

Table SM2. The lone-pair occupancy of the nitrogen atoms (N1) in neutral, protonated and water-complexes [LP(1)_{N1}], the lone-pair occupancy of the neutral nitrogen atoms (N3 and N4), LP(1)_{N3}, and LP(1)_{N4}].

Derivatives	Occupancies (a.u.)				
	LP(1) _{N1}			LP(1) _{N3}	LP(1) _{N4}
	Neutral	Protonated	Complex	Neutral	Neutral
PDPA-H	1.9481	1.6387	1.9330	1.9442	1.9421
PDPA -CH ₃	1.9482	1.6632	1.9313	1.9427	1.9415
PDPA -NH ₂	1.9456	1.7682	1.9336	1.9405	1.941
PDPA -Cl	1.9425	1.6860	1.9278	1.9418	1.9431
PDPA -F	1.9395	1.7072	1.9297	1.9430	1.9437
PDPA -CHO	1.9456	1.6558	1.9380	1.9448	1.9424
PDPA -CN	1.9492	1.6642	1.9405	1.9437	1.9440
PDPA -NO ₂	1.9386	1.6336	1.9379	1.9437	1.9430

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