Electronic Supplementary Material (ESI) for RSC Advances.

Coordinates (in Å) of the optimized geometries of M1-M8

	M1				M2		
Atom	X	Y	Z	Atom	X	Y	Z
C	0.292037	1.014929	0.152394	C	0.514468	0.146881	0.585178
N	-0.948120	0.827799	-0.530926	C	-0.394341	-0.704403	-0.309087
N	-1.766830	0.053950	-0.006760	N	1.922584	0.164158	0.032722
N	-2.615183	-0.603975	0.337079	O	2.442296	-0.920743	-0.183007
N	1.260582	-0.188632	0.000422	O	2.440088	1.251902	-0.160910
O	2.435903	0.059984	0.198264	N	-1.737298	-0.803732	0.288316
O	0.777982	-1.274178	-0.255651	N	-2.540403	0.080834	-0.017765
H	0.816043	1.856364	-0.289460	N	-3.377127	0.816740	-0.224235
H	0.207506	1.143624	1.235500	H	0.584796	-0.288939	1.582252
				H	0.197476	1.185476	0.645816
				H	-0.435042	-0.289429	-1.321327
				H	-0.001352	-1.717254	-0.365223
	M3				M4		
Atom	X	Y	Z	Atom	X	Y	Z
C	1.282180	-0.609961	0.506004	C	-1.728796	0.424935	0.579073
C	-0.008399	-0.215914	-0.208363	C	-0.670502	-0.350467	-0.201707
C	-1.192781	-1.042808	0.308324	C	0.729060	-0.126923	0.384654
N	-2.440803	-0.749019	-0.424505	C	1.798401	-0.908122	-0.386544
N	-3.017752	0.295039	-0.117484	N	-3.107651	0.173039	0.004954
N	-3.649606	1.217068	0.075341	O	-3.727654	1.134450	-0.422577
N	2.440218	0.235818	0.017465	O	-3.503498	-0.982947	0.004106
O	3.391450	-0.343969	-0.481910	N	3.146827	-0.766525	0.205561
O	2.338546	1.444777	0.157630	N	3.726775	0.296204	-0.012401
H	1.571388	-1.642688	0.322078	N	4.367817	1.223512	-0.146139
H	1.223149	-0.422294	1.579983	H	-1.581940	1.502105	0.536646
H	-0.193049	0.848963	-0.048753	H	-1.782754	0.092598	1.617302
H	0.098577	-0.378817	-1.284310	H	-0.925669	-1.412939	-0.179758
H	-1.014949	-2.106971	0.149255	H	-0.693734	-0.031406	-1.249297
H	-1.335480	-0.884903	1.384468	H	0.976251	0.940706	0.365883
				H	0.754123	-0.441710	1.432964
				H	1.583700	-1.976579	-0.352254
				H	1.813879	-0.604949	-1.440394
	M5				M6		
Atom	X	Y	Z	Atom	X	Y	Z
C	2.486840	-0.500277	0.501167	C	3.011427	0.540854	0.555303
C	1.205347	0.013265	-0.152081	C	1.879107	-0.197670	-0.155677
C	-0.029315	-0.731339	0.371239	C	0.511501	0.164493	0.436103
C	-1.327888	-0.240825	-0.280359	C	-0.644809	-0.561148	-0.262449

C	-2.557042	-0.989585	0.242968	C	-2.015323	-0.205622	0.325349
N	3.689201	0.262288	-0.013130	C	-3.158260	-0.943449	-0.377206
O	4.535852	-0.363582	-0.632714	N	-4.484704	-0.660570	0.219521
O	3.724136	1.461348	0.219608	N	-4.962501	0.446548	-0.018788
N	-3.811094	-0.583370	-0.431602	N	-5.512225	1.428816	-0.170478
N	-4.276066	0.506687	-0.103447	N	4.350443	0.153327	-0.034381
N	-4.809291	1.484701	0.116737	O	4.993627	1.022430	-0.603412
H	2.682525	-1.547556	0.280238	O	4.691862	-1.013735	0.088065
H	2.479259	-0.336149	1.580112	H	2.941595	1.621477	0.449216
H	1.113089	1.084092	0.045827	H	3.067285	0.266149	1.609922
H	1.281340	-0.111945	-1.237328	H	2.053866	-1.273469	-0.072840
H	0.084805	-1.806836	0.188475	H	1.901251	0.054519	-1.221347
H	-0.094969	-0.606725	1.459163	H	0.354041	1.247586	0.365575
H	-1.448553	0.832599	-0.094513	H	0.499334	-0.080651	1.505155
H	-1.274476	-0.369931	-1.366168	H	-0.486580	-1.644194	-0.191002
H	-2.463978	-2.057747	0.043546	H	-0.629654	-0.318263	-1.332118
H	-2.655857	-0.861505	1.327988	H	-2.179264	0.875681	0.246599
				H	-2.042054	-0.451960	1.392031
				H	-3.030991	-2.022068	-0.279965
				H	-3.171690	-0.705959	-1.448114

		M7				M8	
Atom	X	Y	Z	Atom	X	Y	Z
C	3.736923	-0.455483	0.475114	C	4.298732	0.606632	0.506165
C	2.461648	0.123831	-0.134271	C	3.128037	-0.129730	-0.142503
C	1.211626	-0.599725	0.381581	C	1.783170	0.331072	0.432814
C	-0.084481	-0.044581	-0.220490	C	0.588690	-0.388255	-0.204762
C	-1.342009	-0.756957	0.291011	C	-0.761977	0.060278	0.364166
C	-2.635673	-0.203410	-0.317930	C	-1.957688	-0.657890	-0.272321
C	-3.880031	-0.929522	0.199764	C	-3.305670	-0.208051	0.303416
N	-5.134569	-0.458904	-0.433696	C	-4.487267	-0.937364	-0.340756
N	-5.543847	0.643469	-0.076370	N	-5.794920	-0.564218	0.249958
N	-6.028108	1.639980	0.174047	N	-6.222679	0.551412	-0.036649
N	4.953729	0.286516	-0.034056	N	-6.727164	1.550804	-0.229867
O	5.748664	-0.332241	-0.725711	N	5.612801	0.122504	-0.067231
O	5.050607	1.465819	0.271643	O	6.274804	0.915069	-0.720609
H	3.893034	-1.499241	0.210401	O	5.916289	-1.041214	0.150664
H	3.753351	-0.332095	1.559200	H	4.272586	1.679309	0.325490
H	2.408158	1.188705	0.106540	H	4.354806	0.402739	1.576614
H	2.516078	0.039198	-1.224910	H	3.257220	-1.203884	0.013676
H	1.286233	-1.670533	0.155397	H	3.149417	0.046877	-1.223279
H	1.168423	-0.517320	1.474750	H	1.672837	1.413085	0.289697
H	-0.157463	1.026719	0.002995	H	1.772492	0.160626	1.516576

H	-0.040656	-0.127119	-1.313315	H	0.701322	-1.470380	-0.063689
H	-1.266082	-1.828973	0.069333	H	0.601134	-0.218325	-1.288611
H	-1.386142	-0.672232	1.384160	H	-0.873515	1.142802	0.223570
H	-2.719120	0.866258	-0.092139	H	-0.773960	-0.109615	1.448076
H	-2.605397	-0.293828	-1.408818	H	-1.845713	-1.740443	-0.132087
H	-3.827154	-1.992147	-0.039606	H	-1.946651	-0.486948	-1.356200
H	-3.955869	-0.838360	1.290395	H	-3.423635	0.872530	0.158889
				H	-3.330156	-0.385903	1.383739
				H	-4.404383	-2.012663	-0.179779
				H	-4.504981	-0.764308	-1.423915