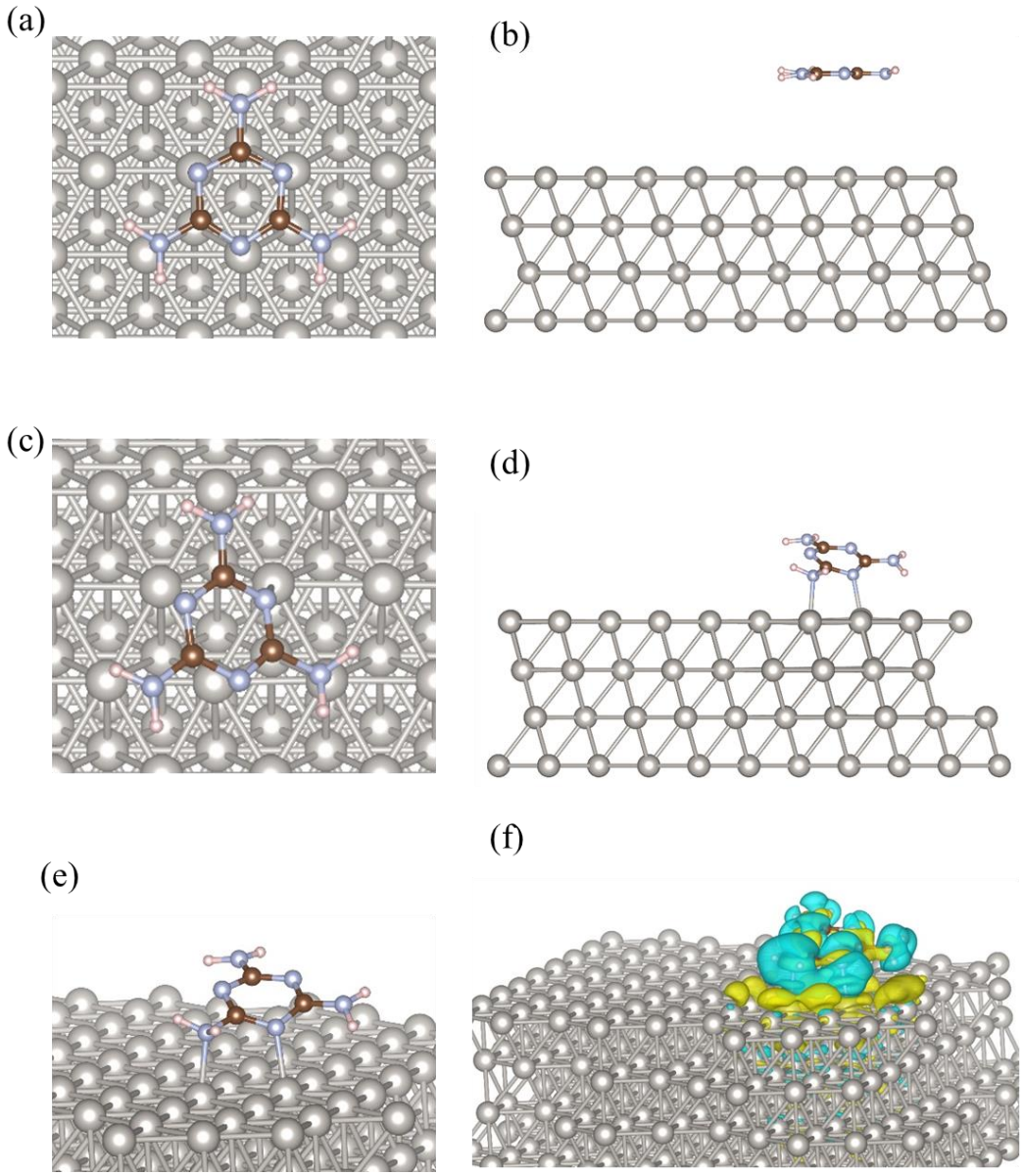

Figure S77. (a) Top and (b) side views of entry 55. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 55. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^3. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

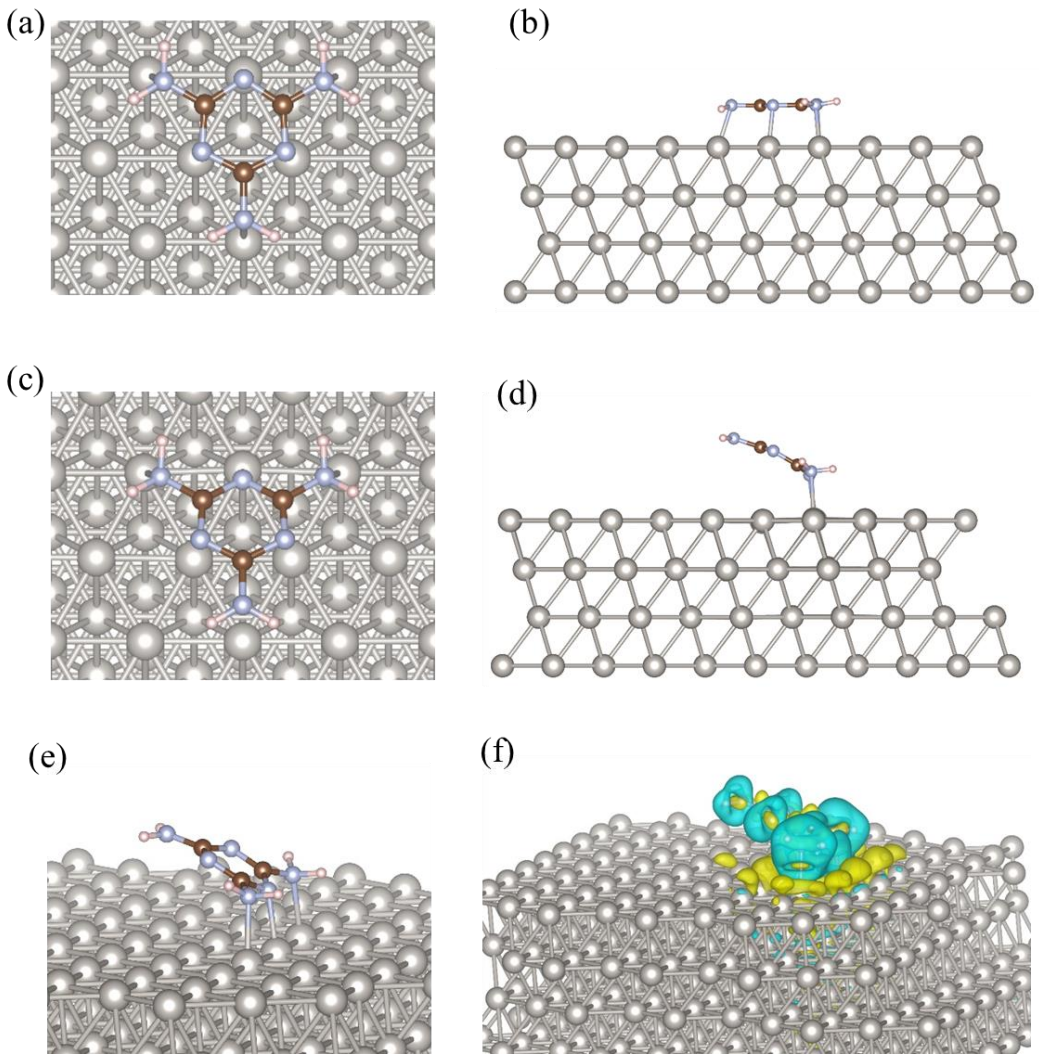

Figure S78. (a) Top and (b) side views of entry 56. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 56. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^3. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

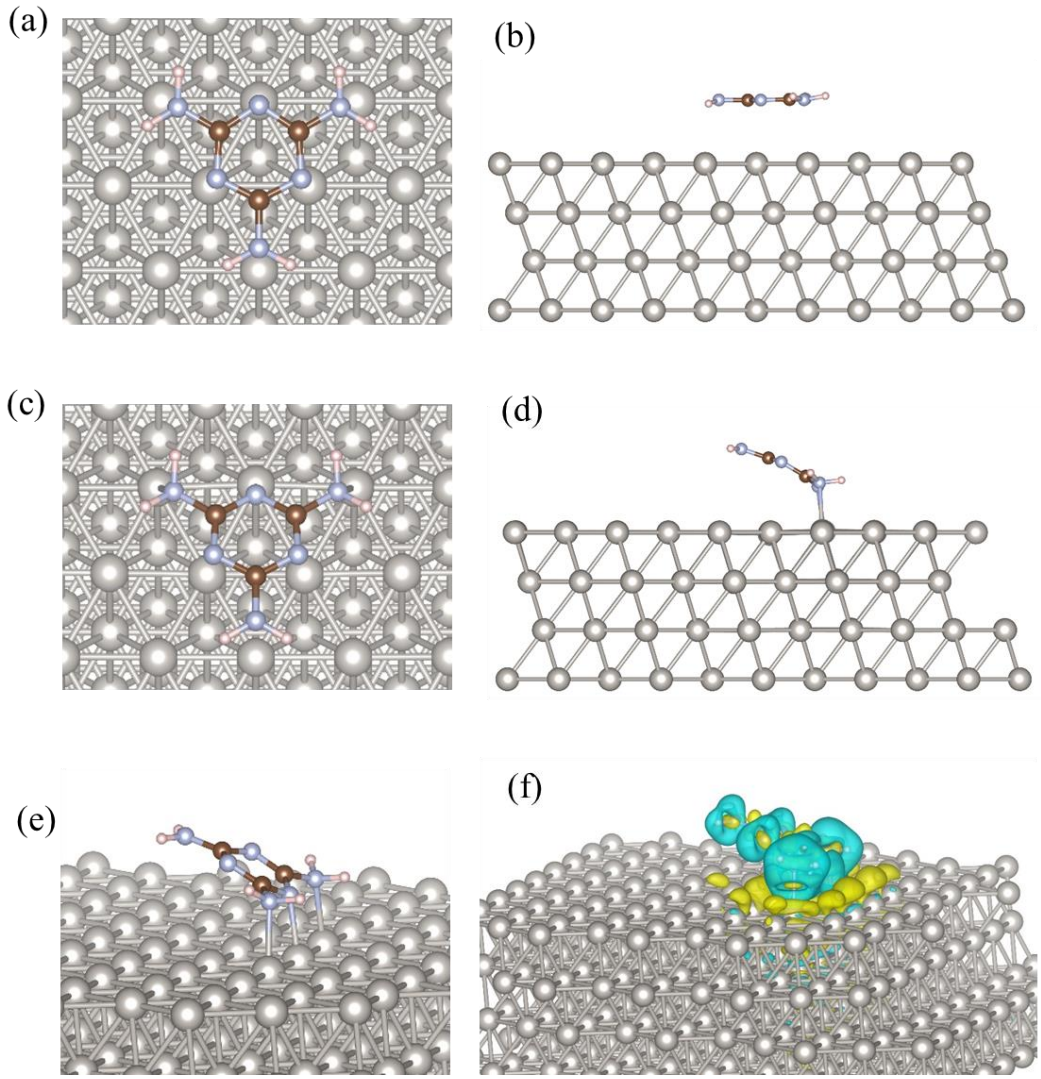

Figure S79. (a) Top and (b) side views of entry 57. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 57. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^3. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

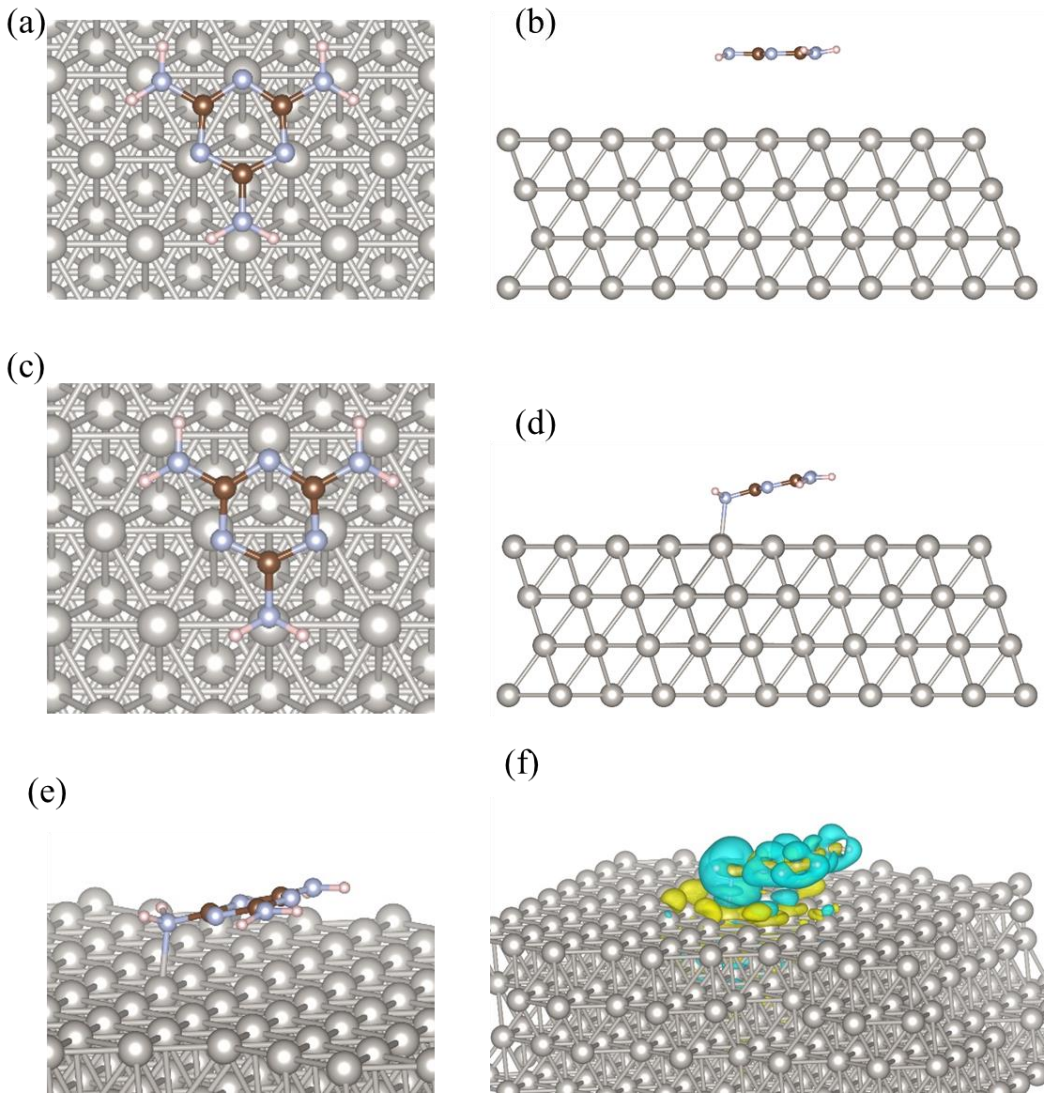

Figure S80. (a) Top and (b) side views of entry 58. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 58. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^3. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

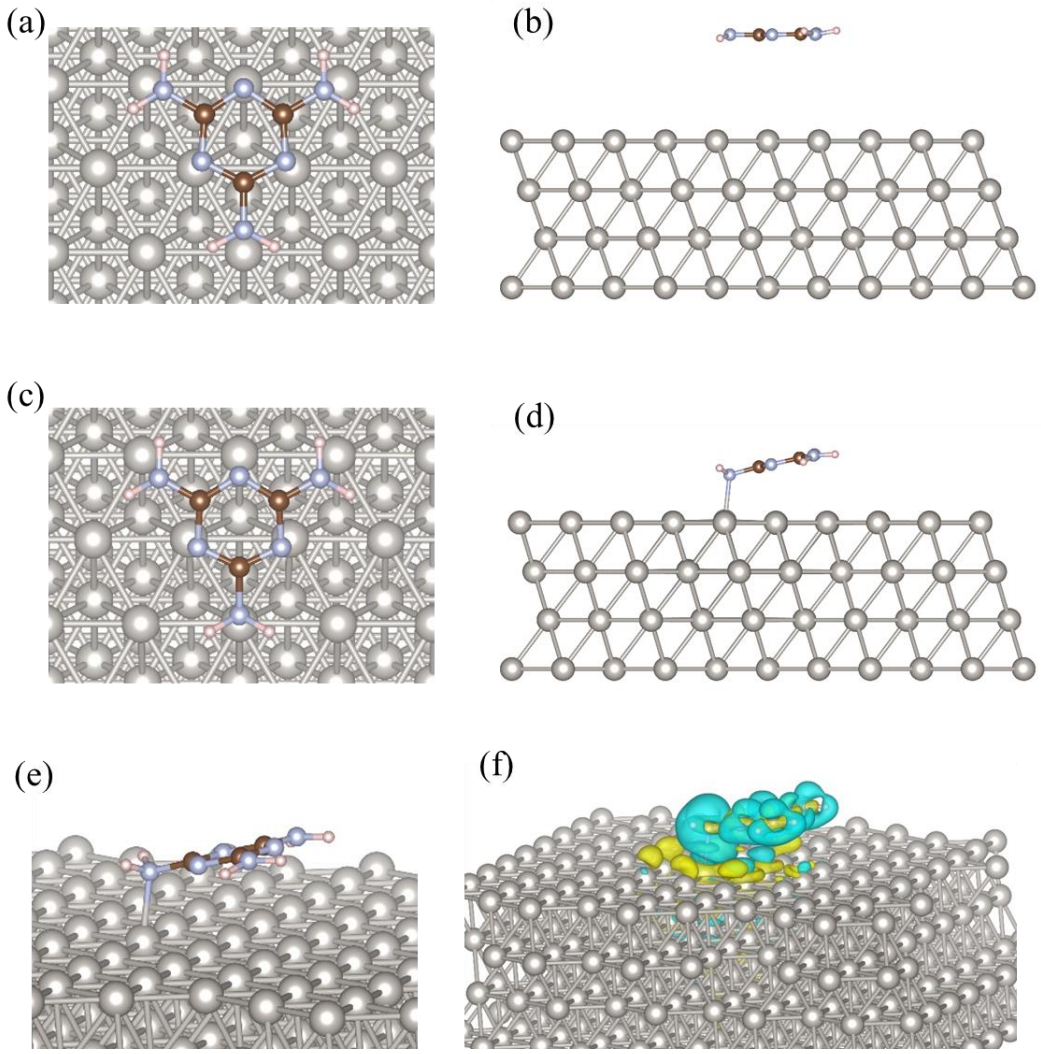

Figure S81. (a) Top and (b) side views of entry 59. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 59. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^3. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

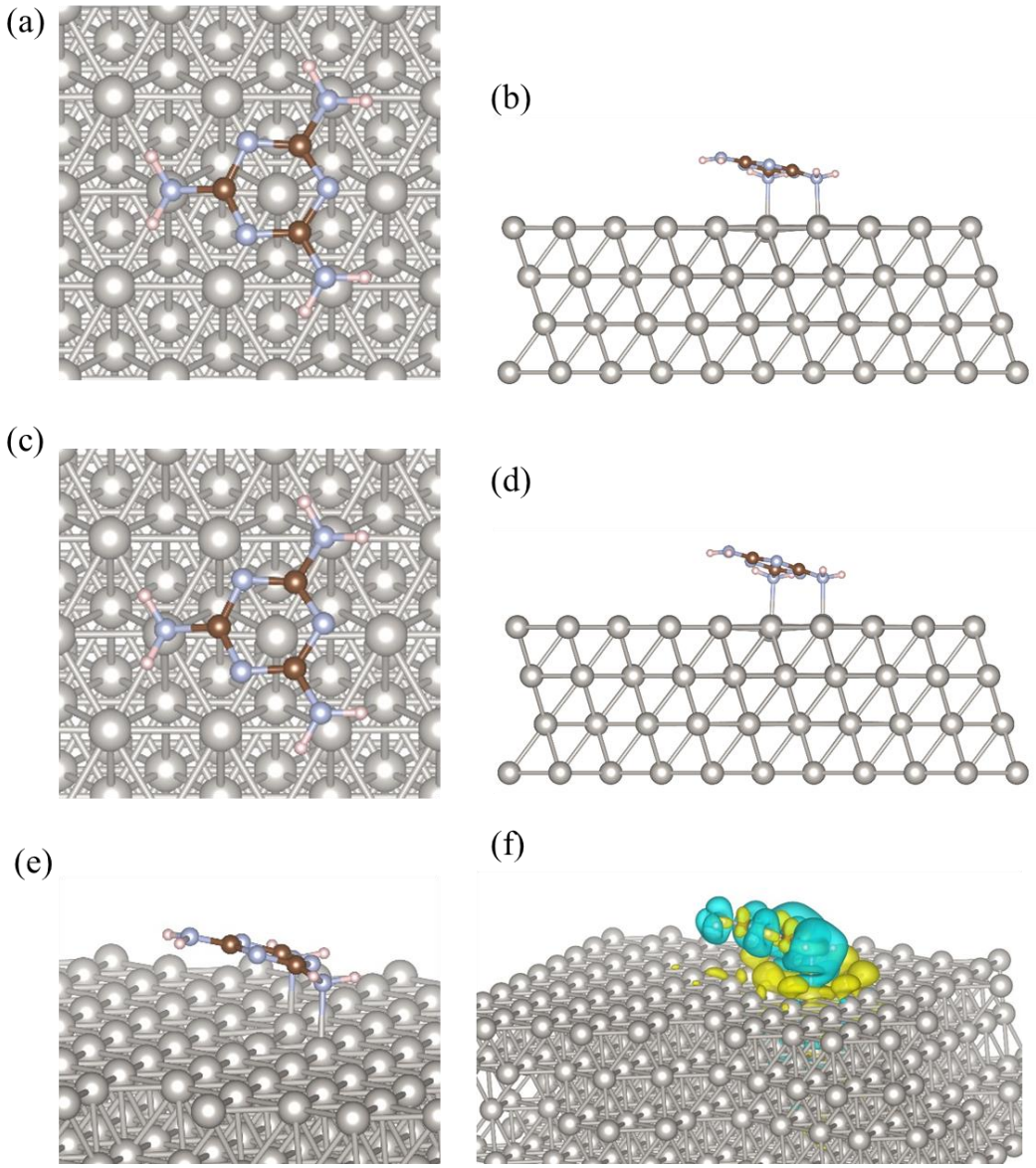

Figure S82. (a) Top and (b) side views of entry 60. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 60. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^3. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

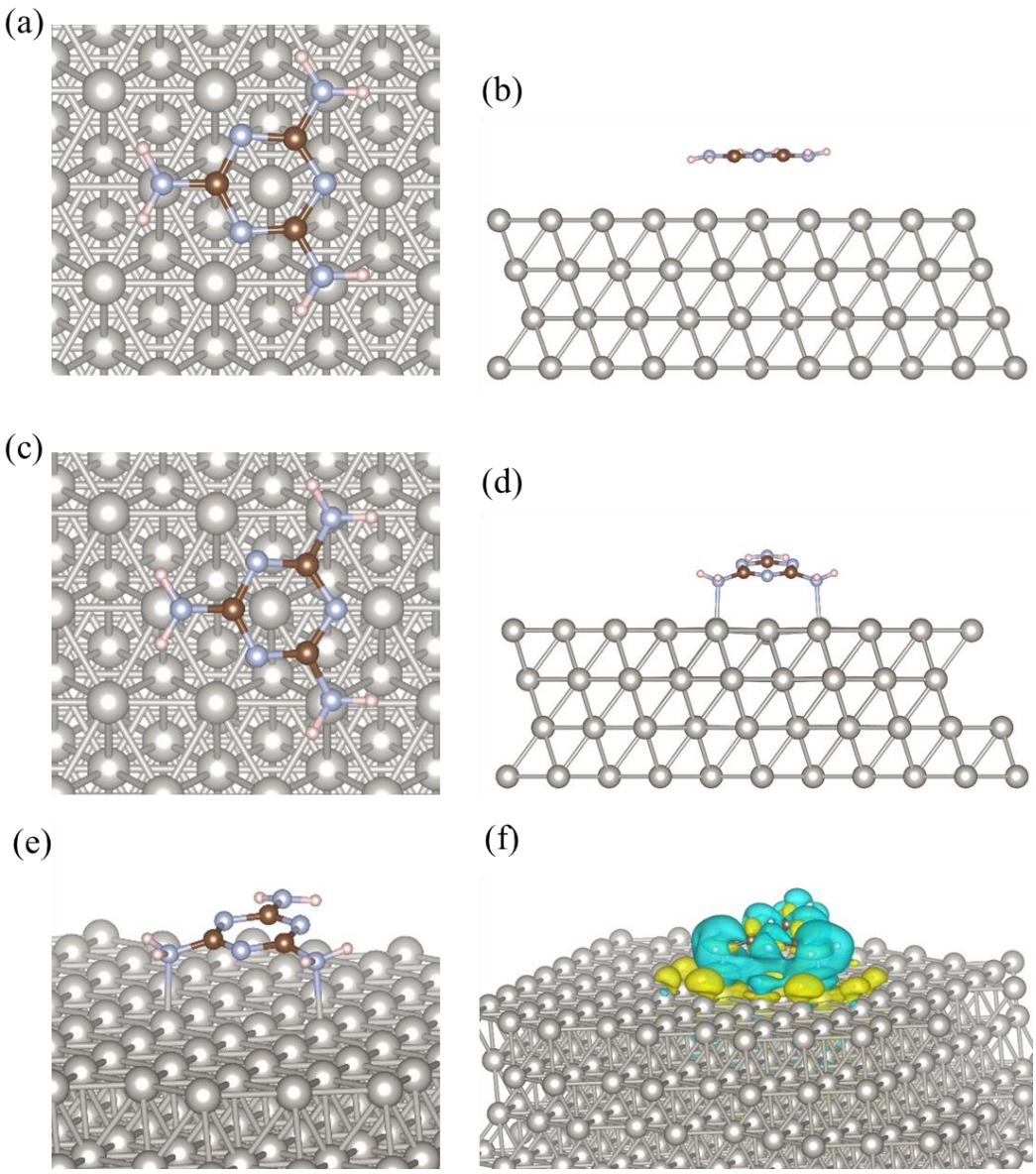

Figure S83. (a) Top and (b) side views of entry 61. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 61. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^{3}. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

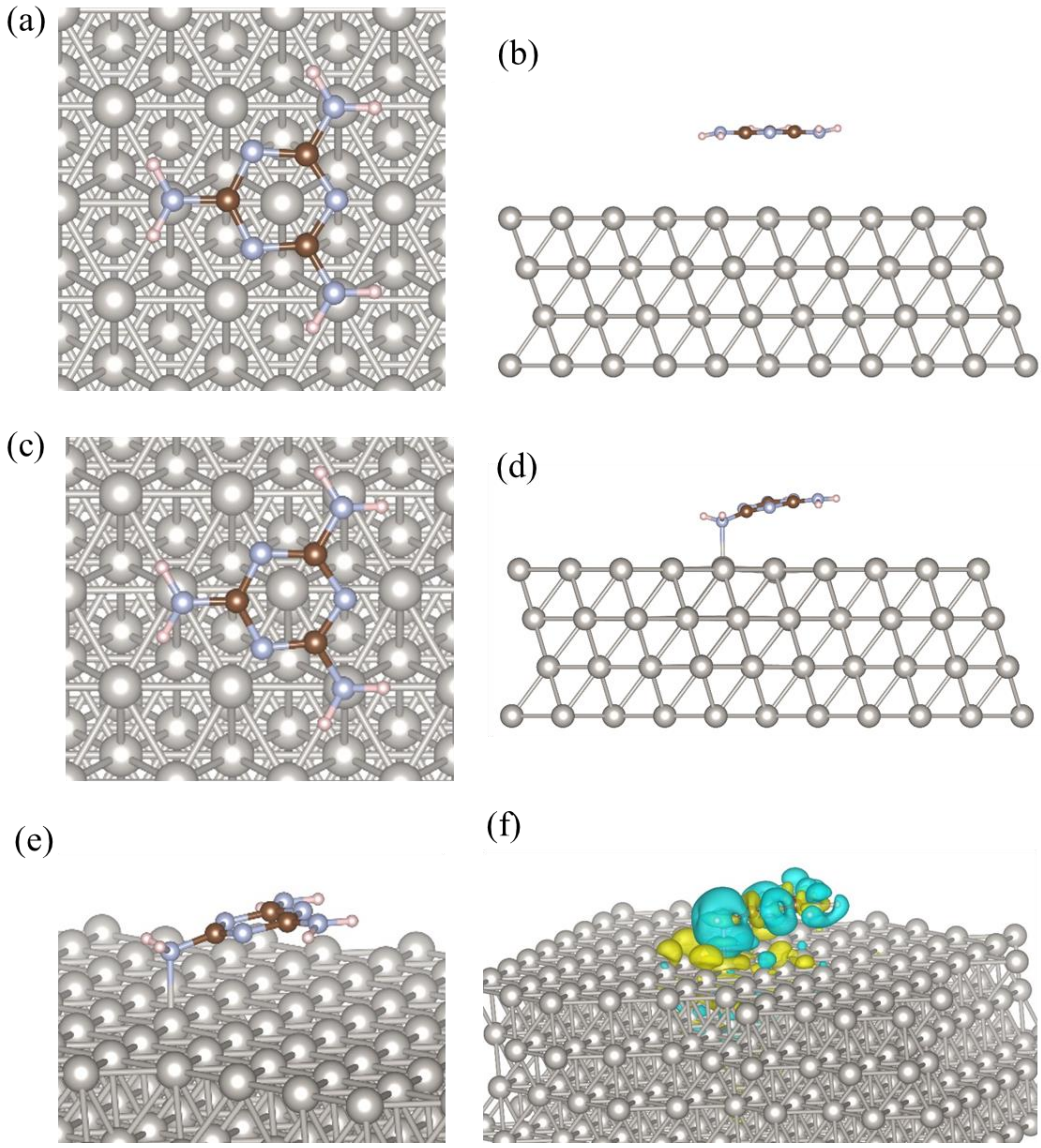

Figure S84. (a) Top and (b) side views of entry 62. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 62. (f) Charge difference distribution of the optimised structure with a threshold of 0.001 e^{-}/Bohr^3. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

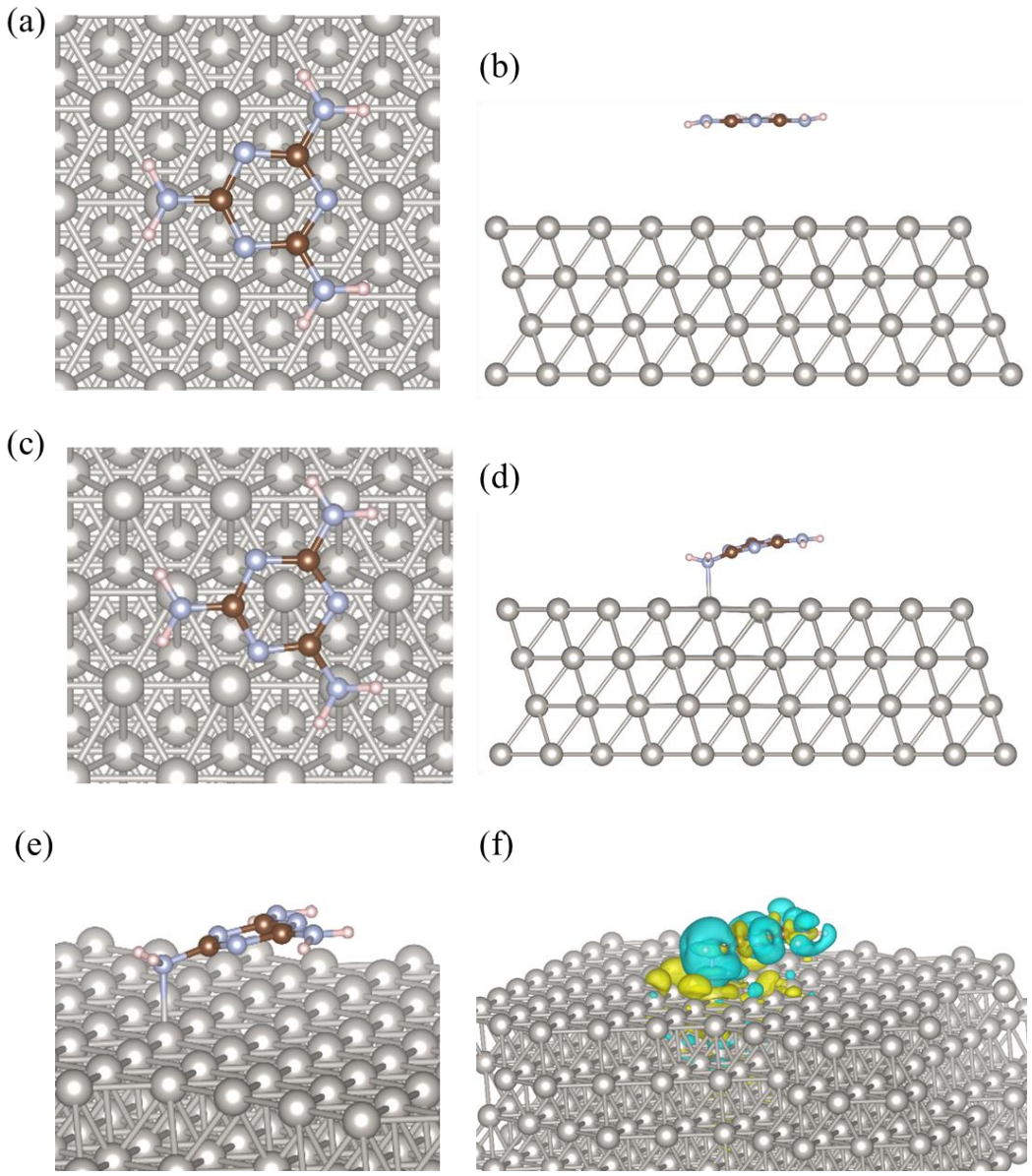

Figure S85. (a) Top and (b) side views of entry 63. (c) Top, (d) side, and (e) perspective views of the optimised structures of entry 63. (f) Charge difference distribution of the optimised structure, and the threshold is 0.001 e^{-}/Bohr^3. Yellow and blue represent decrease and increase of electron density, respectively. The grey, brown, blue, and white balls represent Pt, C, N, and H atoms, respectively.

Table S2. Adsorption type and E_{ads}, E_{int}, E_{dis}(mel.), E_{dis}(Pt), E_{chem}, E_{phys}, $\Delta\rho$(mel.) values of the optimised structures of entries 1–40

Entry	Type	E_{ads} [eV]	E_{int} [eV]	E_{dis}(mel.) [eV]	E_{dis}(Pt) [eV]	E_{chem} [eV]	E_{phys} [eV]	$\Delta\rho$ [e$^-$]
1	B	–2.00	–2.50	0.36	0.14	–1.18	–1.32	–0.334
2	B	–2.11	–2.49	0.35	0.03	–1.17	–1.32	–0.334
3	B	–2.10	–2.46	0.33	0.03	–1.23	–1.23	–0.328
4	B	–2.00	–2.50	0.36	0.14	–1.18	–1.32	–0.336
5	B	–1.99	–2.49	0.36	0.14	–1.16	–1.33	–0.338
6	B	–2.10	–2.50	0.36	0.03	–1.27	–1.23	–0.329
7	B	–1.98	–2.53	0.41	0.13	–1.35	–1.18	–0.338
8[a]	A	–2.05	–2.47	0.25	0.17	–1.18	–1.29	–0.383
9	A	–2.04	–2.49	0.27	0.17	–1.22	–1.27	–0.377
10	B	–1.97	–2.55	0.44	0.13	–1.39	–1.16	–0.337
11	B	–2.09	–2.52	0.40	0.03	–1.35	–1.17	–0.322
12	A	–2.04	–2.43	0.35	0.04	–1.11	–1.32	–0.373
13	A	–2.03	–2.43	0.35	0.04	–1.11	–1.32	–0.373
14	B	–2.09	–2.55	0.37	0.08	–1.38	–1.17	–0.329
15	B	–2.08	–2.52	0.38	0.06	–1.37	–1.15	–0.327
16	A	–2.02	–2.42	0.36	0.05	–1.12	–1.30	–0.371
17	A	–2.03	–2.43	0.36	0.04	–1.13	–1.30	–0.374
18	B	–2.09	–2.51	0.37	0.05	–1.33	–1.18	–0.330
19	B	–2.09	–2.51	0.38	0.04	–1.33	–1.18	–0.328
20	A	–2.03	–2.43	0.37	0.04	–1.14	–1.29	–0.375
21	B	–2.10	–2.57	0.43	0.04	–1.39	–1.18	–0.334
22	C	–1.88	–2.19	0.19	0.12	–0.73	–1.46	–0.315
23	C	–1.88	–2.21	0.20	0.13	–0.75	–1.46	–0.309
24	D	–1.84	–2.05	0.14	0.07	–0.65	–1.40	–0.270
25	B	–1.98	–2.47	0.35	0.13	–1.17	–1.30	–0.333
26[a]	B	–2.12	–2.51	0.35	0.05	–1.20	–1.31	–0.333
27	B	–2.02	–2.54	0.36	0.16	–1.22	–1.32	–0.340
28	C	–1.88	–2.19	0.19	0.12	–0.73	–1.46	–0.315
29	C	–1.88	–2.20	0.20	0.12	–0.74	–1.46	–0.309
30[a]	C	–1.91	–2.22	0.19	0.12	–0.76	–1.46	–0.316
31	C	–1.88	–2.21	0.20	0.13	–0.75	–1.46	–0.309
32	D	–1.84	–2.04	0.14	0.07	–0.64	–1.40	–0.270
33	B	–2.11	-2.49	0.35	0.03	–1.18	–1.31	–0.331
34	D	–1.86	–2.05	0.13	0.06	–0.63	–1.42	–0.302
35	B	–2.10	–2.52	0.34	0.08	–1.27	–1.25	–0.327
36	D	–1.83	–2.02	0.14	0.06	–0.64	–1.38	–0.265
37	D	–1.83	–2.02	0.13	0.05	–0.66	–1.36	–0.268
38	B	–2.01	–2.53	0.36	0.16	–1.21	–1.32	–0.339
39	B	–2.02	–2.54	0.36	0.16	–1.23	–1.31	–0.338
40	D	–1.83	–2.04	0.14	0.07	–0.63	–1.41	–0.263

[a] The entries whose optimised structures are shown in the main text are highlighted in red colour.

Table S3. Adsorption type and E_{ads}, E_{int}, E_{dis}(mel.), E_{dis}(Pt), E_{chem}, E_{phys}, $\Delta\rho$(mel.) values of the optimised structures of entries 41–63

Entry	Type	E_{ads} [eV]	E_{int} [eV]	E_{dis}(mel.) [eV]	E_{dis}(Pt) [eV]	E_{chem} [eV]	E_{phys} [eV]	$\Delta\rho$ [e-]
41	D	–1.84	–2.05	0.14	0.07	–0.65	–1.40	–0.264
42	B	–2.01	–2.51	0.35	0.16	–1.20	–1.31	–0.336
43	B	–2.01	–2.51	0.35	0.16	–1.20	–1.31	–0.337
44	D	–1.85	–2.04	0.13	0.06	–0.63	–1.41	–0.299
45	D	–1.85	–2.03	0.13	0.05	–0.64	–1.39	–0.282
46	D	–1.86	–2.05	0.13	0.05	–0.65	–1.40	–0.297
47 [a]	D	–1.88	–2.06	0.13	0.05	–0.66	–1.40	–0.293
48	B	–2.12	–2.52	0.34	0.06	–1.22	–1.30	–0.330
49	B	–2.11	–2.52	0.34	0.06	–1.24	–1.28	–0.327
50	B	–2.11	–2.51	0.34	0.07	–1.24	–1.27	–0.327
51	B	–2.09	–2.48	0.35	0.04	–1.10	–1.38	–0.349
52	B	–1.99	–2.48	0.36	0.14	–1.15	–1.33	–0.337
53	B	–2.09	–2.50	0.35	0.06	–1.21	–1.29	–0.328
54	B	–1.87	–2.25	0.35	0.03	–1.17	–1.08	–0.329
55	B	–1.88	–2.26	0.35	0.03	–1.18	–1.08	–0.327
56	A	–1.92	–2.42	0.34	0.16	–1.03	–1.39	–0.379
57	A	–1.92	–2.42	0.34	0.16	–1.04	–1.38	–0.379
58	D	–1.87	–2.04	0.13	0.05	–0.62	–1.42	–0.308
59	D	–1.88	–2.07	0.13	0.06	–0.64	–1.43	–0.303
60	C	–1.91	–2.23	0.20	0.13	–0.78	–1.45	–0.309
61	C	–1.88	–2.19	0.19	0.12	–0.73	–1.46	–0.311
62	D	–1.85	–2.04	0.14	0.06	–0.67	–1.37	–0.264
63	D	–1.85	–2.04	0.14	0.06	–0.66	–1.38	–0.271

[a] The entries whose optimised structures are shown in the main text are highlighted in red colour.

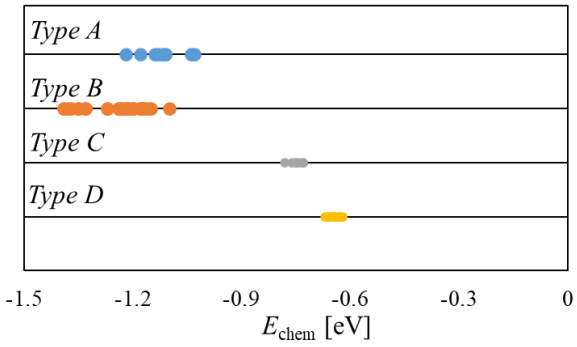

Figure S86. Energy distribution of the E_{chem} of the four types of adsorption structures.

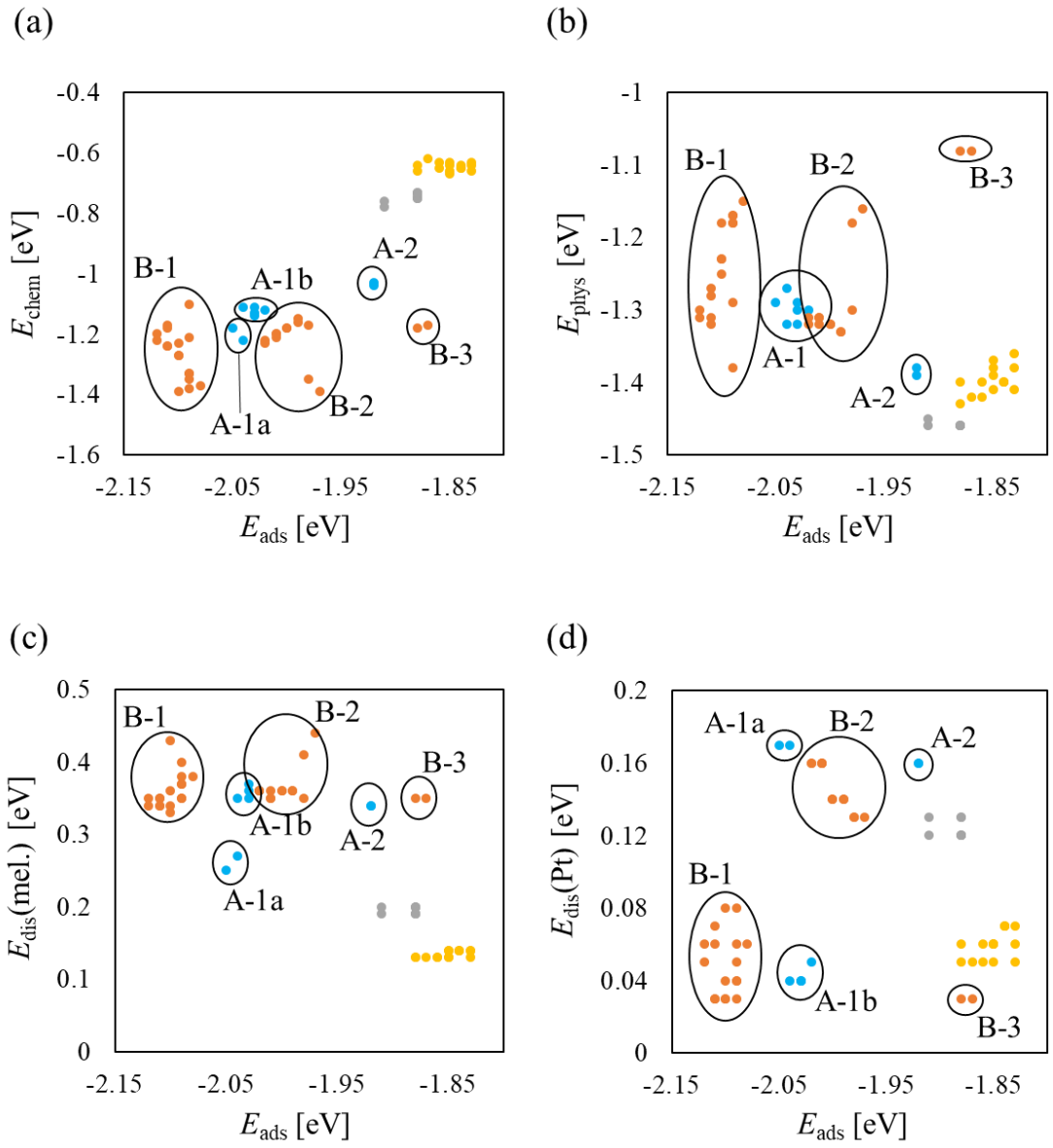

Figure S87. Correlation between (a) adsorption energy of melamine onto Pt (111) (E_{ads}) and chemical interaction energy between Pt and melamine (E_{chem}), (b) E_{ads} and dispersion forces between Pt and melamine (E_{phys}), (c) E_{ads} and distortion energy of melamine (E_{dis}(mel.)), and (d) E_{ads} and distortion energy of Pt (E_{dis}(Pt)). The blue, orange, grey, and yellow dots represent adsorption structure Type A, B, C, and D, respectively.

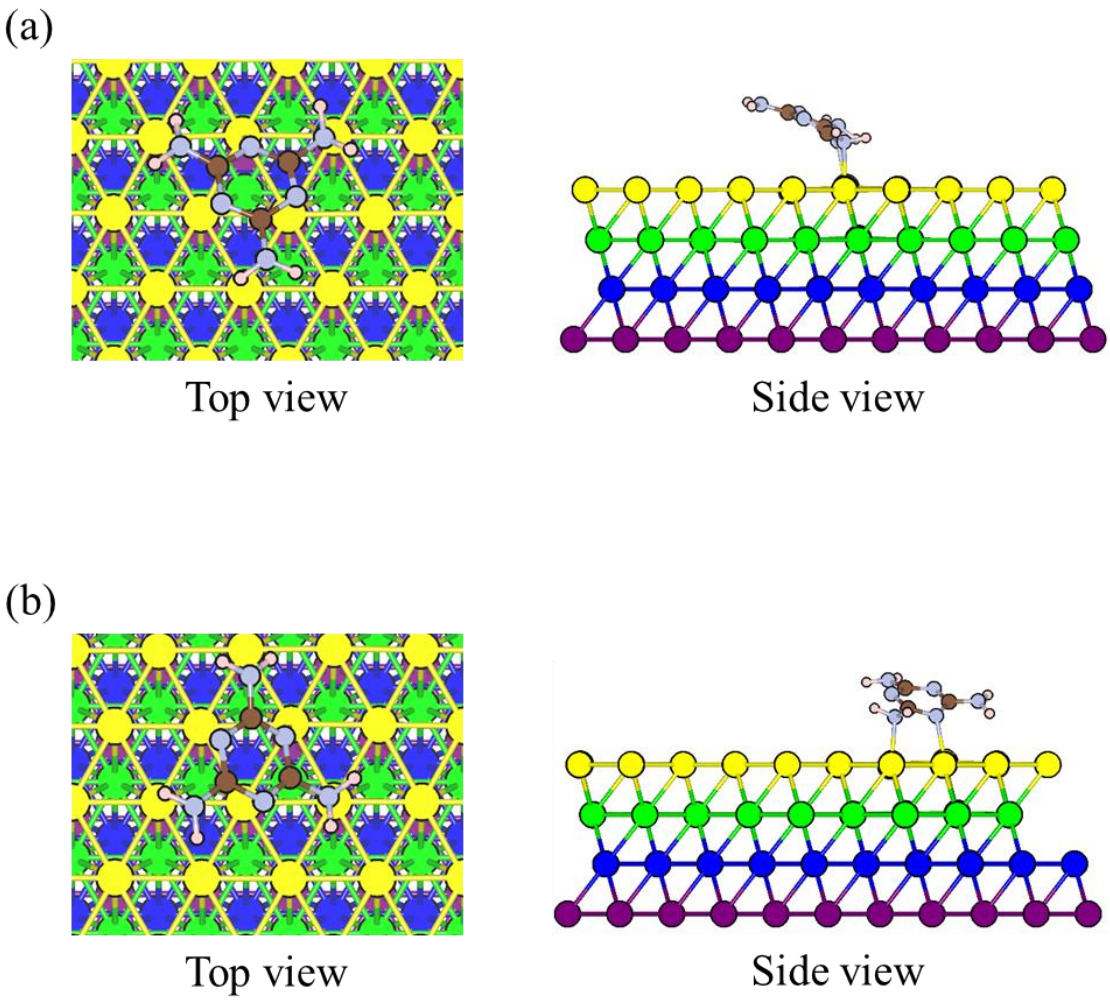

Figure S88. Top and side views of the optimised structures of the Type (a) B-1 and (b) B-2. The Pt atoms in the 1st, 2nd, 3rd, and 4th layers are shown in yellow, green, blue, and purple, respectively.

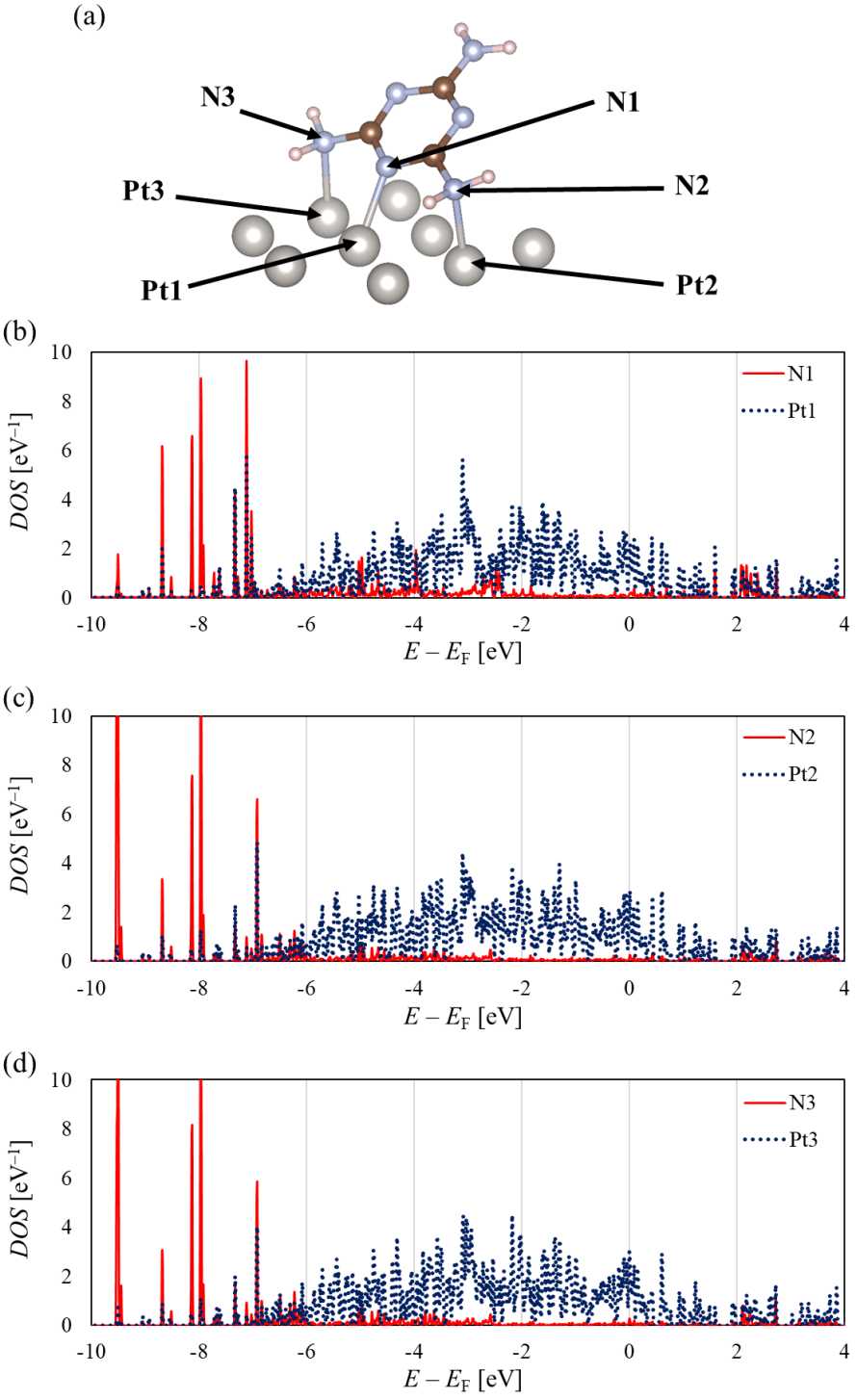

Figure S89. (a) Atom labelling for the Type A structure and (b, c, d) projected density of states (PDOS) of Type A (entry 8 in Table S1). E_F represents the Fermi energy.

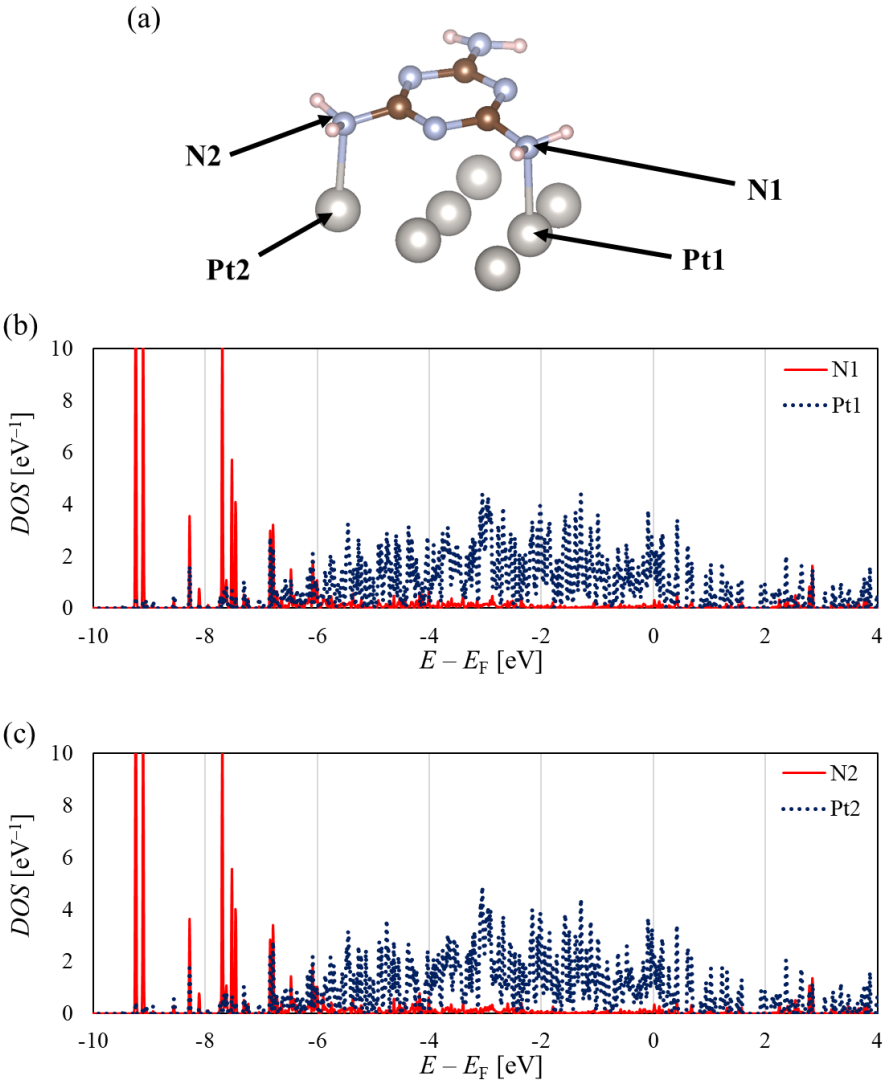

Figure S90. (a) Atom labelling for the Type C structure and (b, c) PDOS of Type C (entry 30 in Table S1). E_F represents the Fermi energy.

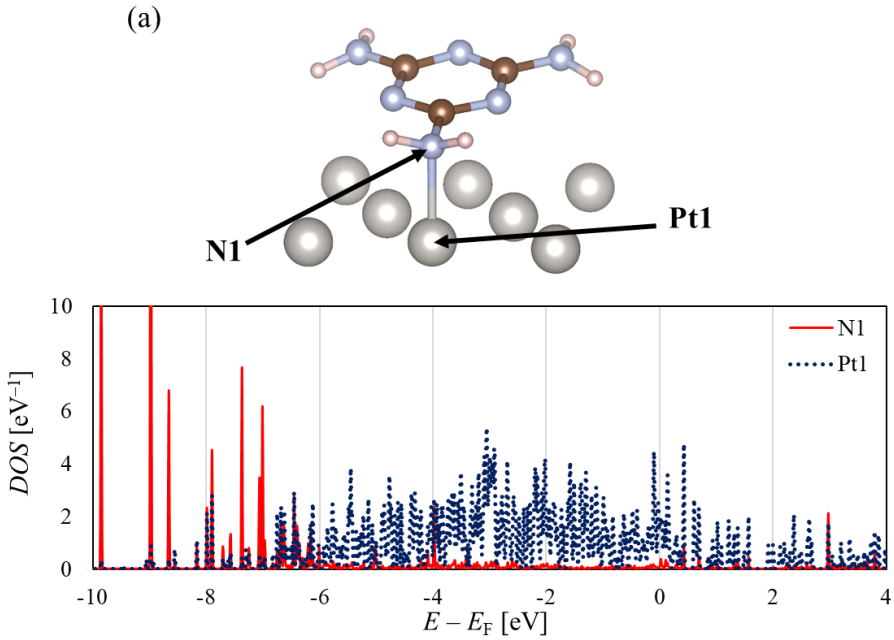

Figure S91. (a) Atom labelling for the Type D structure and (b, c) PDOS of Type D (entry 47 in Table S1). E_F represents the Fermi energy.

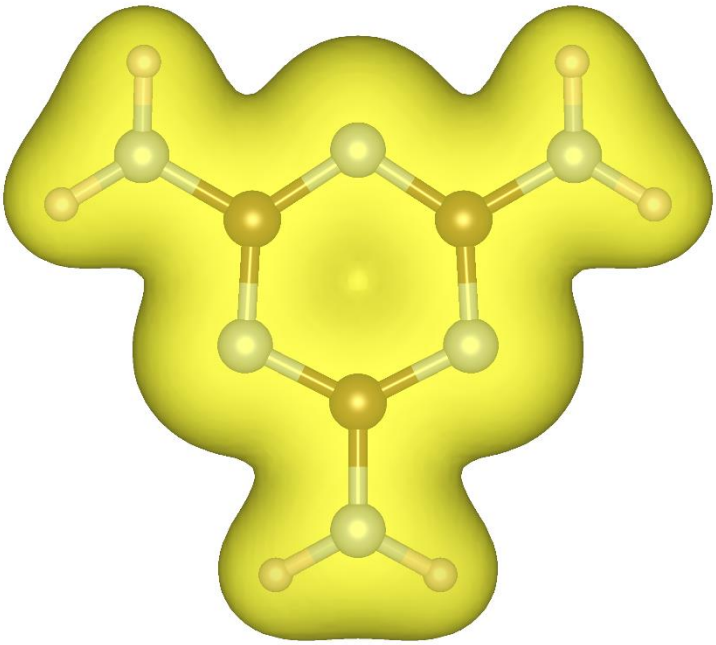

Figure S92. Electron density distribution of melamine calculated by PBE/plane-wave. Threshold is 0.02 e^{-}/Bohr^{3}.

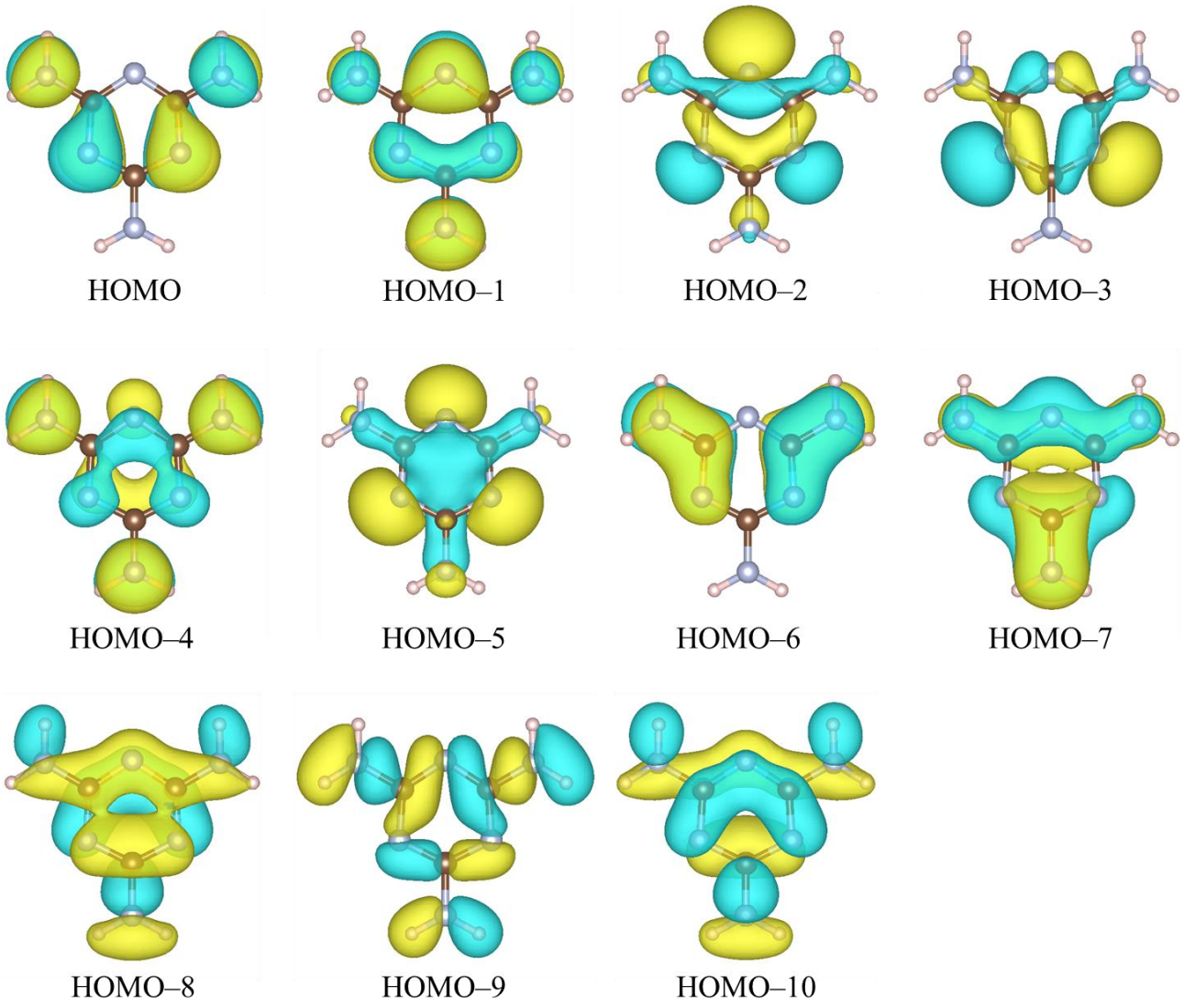

Figure S93. Highest occupied molecular orbitals (HOMO) and HOMO-*n* (*n* = 1–10, where n indicates the nth lower orbital from HOMO) of melamine calculated at the PBE/6-311++G(d,p) level. The optimised structure obtained using PBE/plane-wave was used for the calculation.

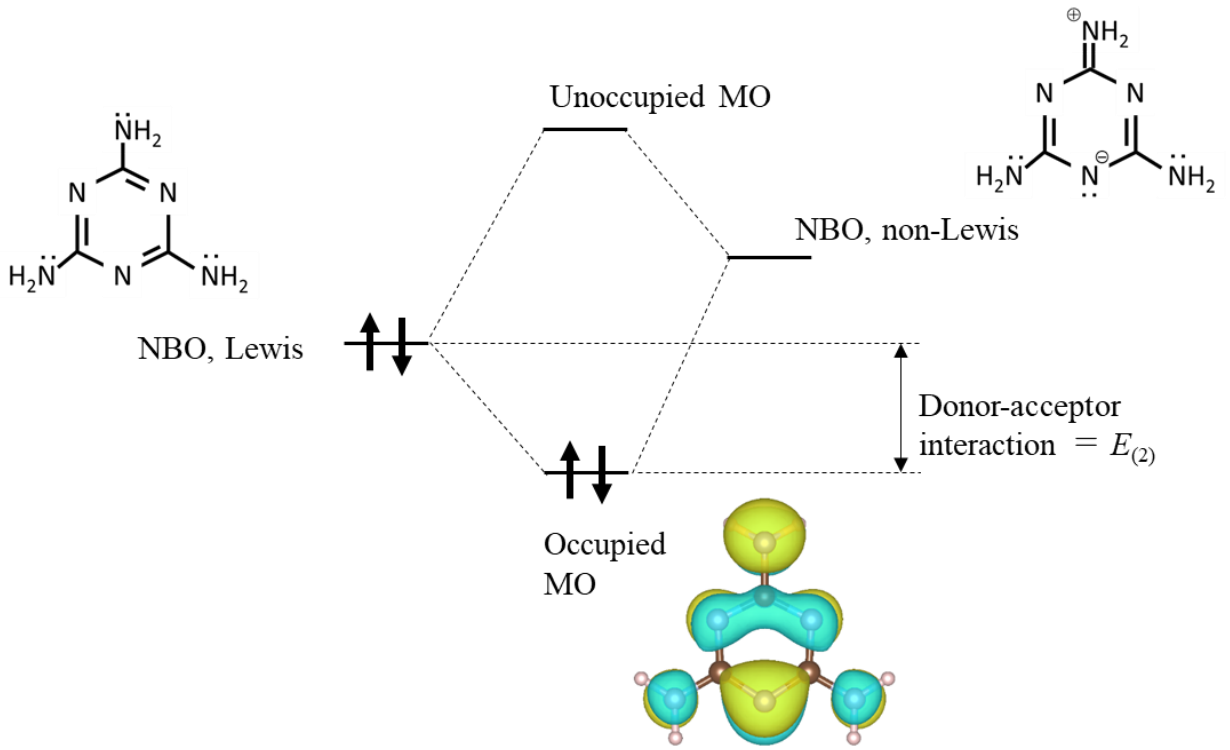

Figure S94. Brief explanation of the donor–acceptor interactions between Lewis and non-Lewis structures. The natural bonding orbitals (NBOs) are localised wavefunctions obtained by the following process: (1) the density matrix obtained from a single-referenced method, such as Hartree–Fock or Kohn–Sham equations, was block-diagonalised using the orbital angular momentum of each atom (= natural atomic orbital); (2) the hybrid orbitals were defined from the natural atomic orbitals; and (3) the wavefunctions were constructed using the hybrid orbitals as a basis set. The resonance between the amino group and the triazine ring was considered electron delocalisation from the occupied Lewis orbital of the amino group to the unoccupied non-Lewis orbital of the triazine ring. In this case, the amino group and triazine ring act as the donor and acceptor, respectively. This interaction stabilises the resonance (electron delocalisation). According to the formalism of quantum chemistry, the donor–acceptor interactions can be defined as the stabilisation caused by the linear combination of localised wavefunctions such as Lewis and non-Lewis to afford delocalised wavefunctions. In other words, the resonance stabilisation can be estimated using NBO (localised wavefunction) and molecular (or Kohn–Sham) orbitals (delocalised function). Specifically, the donor–acceptor interactions can be estimated as the second-order perturbation energy $E_{(2)}$ when the Fock matrix of the NBOs is set to zeroth order and its difference with the Fock matrix of the original molecular (or Kohn–Sham) orbitals is treated as the perturbation.

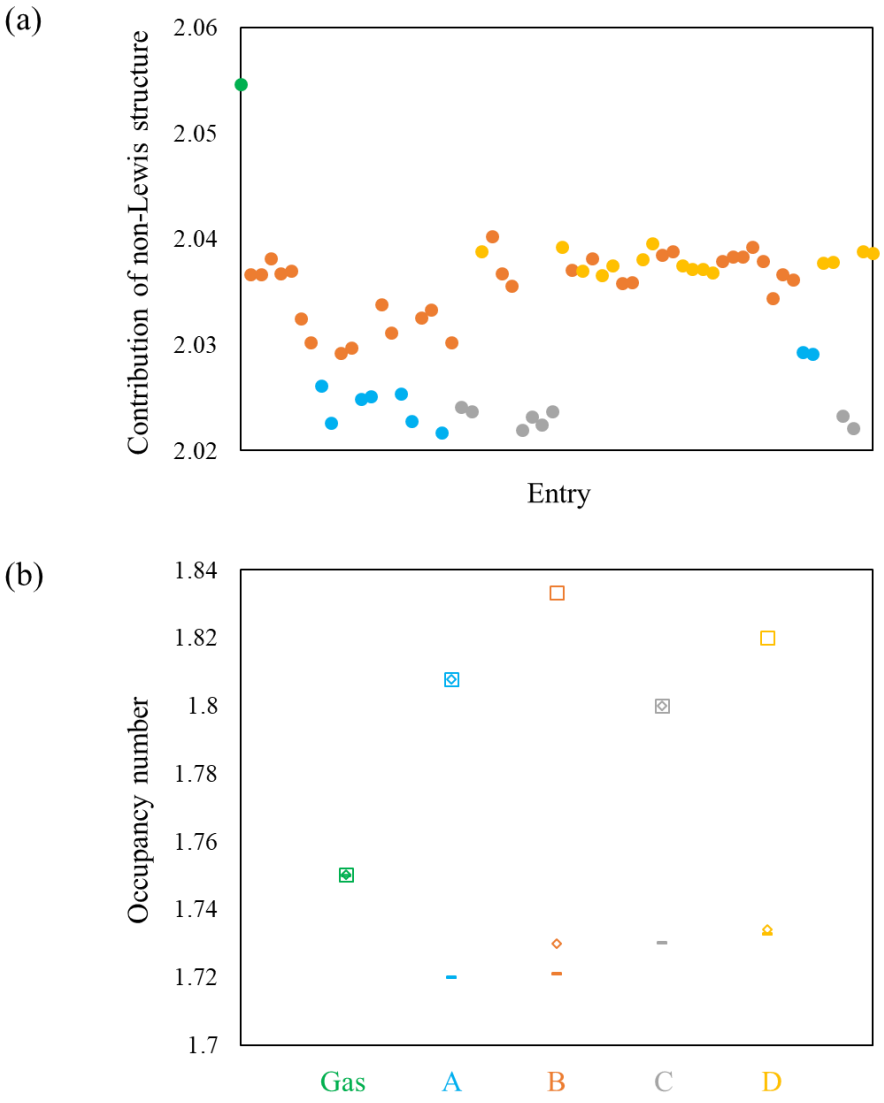

Figure S95. (a) Summation of the occupancies of the non-Lewis structure of melamine molecule with and without distortion caused by Pt(111) adsorption. The green, blue, red-brown, grey, and yellow dots represent melamine molecule in the gas phase and Type A, B, C, and D adsorption structures, respectively. (b) Lone-pair occupancies of NH_2 in the melamine molecule. Green represents the value for the optimised melamine structure in the gas phase, and blue, red-brown, grey, and yellow represent the average values of the melamine molecules in the Type A, B, C, and -D adsorption structures, respectively. The square, diamond, and bar represent maximum, median and minimum values, respectively.

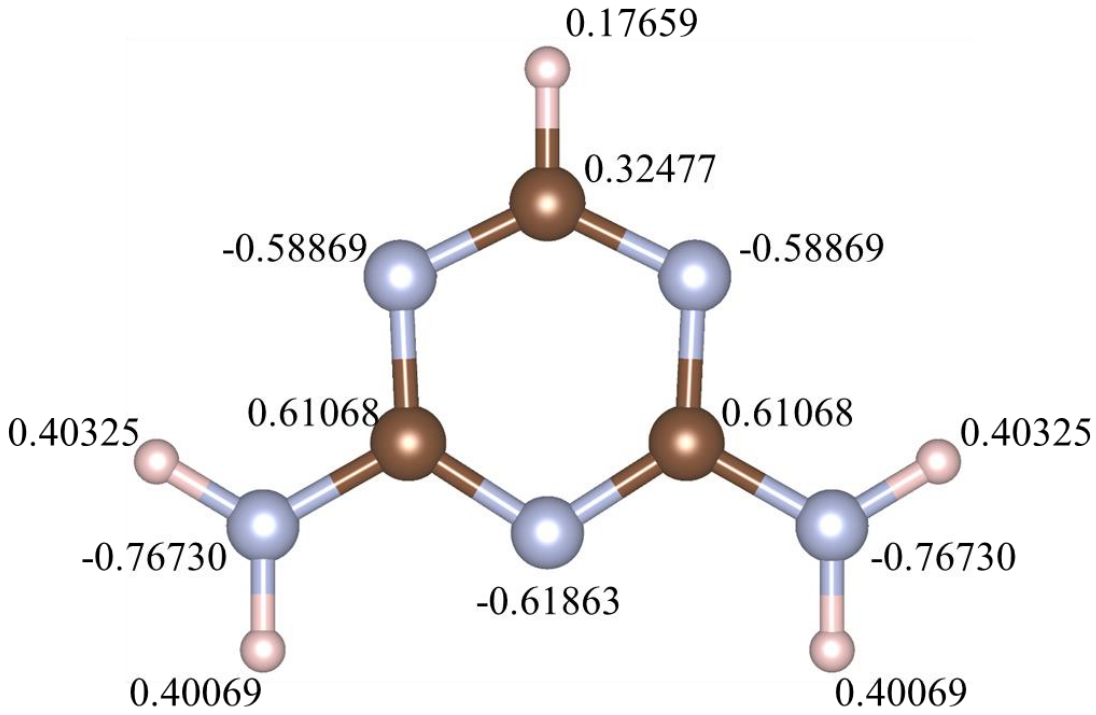

Figure S96. Charges of melamine calculated by NBO analysis. The optimised structure obtained using PBE/plane-wave was used for the calculation.

Table S4. Adsorption angles for the diamino-triazine and amino-triazine molecules

Adsorbed molecule	Adsorption structure	Angles [°]
Diamino triazine	Fig. 8(a)	34.5[a], 30.7[b]
Diamino triazine	Fig. 8(b)	50.2[a], 47.7[b]
Amino triazine	Fig. 8(c)	51.6[a], 50.1[b]

[a] Angle between the Pt surface and the straight line connecting the $N_{triazine}$ adsorbed on Pt and the C atom furthest from the Pt surface.

[b] Angle between the Pt surface and the straight line connecting the $N_{triazine}$ adsorbed on Pt and the substituent (H or N_{amino}) bonded to the C atom furthest from the Pt surface.

Table S5. Atomic coordinates (cartesian; Å) of the Type A structure shown in Fig. 1(a)

Atom label	X [Å]	Y [Å]	Z [Å]
N1	21.40001	0.566739	9.10245
N2	19.93848	1.775349	10.56805
N3	19.92069	18.60483	10.56906
N4	21.31688	2.919444	9.11391
N5	18.42388	0.594354	11.8402
N6	21.30031	17.44185	9.122771
C1	20.88205	1.707614	9.645594
C2	19.44331	0.582587	10.97167
C3	20.86768	18.65663	9.64832
H1	20.93434	3.721698	9.621732
H2	18.00531	1.480304	12.10147
H3	20.92246	16.6392	9.632797
H4	0.140741	2.990063	8.941582
H5	17.98593	18.9433	12.10822
H6	0.122501	17.37699	8.945217
Pt1	0.000000	0.000000	0.000000
Pt2	4.161946	2.4029	0.000000
Pt3	1.387315	2.4029	0.000000
Pt4	0.000000	4.805801	0.000000
Pt5	1.387315	7.208701	0.000000
Pt6	4.161946	7.208701	0.000000
Pt7	2.774631	0.000000	0.000000
Pt8	2.774631	4.805801	0.000000
Pt9	4.16391	8.972542	2.312048
Pt10	1.38661	8.966097	2.310955
Pt11	22.1934	1.755113	2.355223
Pt12	22.19318	6.564805	2.311367
Pt13	2.743786	1.757151	2.343155
Pt14	1.369257	4.160082	2.306647
Pt15	4.14678	4.163841	2.30304
Pt16	2.772258	6.565716	2.305242
Pt17	4.171698	5.971869	4.581313
Pt18	1.396219	5.969439	4.57751
Pt19	22.19281	8.369082	4.593442

Pt20	0.001982	3.571841	4.624292
Pt21	1.331898	1.139481	4.706964
Pt22	4.145037	1.161207	4.600779
Pt23	2.777065	3.560418	4.569412
Pt24	2.776096	8.370546	4.587323
Pt25	0.032461	0.594567	7.062132
Pt26	4.18741	2.952001	6.912399
Pt27	1.465141	2.965103	6.900299
Pt28	0.01165	5.398926	6.891462
Pt29	1.387975	7.75719	6.90309
Pt30	4.161663	7.746493	6.896356
Pt31	2.827703	0.527456	6.938876
Pt32	2.784797	5.351187	6.890677
Pt33	5.549261	0.000000	0.000000
Pt34	9.711207	2.4029	0.000000
Pt35	6.936576	2.4029	0.000000
Pt36	5.549261	4.805801	0.000000
Pt37	6.936576	7.208701	0.000000
Pt38	9.711207	7.208701	0.000000
Pt39	8.323892	0.000000	0.000000
Pt40	8.323892	4.805801	0.000000
Pt41	9.712165	8.978058	2.310937
Pt42	6.939681	8.979013	2.312489
Pt43	5.52103	1.763233	2.31403
Pt44	5.550777	6.572317	2.309215
Pt45	8.310123	1.76573	2.308559
Pt46	6.924907	4.166817	2.308024
Pt47	9.703393	4.16972	2.312472
Pt48	8.324505	6.574048	2.309608
Pt49	9.71134	5.969524	4.58779
Pt50	6.944441	5.969494	4.589003
Pt51	5.5532	8.374937	4.588016
Pt52	5.544621	3.569253	4.584453
Pt53	6.925971	1.168447	4.583584
Pt54	9.702919	1.165264	4.582202
Pt55	8.31885	3.565521	4.588544
Pt56	8.325332	8.374883	4.590719

Pt57	5.562865	0.532577	6.906263
Pt58	9.707758	2.928713	6.899647
Pt59	6.936584	2.937523	6.899536
Pt60	5.560566	5.348723	6.903105
Pt61	6.936756	7.73881	6.905037
Pt62	9.706189	7.737179	6.902529
Pt63	8.317194	0.530334	6.896196
Pt64	8.326599	5.334697	6.905265
Pt65	11.09852	0.000000	0.000000
Pt66	15.26047	2.4029	0.000000
Pt67	12.48584	2.4029	0.000000
Pt68	11.09852	4.805801	0.000000
Pt69	12.48584	7.208701	0.000000
Pt70	15.26047	7.208701	0.000000
Pt71	13.87315	0.000000	0.000000
Pt72	13.87315	4.805801	0.000000
Pt73	15.26095	8.975623	2.314907
Pt74	12.48535	8.978464	2.310877
Pt75	11.0951	1.766413	2.309106
Pt76	11.09999	6.573749	2.311243
Pt77	13.87629	1.764545	2.305233
Pt78	12.48436	4.168624	2.309189
Pt79	15.26906	4.16894	2.312992
Pt80	13.87443	6.572592	2.312837
Pt81	15.25405	5.972271	4.59171
Pt82	12.48057	5.969112	4.593309
Pt83	11.09451	8.374186	4.590144
Pt84	11.09275	3.567252	4.58506
Pt85	12.47958	1.16549	4.584997
Pt86	15.24906	1.171075	4.583795
Pt87	13.8648	3.571535	4.585222
Pt88	13.86392	8.373876	4.589811
Pt89	11.08496	0.528944	6.893311
Pt90	15.23111	2.955639	6.910198
Pt91	12.47452	2.938753	6.897548
Pt92	11.08762	5.334868	6.908158
Pt93	12.47381	7.742626	6.907544

Pt94	15.23843	7.74922	6.905225
Pt95	13.85658	0.536274	6.898794
Pt96	13.85358	5.343372	6.911848
Pt97	16.64778	0.000000	0.000000
Pt98	20.80973	2.4029	0.000000
Pt99	18.0351	2.4029	0.000000
Pt100	16.64778	4.805801	0.000000
Pt101	18.0351	7.208701	0.000000
Pt102	20.80973	7.208701	0.000000
Pt103	19.42241	0.000000	0.000000
Pt104	19.42241	4.805801	0.000000
Pt105	20.80988	8.970779	2.312972
Pt106	18.03542	8.966584	2.309642
Pt107	16.65561	1.762165	2.307549
Pt108	16.65258	6.565321	2.309703
Pt109	19.44034	1.759865	2.313012
Pt110	18.04775	4.160232	2.330996
Pt111	20.80887	4.153682	2.328565
Pt112	19.42932	6.562134	2.312392
Pt113	20.80645	5.973112	4.600154
Pt114	18.03043	5.961747	4.588607
Pt115	16.63863	8.372671	4.589407
Pt116	16.64022	3.569386	4.590831
Pt117	18.01261	1.161361	4.562047
Pt118	20.8008	1.15683	4.651976
Pt119	19.44332	3.555104	4.638415
Pt120	19.4155	8.367677	4.590567
Pt121	16.59063	0.547577	6.919813
Pt122	20.74115	3.030253	6.944507
Pt123	17.96942	2.952031	6.917236
Pt124	16.62827	5.359493	6.911166
Pt125	18.01955	7.756389	6.899998
Pt126	20.80179	7.772514	6.918222
Pt127	19.29913	0.541822	6.840596
Pt128	19.38933	5.399269	6.927378
Pt129	0.000000	9.611602	0.000000
Pt130	4.161946	12.0145	0.000000

Pt131	1.387315	12.0145	0.000000
Pt132	0.000000	14.4174	0.000000
Pt133	1.387315	16.8203	0.000000
Pt134	4.161946	16.8203	0.000000
Pt135	2.774631	9.611602	0.000000
Pt136	2.774631	14.4174	0.000000
Pt137	4.153274	18.58739	2.307876
Pt138	1.377656	18.59218	2.331486
Pt139	22.19444	11.37634	2.310556
Pt140	22.19648	16.19269	2.314524
Pt141	2.770717	11.37376	2.311043
Pt142	1.385895	13.78289	2.310039
Pt143	4.158964	13.7812	2.312873
Pt144	2.774746	16.18629	2.307962
Pt145	4.165037	15.58314	4.593133
Pt146	1.393025	15.57759	4.583685
Pt147	22.19037	17.97863	4.633121
Pt148	22.19438	13.16674	4.580418
Pt149	1.382782	10.76773	4.589979
Pt150	4.15633	10.77506	4.593987
Pt151	2.772748	13.17464	4.591241
Pt152	2.782616	17.98893	4.583293
Pt153	22.18976	10.15253	6.909573
Pt154	4.163179	12.54321	6.906759
Pt155	1.384372	12.53931	6.902078
Pt156	0.013252	14.92348	6.886629
Pt157	1.446948	17.32301	6.877655
Pt158	4.180374	17.34848	6.912513
Pt159	2.766389	10.14796	6.904565
Pt160	2.786005	14.93785	6.906929
Pt161	5.549261	9.611602	0.000000
Pt162	9.711207	12.0145	0.000000
Pt163	6.936576	12.0145	0.000000
Pt164	5.549261	14.4174	0.000000
Pt165	6.936576	16.8203	0.000000
Pt166	9.711207	16.8203	0.000000
Pt167	8.323892	9.611602	0.000000

Pt168	8.323892	14.4174	0.000000
Pt169	9.710956	18.58898	2.311426
Pt170	6.931624	18.58731	2.306014
Pt171	5.543623	11.37695	2.313791
Pt172	5.547323	16.18527	2.311221
Pt173	8.320222	11.38133	2.312109
Pt174	6.929588	13.78287	2.310703
Pt175	9.705632	13.7824	2.311641
Pt176	8.323795	16.18595	2.312941
Pt177	9.710343	15.58195	4.588439
Pt178	6.934485	15.58219	4.591029
Pt179	5.548066	17.98731	4.585106
Pt180	5.544614	13.1784	4.591816
Pt181	6.932445	10.77698	4.590634
Pt182	9.704678	10.77895	4.590791
Pt183	8.316389	13.18034	4.590181
Pt184	8.318304	17.98594	4.587713
Pt185	5.551192	10.13971	6.904883
Pt186	9.705733	12.54799	6.903112
Pt187	6.933482	12.54151	6.906585
Pt188	5.556803	14.93915	6.907526
Pt189	6.934554	17.34562	6.899798
Pt190	9.70779	17.35133	6.90066
Pt191	8.31732	10.14301	6.905017
Pt192	8.323343	14.94704	6.902704
Pt193	11.09852	9.611602	0.000000
Pt194	15.26047	12.0145	0.000000
Pt195	12.48584	12.0145	0.000000
Pt196	11.09852	14.4174	0.000000
Pt197	12.48584	16.8203	0.000000
Pt198	15.26047	16.8203	0.000000
Pt199	13.87315	9.611602	0.000000
Pt200	13.87315	14.4174	0.000000
Pt201	15.27425	18.58265	2.311094
Pt202	12.49247	18.58607	2.309215
Pt203	11.09605	11.38101	2.310366
Pt204	11.10042	16.18576	2.313769

Pt205	13.87223	11.38064	2.313768
Pt206	12.48263	13.78376	2.312516
Pt207	15.2601	13.78007	2.315704
Pt208	13.8774	16.18195	2.309475
Pt209	15.25995	15.5833	4.593706
Pt210	12.48983	15.58162	4.591566
Pt211	11.09465	17.98359	4.584103
Pt212	11.09354	13.18079	4.590986
Pt213	12.47889	10.77795	4.590438
Pt214	15.25172	10.78074	4.594004
Pt215	13.86925	13.18018	4.590781
Pt216	13.87171	17.98724	4.58635
Pt217	11.08918	10.14532	6.902077
Pt218	15.24429	12.54956	6.909816
Pt219	12.47994	12.54775	6.902489
Pt220	11.08778	14.95404	6.905315
Pt221	12.47479	17.35232	6.897566
Pt222	15.23281	17.3507	6.911888
Pt223	13.86072	10.14334	6.907619
Pt224	13.86078	14.94651	6.907677
Pt225	16.64778	9.611602	0.000000
Pt226	20.80973	12.0145	0.000000
Pt227	18.0351	12.0145	0.000000
Pt228	16.64778	14.4174	0.000000
Pt229	18.0351	16.8203	0.000000
Pt230	20.80973	16.8203	0.000000
Pt231	19.42241	9.611602	0.000000
Pt232	19.42241	14.4174	0.000000
Pt233	20.81406	18.58585	2.333784
Pt234	18.04675	18.58256	2.321268
Pt235	16.6443	11.37461	2.313613
Pt236	16.65265	16.17981	2.31345
Pt237	19.41824	11.37433	2.311321
Pt238	18.03013	13.77872	2.310537
Pt239	20.80451	13.78682	2.308966
Pt240	19.426	16.18763	2.324751
Pt241	20.81437	15.567	4.604923

Pt242	18.0308	15.57469	4.602268
Pt243	16.64301	17.98354	4.593217
Pt244	16.64557	13.181	4.597242
Pt245	18.02714	10.77248	4.59031
Pt246	20.80373	10.76848	4.589396
Pt247	19.42123	13.17058	4.586277
Pt248	19.43351	17.95734	4.623674
Pt249	16.63595	10.15449	6.902184
Pt250	20.80373	12.54447	6.903917
Pt251	18.02528	12.54986	6.904894
Pt252	16.62995	14.95369	6.919003
Pt253	17.97257	17.3474	6.922624
Pt254	20.75644	17.35414	6.925287
Pt255	19.412	10.15147	6.901938
Pt256	19.40048	14.92511	6.910419

Table S6. Atomic coordinates (cartesian; Å) of the Type B structure shown in Fig. 1(b)

Atom label	X [Å]	Y [Å]	Z [Å]
N1	21.06255	17.85896	10.19446
N2	19.60525	0.211721	9.148359
N3	18.68879	17.63328	10.43135
N4	21.94804	0.499306	9.110497
N5	17.3795	0.218389	9.84387
N6	20.11065	15.86161	10.84924
C1	20.82093	18.95595	9.512058
C2	18.56165	18.8103	9.813195
C3	19.93399	17.13484	10.47333
H1	21.82681	1.502443	9.301251
H2	17.23589	1.040071	9.248885
H3	19.29799	15.26268	10.9512
H4	0.601695	0.126066	9.54505
H5	16.56301	18.90727	10.12734
H6	21.03408	15.44981	10.76307
Pt1	0.000000	0.000000	0.000000
Pt2	4.161946	2.4029	0.000000
Pt3	1.387315	2.4029	0.000000
Pt4	0.000000	4.805801	0.000000
Pt5	1.387315	7.208701	0.000000
Pt6	4.161946	7.208701	0.000000
Pt7	2.774631	0.000000	0.000000
Pt8	2.774631	4.805801	0.000000
Pt9	4.162022	8.97427	2.313934
Pt10	1.388116	8.971524	2.313255
Pt11	22.18905	1.755522	2.335803
Pt12	22.19447	6.568776	2.314015
Pt13	2.755685	1.763963	2.328835
Pt14	1.374248	4.162365	2.310678
Pt15	4.151305	4.164844	2.308381
Pt16	2.772564	6.569035	2.30981
Pt17	4.167109	5.965908	4.58711
Pt18	1.390688	5.964856	4.5885
Pt19	0.002728	8.367285	4.594021

Pt20	22.19537	3.569289	4.599423
Pt21	1.350914	1.153101	4.643593
Pt22	4.154184	1.162574	4.587803
Pt23	2.771916	3.55735	4.588073
Pt24	2.780052	8.3693	4.59197
Pt25	0.063401	0.546923	6.956252
Pt26	4.172434	2.939095	6.909304
Pt27	1.409037	2.977317	6.921944
Pt28	0.002872	5.360888	6.91355
Pt29	1.3928	7.743841	6.904229
Pt30	4.168393	7.731419	6.902132
Pt31	2.820684	0.527368	6.917543
Pt32	2.780459	5.342256	6.900061
Pt33	5.549261	0.000000	0.000000
Pt34	9.711207	2.4029	0.000000
Pt35	6.936576	2.4029	0.000000
Pt36	5.549261	4.805801	0.000000
Pt37	6.936576	7.208701	0.000000
Pt38	9.711207	7.208701	0.000000
Pt39	8.323892	0.000000	0.000000
Pt40	8.323892	4.805801	0.000000
Pt41	9.711368	8.977673	2.311035
Pt42	6.938248	8.976854	2.311217
Pt43	5.531499	1.76506	2.31056
Pt44	5.549498	6.572408	2.312648
Pt45	8.317951	1.765807	2.308408
Pt46	6.93014	4.167236	2.31089
Pt47	9.709557	4.168991	2.312222
Pt48	8.323995	6.57305	2.31246
Pt49	9.71033	5.964113	4.591278
Pt50	6.940796	5.965975	4.590505
Pt51	5.555704	8.371643	4.591091
Pt52	5.545184	3.563651	4.590494
Pt53	6.933058	1.163853	4.583161
Pt54	9.709733	1.160688	4.586383
Pt55	8.320389	3.563459	4.588107
Pt56	8.326547	8.372808	4.591376

Pt57	5.553224	0.5293	6.90081
Pt58	9.708624	2.925423	6.900749
Pt59	6.939832	2.930989	6.901593
Pt60	5.558651	5.336846	6.906607
Pt61	6.939568	7.733641	6.905678
Pt62	9.710497	7.733275	6.904356
Pt63	8.318906	0.521763	6.893121
Pt64	8.326542	5.329764	6.90735
Pt65	11.09852	0.000000	0.000000
Pt66	15.26047	2.4029	0.000000
Pt67	12.48584	2.4029	0.000000
Pt68	11.09852	4.805801	0.000000
Pt69	12.48584	7.208701	0.000000
Pt70	15.26047	7.208701	0.000000
Pt71	13.87315	0.000000	0.000000
Pt72	13.87315	4.805801	0.000000
Pt73	15.26055	8.973791	2.313278
Pt74	12.48469	8.976764	2.311667
Pt75	11.10293	1.766797	2.30776
Pt76	11.09785	6.573103	2.312961
Pt77	13.89027	1.764806	2.308961
Pt78	12.49039	4.167225	2.311177
Pt79	15.26954	4.163391	2.311344
Pt80	13.87097	6.571777	2.312297
Pt81	15.2541	5.965972	4.588834
Pt82	12.48104	5.967033	4.591828
Pt83	11.09575	8.372077	4.591249
Pt84	11.09676	3.564174	4.587765
Pt85	12.48449	1.166041	4.581109
Pt86	15.26166	1.165365	4.577064
Pt87	13.87107	3.564867	4.592722
Pt88	13.86689	8.371602	4.59123
Pt89	11.10004	0.524814	6.895437
Pt90	15.24019	2.946952	6.914974
Pt91	12.47524	2.931709	6.903592
Pt92	11.09137	5.330012	6.908519
Pt93	12.47968	7.733878	6.90625

Pt94	15.25245	7.736154	6.90215
Pt95	13.85919	0.529603	6.898715
Pt96	13.86023	5.340858	6.91032
Pt97	16.64778	0.000000	0.000000
Pt98	20.80973	2.4029	0.000000
Pt99	18.0351	2.4029	0.000000
Pt100	16.64778	4.805801	0.000000
Pt101	18.0351	7.208701	0.000000
Pt102	20.80973	7.208701	0.000000
Pt103	19.42241	0.000000	0.000000
Pt104	19.42241	4.805801	0.000000
Pt105	20.81042	8.970634	2.313134
Pt106	18.03564	8.972218	2.313718
Pt107	16.67031	1.761951	2.32837
Pt108	16.64635	6.569657	2.310398
Pt109	19.42941	1.756788	2.340159
Pt110	18.04259	4.16336	2.310968
Pt111	20.80677	4.160504	2.310828
Pt112	19.42134	6.56976	2.313805
Pt113	20.80819	5.968682	4.593222
Pt114	18.02849	5.967605	4.590248
Pt115	16.64352	8.369921	4.592038
Pt116	16.64555	3.557768	4.593678
Pt117	18.07532	1.158217	4.65847
Pt118	20.80115	1.164014	4.667205
Pt119	19.41572	3.573827	4.600489
Pt120	19.42078	8.368024	4.59479
Pt121	16.58402	0.523092	6.877568
Pt122	20.80636	2.994869	6.90489
Pt123	18.00593	2.986883	6.930838
Pt124	16.63599	5.346244	6.906122
Pt125	18.02803	7.746914	6.906468
Pt126	20.80875	7.747656	6.909739
Pt127	19.35512	0.589255	7.02482
Pt128	19.41532	5.366721	6.913847
Pt129	0.000000	9.611602	0.000000
Pt130	4.161946	12.0145	0.000000

Pt131	1.387315	12.0145	0.000000
Pt132	0.000000	14.4174	0.000000
Pt133	1.387315	16.8203	0.000000
Pt134	4.161946	16.8203	0.000000
Pt135	2.774631	9.611602	0.000000
Pt136	2.774631	14.4174	0.000000
Pt137	4.157738	18.58526	2.311672
Pt138	1.384359	18.59148	2.323269
Pt139	0.002023	11.375	2.311184
Pt140	0.002435	16.19192	2.302683
Pt141	2.776089	11.3766	2.313186
Pt142	1.387657	13.78239	2.311876
Pt143	4.160396	13.78201	2.312136
Pt144	2.774616	16.18784	2.312155
Pt145	4.162397	15.57797	4.591822
Pt146	1.38685	15.57357	4.586377
Pt147	0.005978	17.97795	4.601684
Pt148	0.000226	13.16532	4.589944
Pt149	1.390083	10.76758	4.592582
Pt150	4.16394	10.77371	4.592282
Pt151	2.772444	13.17435	4.592133
Pt152	2.780273	17.98393	4.597811
Pt153	22.19528	10.13794	6.906517
Pt154	4.162519	12.53895	6.906351
Pt155	1.387535	12.53969	6.905873
Pt156	0.004875	14.9236	6.901923
Pt157	1.404785	17.32282	6.901235
Pt158	4.168842	17.33754	6.9125
Pt159	2.776443	10.13944	6.904381
Pt160	2.782594	14.93534	6.907305
Pt161	5.549261	9.611602	0.000000
Pt162	9.711207	12.0145	0.000000
Pt163	6.936576	12.0145	0.000000
Pt164	5.549261	14.4174	0.000000
Pt165	6.936576	16.8203	0.000000
Pt166	9.711207	16.8203	0.000000
Pt167	8.323892	9.611602	0.000000

Pt168	8.323892	14.4174	0.000000
Pt169	9.711894	18.58986	2.312829
Pt170	6.932793	18.5872	2.311612
Pt171	5.548634	11.37982	2.314038
Pt172	5.549453	16.18542	2.313312
Pt173	8.32324	11.38137	2.311385
Pt174	6.934162	13.78184	2.313064
Pt175	9.71099	13.78228	2.31357
Pt176	8.324499	16.18576	2.313439
Pt177	9.713562	15.57979	4.593592
Pt178	6.93583	15.57917	4.591104
Pt179	5.546824	17.98395	4.594409
Pt180	5.546038	13.17871	4.594703
Pt181	6.936301	10.77713	4.589831
Pt182	9.709996	10.77698	4.590891
Pt183	8.32181	13.17872	4.591047
Pt184	8.322898	17.98122	4.587933
Pt185	5.551984	10.13706	6.903328
Pt186	9.710664	12.54563	6.901654
Pt187	6.9386	12.54104	6.905031
Pt188	5.552114	14.94413	6.908967
Pt189	6.941855	17.3415	6.903055
Pt190	9.71104	17.35	6.90276
Pt191	8.322097	10.13874	6.902584
Pt192	8.323053	14.94213	6.904445
Pt193	11.09852	9.611602	0.000000
Pt194	15.26047	12.0145	0.000000
Pt195	12.48584	12.0145	0.000000
Pt196	11.09852	14.4174	0.000000
Pt197	12.48584	16.8203	0.000000
Pt198	15.26047	16.8203	0.000000
Pt199	13.87315	9.611602	0.000000
Pt200	13.87315	14.4174	0.000000
Pt201	15.2661	18.58539	2.307818
Pt202	12.49038	18.5874	2.310091
Pt203	11.09955	11.38138	2.311797
Pt204	11.09791	16.18611	2.313455

Pt205	13.87375	11.37912	2.314469
Pt206	12.48742	13.78192	2.313154
Pt207	15.26039	13.78085	2.311451
Pt208	13.87275	16.18542	2.312933
Pt209	15.26056	15.57562	4.592079
Pt210	12.48887	15.57887	4.59113
Pt211	11.10256	17.98288	4.589451
Pt212	11.09966	13.17805	4.592016
Pt213	12.48417	10.77704	4.590062
Pt214	15.25784	10.77199	4.592575
Pt215	13.87482	13.17765	4.595158
Pt216	13.8764	17.98493	4.591597
Pt217	11.09842	10.13887	6.902422
Pt218	15.25962	12.5413	6.906656
Pt219	12.48281	12.53955	6.90689
Pt220	11.10161	14.94282	6.905611
Pt221	12.48081	17.33952	6.902629
Pt222	15.25258	17.33638	6.909587
Pt223	13.86808	10.13978	6.902669
Pt224	13.86974	14.94389	6.910862
Pt225	16.64778	9.611602	0.000000
Pt226	20.80973	12.0145	0.000000
Pt227	18.0351	12.0145	0.000000
Pt228	16.64778	14.4174	0.000000
Pt229	18.0351	16.8203	0.000000
Pt230	20.80973	16.8203	0.000000
Pt231	19.42241	9.611602	0.000000
Pt232	19.42241	14.4174	0.000000
Pt233	20.81024	18.59223	2.332333
Pt234	18.04127	18.59205	2.32373
Pt235	16.64744	11.37527	2.312972
Pt236	16.64635	16.18719	2.310182
Pt237	19.42241	11.37526	2.31091
Pt238	18.03388	13.78236	2.31233
Pt239	20.80902	13.78466	2.313875
Pt240	19.4195	16.19352	2.300896
Pt241	20.80951	15.56401	4.565455

Pt242	18.03632	15.57008	4.580924
Pt243	16.64305	17.98133	4.586224
Pt244	16.64762	13.1718	4.591038
Pt245	18.03259	10.7679	4.592513
Pt246	20.81006	10.76596	4.590476
Pt247	19.42057	13.16448	4.59165
Pt248	19.42046	17.98384	4.606065
Pt249	16.64601	10.13934	6.90487
Pt250	20.80871	12.53184	6.907655
Pt251	18.03325	12.53955	6.907358
Pt252	16.63984	14.93162	6.907082
Pt253	18.02208	17.31918	6.874103
Pt254	20.81174	17.28383	6.843224
Pt255	19.42287	10.14114	6.908405
Pt256	19.4188	14.92844	6.90236

Table S7. Atomic coordinates (cartesian; Å) of the Type C structure shown in Fig. 1(c)

Atom label	X [Å]	Y [Å]	Z [Å]
N1	0.264774	17.16751	9.429768
N2	20.46854	18.36825	10.00604
N3	20.46793	15.96375	9.999554
N4	0.150757	0.266776	9.220708
N5	18.55001	17.16521	10.45918
N6	0.146047	14.84678	9.198079
C1	21.73498	18.28754	9.619407
C2	19.85757	17.16619	10.16165
C3	21.73295	16.0468	9.610733
H1	21.87463	1.096483	9.588414
H2	18.04007	18.04118	10.39612
H3	21.86448	14.0129	9.54969
H4	1.167682	0.282885	9.349931
H5	18.03993	16.2897	10.3913
H6	1.16256	14.82293	9.330562
Pt1	0.000000	0.000000	0.000000
Pt2	4.161946	2.4029	0.000000
Pt3	1.387315	2.4029	0.000000
Pt4	0.000000	4.805801	0.000000
Pt5	1.387315	7.208701	0.000000
Pt6	4.161946	7.208701	0.000000
Pt7	2.774631	0.000000	0.000000
Pt8	2.774631	4.805801	0.000000
Pt9	4.162362	8.925941	2.30672
Pt10	1.38714	8.930217	2.307698
Pt11	0.000639	1.713078	2.333679
Pt12	22.19697	6.525274	2.308343
Pt13	2.765736	1.716742	2.312826
Pt14	1.382526	4.11906	2.31046
Pt15	4.157458	4.118914	2.305764
Pt16	2.773768	6.521764	2.306359
Pt17	4.164013	5.857627	4.58039
Pt18	1.387252	5.859387	4.585444
Pt19	7.06E-06	8.259667	4.582059

Pt20	0.000837	3.462056	4.602527
Pt21	1.383094	1.058232	4.62666
Pt22	4.167848	1.054082	4.573949
Pt23	2.776983	3.453952	4.581277
Pt24	2.776018	8.260864	4.58031
Pt25	0.001697	0.416628	6.965666
Pt26	4.173169	2.776815	6.890442
Pt27	1.403721	2.81648	6.908163
Pt28	0.001537	5.195303	6.908011
Pt29	1.390607	7.581211	6.891165
Pt30	4.162643	7.579577	6.887099
Pt31	2.819244	0.376217	6.895179
Pt32	2.782406	5.18061	6.892483
Pt33	5.549261	0.000000	0.000000
Pt34	9.711207	2.4029	0.000000
Pt35	6.936576	2.4029	0.000000
Pt36	5.549261	4.805801	0.000000
Pt37	6.936576	7.208701	0.000000
Pt38	9.711207	7.208701	0.000000
Pt39	8.323892	0.000000	0.000000
Pt40	8.323892	4.805801	0.000000
Pt41	9.711122	8.931976	2.30605
Pt42	6.93529	8.929955	2.308117
Pt43	5.543361	1.720273	2.305032
Pt44	5.54977	6.525278	2.308142
Pt45	8.320786	1.723388	2.303695
Pt46	6.934762	4.126137	2.30655
Pt47	9.710499	4.12733	2.306213
Pt48	8.325931	6.530563	2.308498
Pt49	9.712599	5.86095	4.584096
Pt50	6.939814	5.862666	4.580801
Pt51	5.550862	8.26405	4.584879
Pt52	5.552885	3.459646	4.580317
Pt53	6.939208	1.058181	4.57563
Pt54	9.711268	1.053591	4.579861
Pt55	8.327526	3.459851	4.58182
Pt56	8.325459	8.265522	4.582422

Pt57	5.565899	0.379205	6.89422
Pt58	9.717608	2.768122	6.888025
Pt59	6.949007	2.775062	6.890534
Pt60	5.558302	5.179755	6.888785
Pt61	6.946954	7.575049	6.893241
Pt62	9.716962	7.577498	6.890637
Pt63	8.326434	0.368842	6.887671
Pt64	8.328065	5.173739	6.893352
Pt65	11.09852	0.000000	0.000000
Pt66	15.26047	2.4029	0.000000
Pt67	12.48584	2.4029	0.000000
Pt68	11.09852	4.805801	0.000000
Pt69	12.48584	7.208701	0.000000
Pt70	15.26047	7.208701	0.000000
Pt71	13.87315	0.000000	0.000000
Pt72	13.87315	4.805801	0.000000
Pt73	15.26114	8.932163	2.307861
Pt74	12.48584	8.929969	2.305672
Pt75	11.09663	1.723623	2.306267
Pt76	11.09939	6.526793	2.306546
Pt77	13.87286	1.723642	2.303684
Pt78	12.488	4.124699	2.306704
Pt79	15.2646	4.125289	2.307042
Pt80	13.87311	6.528433	2.305897
Pt81	15.26027	5.861654	4.579247
Pt82	12.48711	5.859147	4.582031
Pt83	11.09859	8.264099	4.579019
Pt84	11.09885	3.458072	4.576662
Pt85	12.48372	1.052245	4.578231
Pt86	15.2562	1.060692	4.576634
Pt87	13.87177	3.457167	4.583406
Pt88	13.87281	8.263206	4.581127
Pt89	11.09982	0.362846	6.887972
Pt90	15.25303	2.772751	6.893474
Pt91	12.48169	2.769074	6.888055
Pt92	11.10145	5.170955	6.889206
Pt93	12.48244	7.577726	6.887807

Pt94	15.25486	7.574131	6.892226
Pt95	13.87122	0.369748	6.887206
Pt96	13.87552	5.173536	6.89115
Pt97	16.64778	0.000000	0.000000
Pt98	20.80973	2.4029	0.000000
Pt99	18.0351	2.4029	0.000000
Pt100	16.64778	4.805801	0.000000
Pt101	18.0351	7.208701	0.000000
Pt102	20.80973	7.208701	0.000000
Pt103	19.42241	0.000000	0.000000
Pt104	19.42241	4.805801	0.000000
Pt105	20.80995	8.927273	2.306784
Pt106	18.03421	8.927048	2.307109
Pt107	16.65498	1.724172	2.309481
Pt108	16.64854	6.528665	2.309236
Pt109	19.4336	1.715919	2.320883
Pt110	18.04109	4.12024	2.307959
Pt111	20.81518	4.117208	2.30956
Pt112	19.4236	6.521117	2.305327
Pt113	20.80876	5.85564	4.584131
Pt114	18.03298	5.859827	4.58159
Pt115	16.64645	8.268795	4.585032
Pt116	16.64833	3.461663	4.585186
Pt117	18.0293	1.060034	4.582908
Pt118	20.82608	1.048233	4.634018
Pt119	19.42319	3.45109	4.584832
Pt120	19.42067	8.260183	4.579487
Pt121	16.62912	0.377394	6.900903
Pt122	20.79569	2.810434	6.91336
Pt123	18.03045	2.776645	6.898554
Pt124	16.64058	5.17714	6.892924
Pt125	18.03694	7.579235	6.886604
Pt126	20.80854	7.578192	6.888449
Pt127	19.38274	0.370373	6.892235
Pt128	19.41723	5.179259	6.891912
Pt129	0.000000	9.611602	0.000000
Pt130	4.161946	12.0145	0.000000

Pt131	1.387315	12.0145	0.000000
Pt132	0.000000	14.4174	0.000000
Pt133	1.387315	16.8203	0.000000
Pt134	4.161946	16.8203	0.000000
Pt135	2.774631	9.611602	0.000000
Pt136	2.774631	14.4174	0.000000
Pt137	4.154818	18.53664	2.314451
Pt138	1.387245	18.54343	2.319418
Pt139	1.95E-05	11.33997	2.307752
Pt140	0.00457	16.14264	2.31174
Pt141	2.774148	11.33283	2.308393
Pt142	1.383649	13.74417	2.324727
Pt143	4.157694	13.73316	2.305212
Pt144	2.768815	16.14083	2.311392
Pt145	4.163018	15.4749	4.577094
Pt146	1.378797	15.46769	4.610228
Pt147	0.008867	17.88264	4.590608
Pt148	0.005151	13.05752	4.619061
Pt149	1.388218	10.66075	4.578549
Pt150	4.164057	10.66448	4.585494
Pt151	2.779054	13.06549	4.587671
Pt152	2.776783	17.86985	4.596386
Pt153	22.19639	9.976097	6.892648
Pt154	4.174832	12.3807	6.900637
Pt155	1.410383	12.35616	6.892859
Pt156	22.19658	14.77824	6.94551
Pt157	1.423856	17.20582	6.895154
Pt158	4.189349	17.18992	6.909925
Pt159	2.783337	9.975881	6.893096
Pt160	2.82328	14.77563	6.887938
Pt161	5.549261	9.611602	0.000000
Pt162	9.711207	12.0145	0.000000
Pt163	6.936576	12.0145	0.000000
Pt164	5.549261	14.4174	0.000000
Pt165	6.936576	16.8203	0.000000
Pt166	9.711207	16.8203	0.000000
Pt167	8.323892	9.611602	0.000000

Pt168	8.323892	14.4174	0.000000
Pt169	9.708517	18.54371	2.307898
Pt170	6.930618	18.54064	2.306563
Pt171	5.547201	11.33222	2.307909
Pt172	5.541804	16.13845	2.306287
Pt173	8.321723	11.33699	2.306004
Pt174	6.931096	13.73634	2.305032
Pt175	9.709864	13.73796	2.306661
Pt176	8.321012	16.14008	2.306041
Pt177	9.71034	15.47433	4.58249
Pt178	6.936226	15.47598	4.576628
Pt179	5.550789	17.87607	4.58675
Pt180	5.547744	13.07251	4.583984
Pt181	6.937464	10.66842	4.579245
Pt182	9.709425	10.66956	4.579162
Pt183	8.320487	13.07349	4.579653
Pt184	8.323294	17.87523	4.58517
Pt185	5.561821	9.978347	6.892483
Pt186	9.716525	12.38555	6.883941
Pt187	6.946264	12.37965	6.891581
Pt188	5.567183	14.78528	6.89463
Pt189	6.946639	17.18847	6.893815
Pt190	9.715883	17.18898	6.89659
Pt191	8.325854	9.97959	6.889642
Pt192	8.324296	14.78515	6.887393
Pt193	11.09852	9.611602	0.000000
Pt194	15.26047	12.0145	0.000000
Pt195	12.48584	12.0145	0.000000
Pt196	11.09852	14.4174	0.000000
Pt197	12.48584	16.8203	0.000000
Pt198	15.26047	16.8203	0.000000
Pt199	13.87315	9.611602	0.000000
Pt200	13.87315	14.4174	0.000000
Pt201	15.25717	18.54307	2.302893
Pt202	12.48483	18.54103	2.306642
Pt203	11.09747	11.33455	2.305223
Pt204	11.09872	16.1379	2.308414

Pt205	13.87257	11.33587	2.305996
Pt206	12.48987	13.73666	2.307353
Pt207	15.26583	13.7363	2.305934
Pt208	13.87767	16.13899	2.305904
Pt209	15.26246	15.47736	4.579486
Pt210	12.48721	15.47112	4.578981
Pt211	11.09713	17.87318	4.579156
Pt212	11.09955	13.07113	4.576006
Pt213	12.48648	10.66819	4.578027
Pt214	15.26028	10.66952	4.579358
Pt215	13.87877	13.07171	4.583187
Pt216	13.87101	17.87489	4.58525
Pt217	11.10062	9.981718	6.886195
Pt218	15.25493	12.37847	6.893019
Pt219	12.48169	12.38452	6.886046
Pt220	11.10038	14.78664	6.887017
Pt221	12.48046	17.18594	6.890299
Pt222	15.2522	17.18884	6.898199
Pt223	13.87486	9.979918	6.88721
Pt224	13.87258	14.78602	6.889026
Pt225	16.64778	9.611602	0.000000
Pt226	20.80973	12.0145	0.000000
Pt227	18.0351	12.0145	0.000000
Pt228	16.64778	14.4174	0.000000
Pt229	18.0351	16.8203	0.000000
Pt230	20.80973	16.8203	0.000000
Pt231	19.42241	9.611602	0.000000
Pt232	19.42241	14.4174	0.000000
Pt233	20.81975	18.5444	2.306978
Pt234	18.03299	18.54248	2.299481
Pt235	16.6495	11.33382	2.310614
Pt236	16.65729	16.13968	2.30785
Pt237	19.42253	11.33016	2.307285
Pt238	18.0396	13.73194	2.306581
Pt239	20.81564	13.73989	2.326878
Pt240	19.42932	16.13799	2.302093
Pt241	20.82327	15.44462	4.590625

Pt242	18.03547	15.47385	4.577579
Pt243	16.63438	17.88402	4.578395
Pt244	16.64941	13.07477	4.586172
Pt245	18.03409	10.66701	4.586886
Pt246	20.81142	10.6584	4.577912
Pt247	19.4188	13.05887	4.590439
Pt248	19.39359	17.88245	4.537146
Pt249	16.64022	9.979562	6.89319
Pt250	20.79174	12.35738	6.896753
Pt251	18.025	12.38602	6.903864
Pt252	16.62738	14.785	6.902508
Pt253	18.00086	17.19643	6.894424
Pt254	20.73752	17.18657	6.754882
Pt255	19.41745	9.977552	6.891182
Pt256	19.37419	14.77704	6.889374

Table S8. Atomic coordinates (cartesian; Å) of the Type D structure shown in Fig. 1(d)

Atom label	X [Å]	Y [Å]	Z [Å]
N1	1.387152	2.132538	10.1675
N2	2.585399	0.105684	9.65862
N3	0.189218	0.105274	9.660005
N4	3.694445	2.0765	10.12756
N5	1.387288	17.38802	9.141545
N6	21.27703	2.076106	10.12874
C1	2.52117	1.435021	9.986852
C2	1.387208	18.76283	9.535515
C3	0.253438	1.434755	9.987659
H1	4.542165	1.613431	9.809989
H2	2.238977	16.90933	9.45289
H3	20.42928	1.612778	9.811483
H4	3.683452	3.089436	10.19724
H5	0.535458	16.90942	9.452841
H6	21.28792	3.089061	10.19779
Pt1	0.000000	0000000	0000000
Pt2	4.161946	2.4029	0000000
Pt3	1.387315	2.4029	0000000
Pt4	0000000	4.805801	0000000
Pt5	1.387315	7.208701	0000000
Pt6	4.161946	7.208701	0000000
Pt7	2.774631	0000000	0000000
Pt8	2.774631	4.805801	0000000
Pt9	4.161234	8.925972	2.30695
Pt10	1.387371	8.929603	2.30664
Pt11	0.004817	1.712391	2.306418
Pt12	0.001102	6.522678	2.308123
Pt13	2.769631	1.712513	2.306357
Pt14	1.387194	4.119707	2.309003
Pt15	4.160071	4.117792	2.306455
Pt16	2.773519	6.522721	2.3082
Pt17	4.164382	5.848488	4.582471
Pt18	1.387231	5.84921	4.587595
Pt19	22.19674	8.250624	4.581927

Pt20	22.19287	3.449544	4.581096
Pt21	1.387302	1.048456	4.599819
Pt22	4.167883	1.044846	4.569445
Pt23	2.77865	3.449464	4.581074
Pt24	2.774736	8.250636	4.581939
Pt25	22.13939	0.378975	6.867084
Pt26	4.175052	2.768554	6.890436
Pt27	1.387117	2.778197	6.87876
Pt28	22.19393	5.164476	6.898268
Pt29	1.387214	7.559949	6.895218
Pt30	4.16249	7.55498	6.888801
Pt31	2.832148	0.37915	6.867285
Pt32	2.777409	5.164334	6.898357
Pt33	5.549261	0000000	0000000
Pt34	9.711207	2.4029	0000000
Pt35	6.936576	2.4029	0000000
Pt36	5.549261	4.805801	0000000
Pt37	6.936576	7.208701	0000000
Pt38	9.711207	7.208701	0000000
Pt39	8.323892	0000000	0000000
Pt40	8.323892	4.805801	0000000
Pt41	9.711	8.927248	2.307553
Pt42	6.936399	8.926471	2.307876
Pt43	5.545816	1.715654	2.306985
Pt44	5.548565	6.523013	2.30816
Pt45	8.32223	1.717985	2.306399
Pt46	6.937567	4.12076	2.306483
Pt47	9.712021	4.121741	2.305831
Pt48	8.323984	6.524537	2.306706
Pt49	9.71359	5.852139	4.581727
Pt50	6.939106	5.851971	4.582031
Pt51	5.549661	8.253566	4.582534
Pt52	5.556638	3.447189	4.579498
Pt53	6.940695	1.04997	4.580739
Pt54	9.713216	1.045787	4.583485
Pt55	8.328145	3.449141	4.582777
Pt56	8.324461	8.255353	4.580523

Pt57	5.57798	0.353464	6.896816
Pt58	9.71698	2.750932	6.891317
Pt59	6.945727	2.757737	6.89847
Pt60	5.551164	5.153795	6.891052
Pt61	6.940613	7.555347	6.886537
Pt62	9.710383	7.554721	6.889314
Pt63	8.329113	0.35183	6.891142
Pt64	8.329279	5.153431	6.889442
Pt65	11.09852	0000000	0000000
Pt66	15.26047	2.4029	0000000
Pt67	12.48584	2.4029	0000000
Pt68	11.09852	4.805801	0000000
Pt69	12.48584	7.208701	0000000
Pt70	15.26047	7.208701	0000000
Pt71	13.87315	0000000	0000000
Pt72	13.87315	4.805801	0000000
Pt73	15.2605	8.927149	2.307523
Pt74	12.48587	8.92603	2.305335
Pt75	11.09796	1.717379	2.306595
Pt76	11.09883	6.523567	2.306184
Pt77	13.87375	1.717458	2.306768
Pt78	12.48577	4.121087	2.306809
Pt79	15.2597	4.121772	2.305918
Pt80	13.87291	6.523559	2.306235
Pt81	15.25799	5.852313	4.581672
Pt82	12.48592	5.850933	4.578773
Pt83	11.09806	8.255693	4.58173
Pt84	11.0995	3.446541	4.581316
Pt85	12.48591	1.044409	4.577336
Pt86	15.25853	1.045762	4.583609
Pt87	13.87213	3.446646	4.581462
Pt88	13.87347	8.255672	4.581754
Pt89	11.10049	0.343994	6.886531
Pt90	15.25455	2.751073	6.89142
Pt91	12.48593	2.744182	6.890718
Pt92	11.10184	5.151156	6.887121
Pt93	12.48579	7.553183	6.885622

Pt94	15.26126	7.554876	6.889179
Pt95	13.87139	0.343856	6.886709
Pt96	13.86972	5.15131	6.88713
Pt97	16.64778	0000000	0000000
Pt98	20.80973	2.4029	0000000
Pt99	18.0351	2.4029	0000000
Pt100	16.64778	4.805801	0000000
Pt101	18.0351	7.208701	0000000
Pt102	20.80973	7.208701	0000000
Pt103	19.42241	0000000	0000000
Pt104	19.42241	4.805801	0000000
Pt105	20.81043	8.926023	2.306773
Pt106	18.03533	8.926572	2.30768
Pt107	16.64938	1.718096	2.306437
Pt108	16.64767	6.524517	2.306727
Pt109	19.42577	1.715657	2.307055
Pt110	18.03428	4.1209	2.306457
Pt111	20.81165	4.117718	2.306407
Pt112	19.42312	6.523088	2.308128
Pt113	20.80699	5.848379	4.58234
Pt114	18.03244	5.852008	4.582023
Pt115	16.64706	8.255498	4.580344
Pt116	16.64358	3.449213	4.582974
Pt117	18.03098	1.050097	4.580872
Pt118	20.80353	1.044822	4.569348
Pt119	19.41491	3.447161	4.579432
Pt120	19.42175	8.253549	4.582322
Pt121	16.64262	0.351795	6.89139
Pt122	20.79662	2.76835	6.890587
Pt123	18.02591	2.757746	6.898626
Pt124	16.64236	5.153528	6.889585
Pt125	18.03083	7.555419	6.886584
Pt126	20.80884	7.555154	6.888801
Pt127	19.39375	0.353309	6.896838
Pt128	19.42021	5.153889	6.891143
Pt129	0000000	9.611602	0000000
Pt130	4.161946	12.0145	0000000

Pt131	1.387315	12.0145	0000000
Pt132	0000000	14.4174	0000000
Pt133	1.387315	16.8203	0000000
Pt134	4.161946	16.8203	0000000
Pt135	2.774631	9.611602	0000000
Pt136	2.774631	14.4174	0000000
Pt137	4.155028	18.5356	2.307292
Pt138	1.387263	18.53549	2.326725
Pt139	4.86E-05	11.33669	2.30684
Pt140	0.005416	16.14397	2.328798
Pt141	2.774579	11.33667	2.306900
Pt142	1.387224	13.74681	2.308798
Pt143	4.161132	13.73832	2.308362
Pt144	2.769058	16.14408	2.328927
Pt145	4.166056	15.46104	4.589931
Pt146	1.387348	15.47081	4.629615
Pt147	0.007721	17.86089	4.618233
Pt148	0.001688	13.06181	4.577646
Pt149	1.387319	10.65513	4.57977
Pt150	4.160058	10.65613	4.578872
Pt151	2.772855	13.06173	4.577651
Pt152	2.766871	17.86095	4.618443
Pt153	0.000156	9.955987	6.886784
Pt154	4.16633	12.35782	6.888344
Pt155	1.387177	12.3557	6.887122
Pt156	22.18208	14.74438	6.896811
Pt157	1.387231	17.18167	6.963776
Pt158	4.211547	17.16186	6.882558
Pt159	2.774215	9.955879	6.886855
Pt160	2.78975	14.74444	6.897028
Pt161	5.549261	9.611602	0000000
Pt162	9.711207	12.0145	0000000
Pt163	6.936576	12.0145	0000000
Pt164	5.549261	14.4174	0000000
Pt165	6.936576	16.8203	0000000
Pt166	9.711207	16.8203	0000000
Pt167	8.323892	9.611602	0000000

Pt168	8.323892	14.4174	0000000
Pt169	9.707172	18.53834	2.305033
Pt170	6.929861	18.5373	2.305518
Pt171	5.54955	11.3292	2.306493
Pt172	5.545371	16.13326	2.305769
Pt173	8.322702	11.32959	2.307369
Pt174	6.935345	13.73308	2.307874
Pt175	9.710958	13.7325	2.306104
Pt176	8.321593	16.13471	2.305179
Pt177	9.707822	15.46356	4.580679
Pt178	6.936206	15.46557	4.582164
Pt179	5.55078	17.86933	4.574761
Pt180	5.548894	13.0608	4.584276
Pt181	6.934776	10.65873	4.583741
Pt182	9.70929	10.65729	4.5826
Pt183	8.323216	13.06012	4.58124
Pt184	8.323374	17.87116	4.576431
Pt185	5.546302	9.959226	6.88614
Pt186	9.711479	12.35944	6.888677
Pt187	6.94131	12.35767	6.89114
Pt188	5.559623	14.76098	6.898967
Pt189	6.954469	17.16643	6.889983
Pt190	9.710928	17.16539	6.88325
Pt191	8.326663	9.955768	6.8906
Pt192	8.330168	14.75835	6.888996
Pt193	11.09852	9.611602	0000000
Pt194	15.26047	12.0145	0000000
Pt195	12.48584	12.0145	0000000
Pt196	11.09852	14.4174	0000000
Pt197	12.48584	16.8203	0000000
Pt198	15.26047	16.8203	0000000
Pt199	13.87315	9.611602	0000000
Pt200	13.87315	14.4174	0000000
Pt201	15.26437	18.53831	2.305049
Pt202	12.48575	18.53729	2.304622
Pt203	11.09834	11.32957	2.307406
Pt204	11.09711	16.13546	2.306158

Pt205	13.87325	11.32956	2.307412
Pt206	12.48586	13.73238	2.30764
Pt207	15.26079	13.73248	2.306043
Pt208	13.87461	16.13549	2.306107
Pt209	15.26385	15.46351	4.580674
Pt210	12.48592	15.46096	4.57575
Pt211	11.09772	17.8648	4.5765
Pt212	11.09672	13.05939	4.580549
Pt213	12.48573	10.65775	4.580877
Pt214	15.26227	10.65741	4.582507
Pt215	13.87499	13.05937	4.580657
Pt216	13.87398	17.86487	4.576482
Pt217	11.10034	9.958275	6.887569
Pt218	15.2601	12.35931	6.888703
Pt219	12.48575	12.36142	6.888036
Pt220	11.1022	14.76343	6.884462
Pt221	12.48598	17.16616	6.879366
Pt222	15.26086	17.16526	6.883265
Pt223	13.87142	9.958226	6.887546
Pt224	13.86945	14.76329	6.884538
Pt225	16.64778	9.611602	0000000
Pt226	20.80973	12.0145	0000000
Pt227	18.0351	12.0145	0000000
Pt228	16.64778	14.4174	0000000
Pt229	18.0351	16.8203	0000000
Pt230	20.80973	16.8203	0000000
Pt231	19.42241	9.611602	0000000
Pt232	19.42241	14.4174	0000000
Pt233	20.81649	18.53553	2.307261
Pt234	18.04173	18.5374	2.305479
Pt235	16.64896	11.32953	2.307394
Pt236	16.65005	16.13471	2.305091
Pt237	19.42204	11.32912	2.30654
Pt238	18.03633	13.73297	2.307886
Pt239	20.81039	13.73823	2.308331
Pt240	19.42616	16.13314	2.305567
Pt241	20.80536	15.4609	4.589828

Pt242	18.03527	15.46563	4.582078
Pt243	16.64832	17.87118	4.576441
Pt244	16.64851	13.06015	4.581186
Pt245	18.03682	10.65882	4.583738
Pt246	20.81153	10.65602	4.578671
Pt247	19.42267	13.06088	4.584297
Pt248	19.4207	17.86933	4.574764
Pt249	16.6451	9.955704	6.890567
Pt250	20.80522	12.35775	6.888311
Pt251	18.03036	12.35751	6.891225
Pt252	16.64149	14.75804	6.889051
Pt253	18.01706	17.16625	6.889827
Pt254	20.76001	17.16176	6.882392
Pt255	19.42521	9.959217	6.885968
Pt256	19.41207	14.76089	6.898972

Table S9. Atomic coordinates (cartesian; Å) of the diamino-triazine/Pt(111) structure shown in Fig. 8(a)

Atom label	X [Å]	Y [Å]	Z [Å]
N1	21.10721	17.92102	10.2909
N2	19.59279	0.063238	9.060017
N3	18.74617	17.5014	10.3907
N4	21.90244	0.558288	9.131257
N5	20.27489	15.92354	11.10034
C1	20.82659	18.95665	9.523402
C2	18.57525	18.55571	9.619104
C3	20.03975	17.12943	10.57588
H1	21.69951	1.56273	9.22833
H2	19.4934	15.29369	11.25054
H3	0.567793	0.285587	9.613045
H4	21.22809	15.58135	11.16131
H5	17.56186	18.90842	9.410263
Pt1	0.000000	0.000000	0.000000
Pt2	4.161946	2.4029	0.000000
Pt3	1.387315	2.4029	0.000000
Pt4	0.000000	4.805801	0.000000
Pt5	1.387315	7.208701	0.000000
Pt6	4.161946	7.208701	0.000000
Pt7	2.774631	0.000000	0.000000
Pt8	2.774631	4.805801	0.000000
Pt9	4.161745	8.973887	2.31401
Pt10	1.38751	8.971317	2.313741
Pt11	22.18648	1.755677	2.332442
Pt12	22.19483	6.568706	2.313713
Pt13	2.754805	1.763134	2.329753
Pt14	1.374151	4.162116	2.310816
Pt15	4.151497	4.162969	2.308153
Pt16	2.772874	6.568735	2.309588
Pt17	4.166276	5.963641	4.586689
Pt18	1.390155	5.963971	4.588181
Pt19	0.00054	8.365988	4.593786
Pt20	22.19602	3.566896	4.598684
Pt21	1.352033	1.151558	4.639212

Pt22	4.154328	1.16125	4.587208
Pt23	2.772138	3.556578	4.588457
Pt24	2.778833	8.367981	4.592364
Pt25	0.068239	0.54637	6.949937
Pt26	4.172776	2.93548	6.908198
Pt27	1.409109	2.972679	6.92277
Pt28	0.002254	5.356677	6.913341
Pt29	1.389933	7.738686	6.902309
Pt30	4.166634	7.728344	6.902941
Pt31	2.821012	0.52452	6.919013
Pt32	2.780303	5.33736	6.900341
Pt33	5.549261	0.000000	0.000000
Pt34	9.711207	2.4029	0.000000
Pt35	6.936576	2.4029	0.000000
Pt36	5.549261	4.805801	0.000000
Pt37	6.936576	7.208701	0.000000
Pt38	9.711207	7.208701	0.000000
Pt39	8.323892	0.000000	0.000000
Pt40	8.323892	4.805801	0.000000
Pt41	9.710928	8.976772	2.311185
Pt42	6.93763	8.97508	2.311407
Pt43	5.531672	1.762948	2.310016
Pt44	5.549616	6.571336	2.311741
Pt45	8.318326	1.764709	2.308361
Pt46	6.930236	4.165855	2.310194
Pt47	9.710339	4.16849	2.311881
Pt48	8.323958	6.572242	2.311968
Pt49	9.709679	5.962626	4.590768
Pt50	6.939524	5.963215	4.589528
Pt51	5.553451	8.368994	4.591285
Pt52	5.545881	3.561028	4.588951
Pt53	6.932597	1.160701	4.583099
Pt54	9.708711	1.15855	4.586332
Pt55	8.320939	3.561341	4.586614
Pt56	8.324667	8.369254	4.591161
Pt57	5.552909	0.525827	6.899505
Pt58	9.708698	2.922192	6.899837

Pt59	6.940686	2.928432	6.900007
Pt60	5.557677	5.334076	6.905584
Pt61	6.939175	7.73094	6.905317
Pt62	9.709134	7.729796	6.904289
Pt63	8.318458	0.519415	6.893516
Pt64	8.325494	5.326495	6.906732
Pt65	11.09852	0.000000	0.000000
Pt66	15.26047	2.4029	0.000000
Pt67	12.48584	2.4029	0.000000
Pt68	11.09852	4.805801	0.000000
Pt69	12.48584	7.208701	0.000000
Pt70	15.26047	7.208701	0.000000
Pt71	13.87315	0.000000	0.000000
Pt72	13.87315	4.805801	0.000000
Pt73	15.25984	8.972549	2.313688
Pt74	12.48441	8.975381	2.311569
Pt75	11.10349	1.765766	2.308431
Pt76	11.09819	6.572206	2.312937
Pt77	13.88972	1.762227	2.308664
Pt78	12.49079	4.166121	2.310949
Pt79	15.2691	4.162092	2.309782
Pt80	13.87151	6.57023	2.311504
Pt81	15.25511	5.963544	4.586357
Pt82	12.48108	5.965217	4.59088
Pt83	11.0944	8.370131	4.59117
Pt84	11.09736	3.562834	4.586941
Pt85	12.48426	1.163194	4.581515
Pt86	15.26329	1.160505	4.580097
Pt87	13.87226	3.56165	4.590314
Pt88	13.86684	8.36919	4.591096
Pt89	11.09899	0.521877	6.895462
Pt90	15.24306	2.941983	6.909873
Pt91	12.4757	2.928946	6.900474
Pt92	11.09148	5.326901	6.906859
Pt93	12.47891	7.730326	6.905394
Pt94	15.25302	7.731146	6.901069
Pt95	13.86092	0.527926	6.896322

Pt96	13.86171	5.336978	6.906756
Pt97	16.64778	0.000000	0.000000
Pt98	20.80973	2.4029	0.000000
Pt99	18.0351	2.4029	0.000000
Pt100	16.64778	4.805801	0.000000
Pt101	18.0351	7.208701	0.000000
Pt102	20.80973	7.208701	0.000000
Pt103	19.42241	0.000000	0.000000
Pt104	19.42241	4.805801	0.000000
Pt105	20.8093	8.969342	2.31272
Pt106	18.03382	8.971529	2.313758
Pt107	16.66673	1.762301	2.327907
Pt108	16.64767	6.569124	2.310039
Pt109	19.42569	1.755583	2.341394
Pt110	18.04288	4.162562	2.309033
Pt111	20.80643	4.16022	2.311134
Pt112	19.42177	6.569109	2.313293
Pt113	20.8082	5.966446	4.592991
Pt114	18.02955	5.966813	4.58959
Pt115	16.64277	8.369139	4.592954
Pt116	16.64727	3.555728	4.590106
Pt117	18.07404	1.155575	4.663895
Pt118	20.79915	1.160558	4.663095
Pt119	19.4162	3.571725	4.599898
Pt120	19.41928	8.366569	4.594328
Pt121	16.58552	0.530249	6.90013
Pt122	20.80815	2.99043	6.903558
Pt123	18.00687	2.981087	6.925874
Pt124	16.63672	5.341282	6.902623
Pt125	18.02768	7.741903	6.906696
Pt126	20.80663	7.742815	6.909239
Pt127	19.35144	0.570504	7.014978
Pt128	19.41556	5.360411	6.913084
Pt129	0.000000	9.611602	0.000000
Pt130	4.161946	12.0145	0.000000
Pt131	1.387315	12.0145	0.000000
Pt132	0.000000	14.4174	0.000000

Pt133	1.387315	16.8203	0.000000
Pt134	4.161946	16.8203	0.000000
Pt135	2.774631	9.611602	0.000000
Pt136	2.774631	14.4174	0.000000
Pt137	4.15671	18.58424	2.311567
Pt138	1.383683	18.59107	2.321964
Pt139	0.000912	11.37406	2.310939
Pt140	0.00297	16.19123	2.30245
Pt141	2.775042	11.3759	2.313516
Pt142	1.38761	13.78176	2.312345
Pt143	4.159787	13.78072	2.311424
Pt144	2.774573	16.18708	2.312903
Pt145	4.161024	15.57611	4.5922
Pt146	1.385879	15.57308	4.587838
Pt147	0.005397	17.97738	4.597744
Pt148	0.001274	13.16211	4.590568
Pt149	1.389407	10.7666	4.593643
Pt150	4.162131	10.77132	4.593472
Pt151	2.77334	13.17266	4.592583
Pt152	2.778594	17.98281	4.598438
Pt153	22.19413	10.1347	6.906183
Pt154	4.163249	12.53617	6.907306
Pt155	1.388092	12.53682	6.90643
Pt156	0.00437	14.91895	6.903196
Pt157	1.404554	17.32285	6.904577
Pt158	4.166554	17.33365	6.912991
Pt159	2.775743	10.13504	6.905186
Pt160	2.781588	14.93132	6.907864
Pt161	5.549261	9.611602	0.000000
Pt162	9.711207	12.0145	0.000000
Pt163	6.936576	12.0145	0.000000
Pt164	5.549261	14.4174	0.000000
Pt165	6.936576	16.8203	0.000000
Pt166	9.711207	16.8203	0.000000
Pt167	8.323892	9.611602	0.000000
Pt168	8.323892	14.4174	0.000000
Pt169	9.711184	18.58907	2.31293

Pt170	6.932166	18.58557	2.310815
Pt171	5.547503	11.37824	2.314432
Pt172	5.548929	16.18399	2.312975
Pt173	8.322155	11.37997	2.31142
Pt174	6.933615	13.78038	2.31282
Pt175	9.710172	13.78152	2.313802
Pt176	8.323947	16.18456	2.313383
Pt177	9.7116	15.57778	4.593324
Pt178	6.934245	15.57684	4.590836
Pt179	5.544726	17.98119	4.593209
Pt180	5.545535	13.17615	4.594056
Pt181	6.934876	10.77352	4.590085
Pt182	9.708902	10.7737	4.591765
Pt183	8.320718	13.17525	4.591079
Pt184	8.320843	17.97851	4.587934
Pt185	5.551117	10.13394	6.90445
Pt186	9.709705	12.543	6.901656
Pt187	6.938256	12.53732	6.905125
Pt188	5.551113	14.94073	6.909343
Pt189	6.939068	17.33829	6.901968
Pt190	9.709984	17.34834	6.903573
Pt191	8.321076	10.1354	6.902553
Pt192	8.321472	14.94018	6.903808
Pt193	11.09852	9.611602	0.000000
Pt194	15.26047	12.0145	0.000000
Pt195	12.48584	12.0145	0.000000
Pt196	11.09852	14.4174	0.000000
Pt197	12.48584	16.8203	0.000000
Pt198	15.26047	16.8203	0.000000
Pt199	13.87315	9.611602	0.000000
Pt200	13.87315	14.4174	0.000000
Pt201	15.26522	18.58407	2.308728
Pt202	12.48956	18.58572	2.310448
Pt203	11.09853	11.38039	2.312371
Pt204	11.09767	16.18514	2.31325
Pt205	13.87288	11.37786	2.314543
Pt206	12.4867	13.78079	2.313138

Pt207	15.25965	13.78009	2.311723
Pt208	13.87318	16.18386	2.312808
Pt209	15.2601	15.57453	4.593156
Pt210	12.487	15.57626	4.59016
Pt211	11.10013	17.98094	4.589006
Pt212	11.09826	13.17564	4.591843
Pt213	12.48235	10.77405	4.590352
Pt214	15.25665	10.77017	4.593651
Pt215	13.87359	13.17445	4.595345
Pt216	13.8749	17.98101	4.591062
Pt217	11.09754	10.13531	6.904263
Pt218	15.25742	12.53697	6.906625
Pt219	12.48101	12.53617	6.906621
Pt220	11.09985	14.94019	6.905034
Pt221	12.47911	17.33735	6.901
Pt222	15.24838	17.33667	6.910605
Pt223	13.86629	10.13444	6.903284
Pt224	13.86795	14.94043	6.90952
Pt225	16.64778	9.611602	0.000000
Pt226	20.80973	12.0145	0.000000
Pt227	18.0351	12.0145	0.000000
Pt228	16.64778	14.4174	0.000000
Pt229	18.0351	16.8203	0.000000
Pt230	20.80973	16.8203	0.000000
Pt231	19.42241	9.611602	0.000000
Pt232	19.42241	14.4174	0.000000
Pt233	20.80917	18.59062	2.328539
Pt234	18.03891	18.59284	2.32539
Pt235	16.64628	11.37568	2.313529
Pt236	16.64665	16.18721	2.311974
Pt237	19.42043	11.3742	2.310742
Pt238	18.03394	13.78231	2.312957
Pt239	20.80965	13.78308	2.313949
Pt240	19.41861	16.19221	2.300118
Pt241	20.80883	15.55854	4.56238
Pt242	18.03592	15.57183	4.583974
Pt243	16.64159	17.98321	4.592061

Pt244	16.64656	13.17126	4.59179
Pt245	18.03084	10.76686	4.592943
Pt246	20.80896	10.7635	4.589731
Pt247	19.42008	13.16161	4.591506
Pt248	19.4177	17.97903	4.60189
Pt249	16.64484	10.1359	6.90595
Pt250	20.80847	12.5267	6.907081
Pt251	18.03208	12.53564	6.907813
Pt252	16.63871	14.92798	6.906686
Pt253	18.01332	17.31429	6.884556
Pt254	20.81757	17.26966	6.831068
Pt255	19.42116	10.13673	6.907145
Pt256	19.41813	14.92148	6.90262

Table S10. Atomic coordinates (cartesian; Å) of the diamino-triazine/Pt(111) structure shown in Fig. 8(b)

Atom label	X [Å]	Y [Å]	Z [Å]
N1	21.14361	18.35278	10.67111
N2	19.65528	0.24182	9.175271
N3	18.80011	18.17442	11.00141
N4	21.99516	0.618364	9.097229
N5	17.42162	0.401184	9.861097
C1	20.88247	19.1796	9.671002
C2	18.62677	19.08162	10.01211
C3	20.04688	17.79865	11.22916
H1	21.89656	1.645509	9.145535
H2	17.22094	1.019637	9.059724
H3	0.655471	0.307714	9.567522
H4	16.6472	19.21238	10.37413
H5	20.21117	16.99799	11.95515
Pt1	0.000000	0.000000	0.000000
Pt2	4.161946	2.4029	0.000000
Pt3	1.387315	2.4029	0.000000
Pt4	0.000000	4.805801	0.000000
Pt5	1.387315	7.208701	0.000000
Pt6	4.161946	7.208701	0.000000
Pt7	2.774631	0.000000	0.000000
Pt8	2.774631	4.805801	0.000000
Pt9	4.161607	8.973641	2.314051
Pt10	1.387276	8.96964	2.312789
Pt11	22.18621	1.754106	2.331303
Pt12	22.19424	6.567214	2.312964
Pt13	2.756244	1.761431	2.323521
Pt14	1.374555	4.160211	2.30889
Pt15	4.152489	4.162587	2.306909
Pt16	2.77312	6.567607	2.309282
Pt17	4.166345	5.963433	4.586543
Pt18	1.390329	5.961623	4.586821
Pt19	0.001696	8.364557	4.593062
Pt20	22.1943	3.565205	4.595144
Pt21	1.354921	1.149082	4.631542

Pt22	4.154419	1.159984	4.583868
Pt23	2.773352	3.555196	4.583747
Pt24	2.77919	8.366852	4.591493
Pt25	0.058507	0.527368	6.944976
Pt26	4.171741	2.93365	6.905716
Pt27	1.408622	2.968089	6.910282
Pt28	0.002961	5.353741	6.909079
Pt29	1.391471	7.738006	6.90168
Pt30	4.166603	7.72775	6.903143
Pt31	2.81978	0.519877	6.909206
Pt32	2.779848	5.336411	6.898938
Pt33	5.549261	0.000000	0.000000
Pt34	9.711207	2.4029	0.000000
Pt35	6.936576	2.4029	0.000000
Pt36	5.549261	4.805801	0.000000
Pt37	6.936576	7.208701	0.000000
Pt38	9.711207	7.208701	0.000000
Pt39	8.323892	0.000000	0.000000
Pt40	8.323892	4.805801	0.000000
Pt41	9.710993	8.975938	2.310653
Pt42	6.93718	8.97518	2.310921
Pt43	5.532113	1.762093	2.309329
Pt44	5.549776	6.571271	2.312257
Pt45	8.318233	1.763573	2.307642
Pt46	6.931075	4.165476	2.310336
Pt47	9.710205	4.167129	2.311224
Pt48	8.324136	6.571507	2.311716
Pt49	9.710301	5.961061	4.589697
Pt50	6.939701	5.962895	4.589171
Pt51	5.553566	8.369003	4.591165
Pt52	5.546295	3.56067	4.588435
Pt53	6.932249	1.159962	4.581861
Pt54	9.710079	1.157859	4.585608
Pt55	8.321166	3.55966	4.586592
Pt56	8.325143	8.368473	4.590372
Pt57	5.553126	0.525438	6.899735
Pt58	9.70906	2.922588	6.899328

Pt59	6.94053	2.926772	6.900467
Pt60	5.556982	5.331881	6.904699
Pt61	6.939025	7.729295	6.904634
Pt62	9.709081	7.729136	6.903291
Pt63	8.319135	0.518738	6.891096
Pt64	8.325621	5.326498	6.905332
Pt65	11.09852	0.000000	0.000000
Pt66	15.26047	2.4029	0.000000
Pt67	12.48584	2.4029	0.000000
Pt68	11.09852	4.805801	0.000000
Pt69	12.48584	7.208701	0.000000
Pt70	15.26047	7.208701	0.000000
Pt71	13.87315	0.000000	0.000000
Pt72	13.87315	4.805801	0.000000
Pt73	15.26065	8.972006	2.31282
Pt74	12.485	8.975319	2.311653
Pt75	11.10372	1.76488	2.30748
Pt76	11.09806	6.571383	2.3126
Pt77	13.8931	1.761944	2.307675
Pt78	12.49174	4.164871	2.310251
Pt79	15.27113	4.15869	2.309698
Pt80	13.87114	6.569604	2.311381
Pt81	15.2548	5.961303	4.586101
Pt82	12.48179	5.964364	4.590143
Pt83	11.09535	8.369437	4.590915
Pt84	11.09805	3.561439	4.586165
Pt85	12.48602	1.164168	4.578208
Pt86	15.26544	1.160786	4.576871
Pt87	13.87364	3.561339	4.591356
Pt88	13.86788	8.36872	4.59057
Pt89	11.10071	0.52191	6.894424
Pt90	15.24244	2.938221	6.911777
Pt91	12.47587	2.927009	6.901248
Pt92	11.09221	5.325533	6.905883
Pt93	12.47904	7.728902	6.904969
Pt94	15.25323	7.730428	6.900114
Pt95	13.85778	0.526402	6.896245

Pt96	13.8625	5.336047	6.907225
Pt97	16.64778	0.000000	0.000000
Pt98	20.80973	2.4029	0.000000
Pt99	18.0351	2.4029	0.000000
Pt100	16.64778	4.805801	0.000000
Pt101	18.0351	7.208701	0.000000
Pt102	20.80973	7.208701	0.000000
Pt103	19.42241	0.000000	0.000000
Pt104	19.42241	4.805801	0.000000
Pt105	20.80966	8.970343	2.31335
Pt106	18.0354	8.971372	2.313353
Pt107	16.67479	1.758302	2.332111
Pt108	16.64646	6.566912	2.309165
Pt109	19.42822	1.755009	2.346567
Pt110	18.04302	4.161162	2.309018
Pt111	20.80606	4.159435	2.308685
Pt112	19.42129	6.568979	2.312873
Pt113	20.80747	5.966284	4.591236
Pt114	18.02885	5.964763	4.588431
Pt115	16.64377	8.366194	4.590666
Pt116	16.64899	3.551688	4.592707
Pt117	18.08617	1.154252	4.683324
Pt118	20.80268	1.161547	4.67365
Pt119	19.41649	3.572083	4.599474
Pt120	19.42018	8.366438	4.594033
Pt121	16.58258	0.509493	6.877375
Pt122	20.80704	2.991526	6.905879
Pt123	18.00938	2.980784	6.932709
Pt124	16.63644	5.337775	6.902006
Pt125	18.02807	7.740112	6.904948
Pt126	20.80734	7.741171	6.907499
Pt127	19.36368	0.577364	7.079425
Pt128	19.41612	5.360478	6.911955
Pt129	0.000000	9.611602	0.000000
Pt130	4.161946	12.0145	0.000000
Pt131	1.387315	12.0145	0.000000
Pt132	0.000000	14.4174	0.000000

Pt133	1.387315	16.8203	0.000000
Pt134	4.161946	16.8203	0.000000
Pt135	2.774631	9.611602	0.000000
Pt136	2.774631	14.4174	0.000000
Pt137	4.155372	18.583	2.310733
Pt138	1.380852	18.58921	2.324595
Pt139	0.001135	11.37523	2.310769
Pt140	0.000882	16.19198	2.307114
Pt141	2.775113	11.37545	2.312963
Pt142	1.387273	13.78218	2.311623
Pt143	4.160028	13.78062	2.31146
Pt144	2.773733	16.18659	2.313501
Pt145	4.162507	15.57513	4.592498
Pt146	1.386086	15.57162	4.588644
Pt147	0.003866	17.97473	4.615053
Pt148	22.19704	13.1659	4.588881
Pt149	1.388888	10.76579	4.591393
Pt150	4.162813	10.77135	4.592576
Pt151	2.773159	13.17196	4.591171
Pt152	2.777981	17.97784	4.598591
Pt153	22.19502	10.13317	6.904168
Pt154	4.162906	12.53559	6.9061
Pt155	1.389004	12.53568	6.903669
Pt156	0.003945	14.92173	6.902293
Pt157	1.406344	17.31525	6.910903
Pt158	4.169118	17.33229	6.913804
Pt159	2.776074	10.13492	6.904057
Pt160	2.782916	14.9303	6.907288
Pt161	5.549261	9.611602	0.000000
Pt162	9.711207	12.0145	0.000000
Pt163	6.936576	12.0145	0.000000
Pt164	5.549261	14.4174	0.000000
Pt165	6.936576	16.8203	0.000000
Pt166	9.711207	16.8203	0.000000
Pt167	8.323892	9.611602	0.000000
Pt168	8.323892	14.4174	0.000000
Pt169	9.711634	18.58889	2.312178

Pt170	6.931501	18.58479	2.310582
Pt171	5.547873	11.37845	2.314378
Pt172	5.549117	16.18353	2.3128
Pt173	8.322508	11.3797	2.311141
Pt174	6.934201	13.78031	2.312987
Pt175	9.710457	13.78139	2.313799
Pt176	8.32419	16.18472	2.312602
Pt177	9.711882	15.57626	4.592704
Pt178	6.935759	15.57583	4.590656
Pt179	5.544807	17.98091	4.593166
Pt180	5.545873	13.17611	4.59432
Pt181	6.934705	10.77344	4.590445
Pt182	9.70847	10.77237	4.591392
Pt183	8.321358	13.17447	4.591567
Pt184	8.321041	17.97826	4.586407
Pt185	5.551215	10.13275	6.904094
Pt186	9.710363	12.54122	6.90304
Pt187	6.938804	12.53696	6.905344
Pt188	5.553175	14.93932	6.909418
Pt189	6.940016	17.33844	6.901405
Pt190	9.710348	17.34735	6.899872
Pt191	8.320816	10.13423	6.902769
Pt192	8.322313	14.93941	6.904472
Pt193	11.09852	9.611602	0.000000
Pt194	15.26047	12.0145	0.000000
Pt195	12.48584	12.0145	0.000000
Pt196	11.09852	14.4174	0.000000
Pt197	12.48584	16.8203	0.000000
Pt198	15.26047	16.8203	0.000000
Pt199	13.87315	9.611602	0.000000
Pt200	13.87315	14.4174	0.000000
Pt201	15.26901	18.58326	2.308796
Pt202	12.49155	18.58609	2.309382
Pt203	11.09898	11.37967	2.312757
Pt204	11.0974	16.18524	2.313009
Pt205	13.87328	11.37729	2.314697
Pt206	12.48657	13.78063	2.313206

Pt207	15.25938	13.7797	2.311064
Pt208	13.87286	16.18421	2.312346
Pt209	15.25894	15.57293	4.591332
Pt210	12.4869	15.57617	4.589862
Pt211	11.10162	17.98111	4.587466
Pt212	11.09834	13.17401	4.59228
Pt213	12.48342	10.77353	4.590757
Pt214	15.25801	10.76823	4.592061
Pt215	13.87291	13.17394	4.595115
Pt216	13.87754	17.98181	4.590935
Pt217	11.09745	10.13356	6.903278
Pt218	15.25836	12.53707	6.905543
Pt219	12.48144	12.53491	6.906925
Pt220	11.10046	14.93892	6.904556
Pt221	12.4804	17.3362	6.89974
Pt222	15.25311	17.33015	6.909509
Pt223	13.86798	10.13425	6.902658
Pt224	13.86844	14.93932	6.90936
Pt225	16.64778	9.611602	0.000000
Pt226	20.80973	12.0145	0.000000
Pt227	18.0351	12.0145	0.000000
Pt228	16.64778	14.4174	0.000000
Pt229	18.0351	16.8203	0.000000
Pt230	20.80973	16.8203	0.000000
Pt231	19.42241	9.611602	0.000000
Pt232	19.42241	14.4174	0.000000
Pt233	20.80952	18.59144	2.339694
Pt234	18.04528	18.59248	2.33144
Pt235	16.64715	11.37507	2.312819
Pt236	16.64762	16.18642	2.311272
Pt237	19.42178	11.37582	2.310695
Pt238	18.03426	13.78308	2.312267
Pt239	20.80878	13.78585	2.313897
Pt240	19.42043	16.1946	2.305707
Pt241	20.80824	15.56994	4.573574
Pt242	18.03589	15.57285	4.585098
Pt243	16.64745	17.97715	4.590141

Pt244	16.64675	13.16977	4.589353
Pt245	18.03265	10.7667	4.591267
Pt246	20.80924	10.76563	4.589134
Pt247	19.42002	13.16737	4.589922
Pt248	19.4224	17.98566	4.625687
Pt249	16.64526	10.13341	6.903808
Pt250	20.80882	12.52801	6.901182
Pt251	18.03226	12.53447	6.903755
Pt252	16.63986	14.92643	6.905183
Pt253	18.02312	17.31694	6.893778
Pt254	20.81023	17.28483	6.875721
Pt255	19.42177	10.13662	6.905937
Pt256	19.41895	14.92685	6.901448

Table S11. Atomic coordinates (cartesian; Å) of the amino-triazine/Pt(111) structure shown in Fig. 8(c)

Atom label	X [Å]	Y [Å]	Z [Å]
N1	21.11244	18.40974	10.69366
N2	19.61592	0.077919	9.073682
N3	18.80149	17.84954	10.77347
N4	21.87693	0.762181	9.152683
C1	20.83511	19.21329	9.667524
C2	18.61399	18.64671	9.727797
C3	20.07626	17.70935	11.16737
H1	21.63055	1.759412	9.015029
H2	0.538444	0.638774	9.697672
H3	17.60379	18.80629	9.341709
H4	20.28579	16.98258	11.95633
Pt1	0.000000	0.000000	0.000000
Pt2	4.161946	2.4029	0.000000
Pt3	1.387315	2.4029	0.000000
Pt4	0.000000	4.805801	0.000000
Pt5	1.387315	7.208701	0.000000
Pt6	4.161946	7.208701	0.000000
Pt7	2.774631	0.000000	0.000000
Pt8	2.774631	4.805801	0.000000
Pt9	4.161964	8.974292	2.313444
Pt10	1.387738	8.971813	2.31321
Pt11	22.18432	1.755468	2.327726
Pt12	22.1954	6.56859	2.312699
Pt13	2.755908	1.762209	2.326536
Pt14	1.375917	4.161357	2.308568
Pt15	4.153672	4.163211	2.307682
Pt16	2.774053	6.568846	2.309674
Pt17	4.167289	5.964333	4.587055
Pt18	1.391895	5.962848	4.586732
Pt19	0.002787	8.365341	4.593011
Pt20	0.000591	3.564222	4.592689
Pt21	1.359319	1.149348	4.626709
Pt22	4.155883	1.161672	4.587055
Pt23	2.775291	3.556548	4.585664

Pt24	2.779967	8.367968	4.59133
Pt25	0.077423	0.543089	6.94252
Pt26	4.176401	2.937794	6.908304
Pt27	1.413069	2.971624	6.91162
Pt28	0.007653	5.356025	6.910111
Pt29	1.393077	7.73799	6.901714
Pt30	4.169668	7.729842	6.902332
Pt31	2.822998	0.526476	6.917837
Pt32	2.784469	5.338628	6.900474
Pt33	5.549261	0.000000	0.000000
Pt34	9.711207	2.4029	0.000000
Pt35	6.936576	2.4029	0.000000
Pt36	5.549261	4.805801	0.000000
Pt37	6.936576	7.208701	0.000000
Pt38	9.711207	7.208701	0.000000
Pt39	8.323892	0.000000	0.000000
Pt40	8.323892	4.805801	0.000000
Pt41	9.711029	8.976199	2.310848
Pt42	6.937823	8.975063	2.310908
Pt43	5.534047	1.762248	2.310566
Pt44	5.550183	6.571389	2.312121
Pt45	8.321029	1.764407	2.308716
Pt46	6.931997	4.165585	2.310739
Pt47	9.712011	4.168176	2.311634
Pt48	8.324597	6.571562	2.311527
Pt49	9.709963	5.962818	4.590983
Pt50	6.939995	5.963357	4.589456
Pt51	5.554909	8.369732	4.590341
Pt52	5.548259	3.561609	4.589235
Pt53	6.934836	1.160788	4.583487
Pt54	9.712206	1.158834	4.586083
Pt55	8.323083	3.561112	4.58705
Pt56	8.32628	8.369239	4.590804
Pt57	5.555024	0.526291	6.898797
Pt58	9.71077	2.922207	6.900381
Pt59	6.94336	2.929137	6.901286
Pt60	5.559742	5.334669	6.906779

Pt61	6.94191	7.730581	6.904824
Pt62	9.710695	7.730597	6.904494
Pt63	8.321407	0.521183	6.893064
Pt64	8.326831	5.327926	6.906646
Pt65	11.09852	0.000000	0.000000
Pt66	15.26047	2.4029	0.000000
Pt67	12.48584	2.4029	0.000000
Pt68	11.09852	4.805801	0.000000
Pt69	12.48584	7.208701	0.000000
Pt70	15.26047	7.208701	0.000000
Pt71	13.87315	0.000000	0.000000
Pt72	13.87315	4.805801	0.000000
Pt73	15.26047	8.972427	2.313456
Pt74	12.48535	8.975367	2.311504
Pt75	11.10633	1.765336	2.308727
Pt76	11.09843	6.571662	2.31327
Pt77	13.89381	1.760804	2.308913
Pt78	12.49304	4.165309	2.310306
Pt79	15.27127	4.160044	2.309076
Pt80	13.87123	6.569869	2.311039
Pt81	15.25521	5.962795	4.585398
Pt82	12.48138	5.964334	4.590108
Pt83	11.09562	8.369695	4.591086
Pt84	11.09912	3.562505	4.586983
Pt85	12.48831	1.163515	4.581314
Pt86	15.26762	1.158377	4.583131
Pt87	13.8748	3.560632	4.590095
Pt88	13.86794	8.368294	4.59078
Pt89	11.10231	0.522251	6.894987
Pt90	15.24572	2.938374	6.909658
Pt91	12.47749	2.929326	6.900833
Pt92	11.09369	5.326736	6.905995
Pt93	12.48026	7.729634	6.904978
Pt94	15.25504	7.729651	6.900983
Pt95	13.86273	0.526134	6.898362
Pt96	13.86479	5.335314	6.904807
Pt97	16.64778	0	0

Pt98	20.80973	2.4029	0.000000
Pt99	18.0351	2.4029	0.000000
Pt100	16.64778	4.805801	0.000000
Pt101	18.0351	7.208701	0.000000
Pt102	20.80973	7.208701	0.000000
Pt103	19.42241	0.000000	0.000000
Pt104	19.42241	4.805801	0.000000
Pt105	20.80966	8.970559	2.31292
Pt106	18.03472	8.97111	2.313209
Pt107	16.67131	1.760267	2.331538
Pt108	16.6472	6.567733	2.3095
Pt109	19.42615	1.754887	2.3474
Pt110	18.04295	4.161788	2.307568
Pt111	20.80608	4.160828	2.309727
Pt112	19.42212	6.569374	2.312964
Pt113	20.80988	5.965742	4.591595
Pt114	18.03027	5.965715	4.588071
Pt115	16.64403	8.36714	4.591921
Pt116	16.64941	3.553073	4.590926
Pt117	18.08056	1.153345	4.683748
Pt118	20.80105	1.160206	4.668184
Pt119	19.41588	3.5718	4.597727
Pt120	19.42144	8.365949	4.593595
Pt121	16.58796	0.526017	6.907427
Pt122	20.81244	2.994247	6.90079
Pt123	18.01333	2.972845	6.927388
Pt124	16.63957	5.337795	6.899361
Pt125	18.02978	7.740033	6.904767
Pt126	20.80998	7.741281	6.906942
Pt127	19.36431	0.550183	7.046954
Pt128	19.41843	5.357047	6.910207
Pt129	0.000000	9.611602	0.000000
Pt130	4.161946	12.0145	0.000000
Pt131	1.387315	12.0145	0.000000
Pt132	0.000000	14.4174	0.000000
Pt133	1.387315	16.8203	0.000000
Pt134	4.161946	16.8203	0.000000

Pt135	2.774631	9.611602	0.000000
Pt136	2.774631	14.4174	0.000000
Pt137	4.156363	18.58394	2.311624
Pt138	1.38194	18.58915	2.322975
Pt139	0.002115	11.37503	2.310952
Pt140	0.001828	16.19205	2.306864
Pt141	2.776041	11.37641	2.313116
Pt142	1.388776	13.78267	2.311527
Pt143	4.161599	13.78108	2.312043
Pt144	2.774175	16.18666	2.313557
Pt145	4.162283	15.57566	4.592321
Pt146	1.386972	15.57444	4.590265
Pt147	0.005718	17.97804	4.609755
Pt148	0.001837	13.16529	4.588214
Pt149	1.39076	10.76699	4.592426
Pt150	4.164906	10.77199	4.591947
Pt151	2.774193	13.17319	4.591679
Pt152	2.778856	17.98083	4.600039
Pt153	22.19601	10.13426	6.90488
Pt154	4.164628	12.53706	6.906323
Pt155	1.390138	12.53648	6.903278
Pt156	0.006801	14.92232	6.901203
Pt157	1.407723	17.32608	6.914698
Pt158	4.17041	17.33457	6.912253
Pt159	2.778896	10.1348	6.90259
Pt160	2.783718	14.93322	6.908075
Pt161	5.549261	9.611602	0.000000
Pt162	9.711207	12.0145	0.000000
Pt163	6.936576	12.0145	0.000000
Pt164	5.549261	14.4174	0.000000
Pt165	6.936576	16.8203	0.000000
Pt166	9.711207	16.8203	0.000000
Pt167	8.323892	9.611602	0.000000
Pt168	8.323892	14.4174	0.000000
Pt169	9.711968	18.58916	2.312719
Pt170	6.932294	18.58553	2.310714
Pt171	5.548746	11.37894	2.314424

Pt172	5.549405	16.18359	2.312897
Pt173	8.32415	11.37964	2.310606
Pt174	6.935892	13.78021	2.313606
Pt175	9.711853	13.78165	2.313551
Pt176	8.324247	16.18479	2.313129
Pt177	9.713081	15.5779	4.592682
Pt178	6.936377	15.5761	4.590791
Pt179	5.546034	17.98086	4.59238
Pt180	5.547895	13.17599	4.594819
Pt181	6.938546	10.7736	4.589108
Pt182	9.712869	10.77348	4.591474
Pt183	8.32407	13.17472	4.591513
Pt184	8.322498	17.97924	4.587083
Pt185	5.554144	10.13441	6.90263
Pt186	9.711447	12.54328	6.902569
Pt187	6.939798	12.53816	6.905292
Pt188	5.553387	14.94079	6.909376
Pt189	6.941378	17.34049	6.900845
Pt190	9.71119	17.34852	6.901573
Pt191	8.323214	10.13688	6.902384
Pt192	8.323744	14.94106	6.904176
Pt193	11.09852	9.611602	0.000000
Pt194	15.26047	12.0145	0.000000
Pt195	12.48584	12.0145	0.000000
Pt196	11.09852	14.4174	0.000000
Pt197	12.48584	16.8203	0.000000
Pt198	15.26047	16.8203	0.000000
Pt199	13.87315	9.611602	0.000000
Pt200	13.87315	14.4174	0.000000
Pt201	15.26775	18.58378	2.3098
Pt202	12.49135	18.58607	2.309735
Pt203	11.10015	11.38006	2.312479
Pt204	11.09799	16.1857	2.31299
Pt205	13.87411	11.37806	2.314261
Pt206	12.48766	13.78108	2.312823
Pt207	15.26056	13.78043	2.311091
Pt208	13.87347	16.18455	2.312703

Pt209	15.26009	15.57492	4.593098
Pt210	12.48753	15.57667	4.589993
Pt211	11.10271	17.98204	4.588458
Pt212	11.10111	13.17514	4.592027
Pt213	12.48573	10.77318	4.590895
Pt214	15.25917	10.76904	4.592844
Pt215	13.87482	13.17442	4.594189
Pt216	13.87778	17.98154	4.591711
Pt217	11.09946	10.13509	6.904443
Pt218	15.2579	12.53654	6.905565
Pt219	12.48349	12.53659	6.907503
Pt220	11.10081	14.9401	6.904966
Pt221	12.48167	17.3367	6.900291
Pt222	15.25307	17.33554	6.913025
Pt223	13.86827	10.13355	6.903208
Pt224	13.8689	14.93957	6.908999
Pt225	16.64778	9.611602	0.000000
Pt226	20.80973	12.0145	0.000000
Pt227	18.0351	12.0145	0.000000
Pt228	16.64778	14.4174	0.000000
Pt229	18.0351	16.8203	0.000000
Pt230	20.80973	16.8203	0.000000
Pt231	19.42241	9.611602	0.000000
Pt232	19.42241	14.4174	0.000000
Pt233	20.80957	18.59093	2.333794
Pt234	18.04146	18.59348	2.331196
Pt235	16.64789	11.37523	2.312984
Pt236	16.64672	16.18796	2.312397
Pt237	19.42218	11.37518	2.310663
Pt238	18.03491	13.7831	2.312182
Pt239	20.81047	13.78432	2.313445
Pt240	19.42027	16.19359	2.303315
Pt241	20.80919	15.56404	4.569058
Pt242	18.03609	15.57152	4.583121
Pt243	16.64608	17.98229	4.596286
Pt244	16.64703	13.17025	4.589514
Pt245	18.03343	10.76619	4.591321

Pt246	20.81082	10.76426	4.588669
Pt247	19.42082	13.16411	4.58967
Pt248	19.42206	17.9801	4.614056
Pt249	16.64661	10.1344	6.904634
Pt250	20.811	12.52643	6.901941
Pt251	18.03312	12.53357	6.903808
Pt252	16.6407	14.92573	6.905116
Pt253	18.01714	17.30429	6.890402
Pt254	20.82017	17.2769	6.857469
Pt255	19.42291	10.13602	6.90605
Pt256	19.42124	14.92109	6.901226