

Effect of backbone conformation and its defects on electronic properties and assessment of the stabilizing role of π - π interactions in aryl substituted polysilylenes studied by DFT on deca[methyl(phenyl)silylene]s

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Additional data file 4

Molecular energies calculated for all studied deca[methyl(phenyl)silylene]s obtained with B3LYP, M06 and ω B97X-D functionals.

Table S2 Molecular energies of all studied OMPSi₁₀ calculated with B3LYP, M06 and ω B97X-D functionals (ω – dihedral angle).

ω [°]	B3LYP [eV]	M06 [eV]	ω B97X-D [eV]
10A			
120	-154849.900	-154885.444	-154925.534
130	-154850.264	-154885.934	-154925.955
140	-154850.668	-154886.582	-154926.581
150	-154850.899	-154886.857	-154926.870
160	-154850.955	-154887.013	-154927.033
170	-154850.808	-154886.859	-154926.867
180	-154850.712	-154886.446	-154926.495
opt	-154850.980	-154886.893	-154926.909
10B			
120	-154850.087	-154885.747	-154925.820
130	-154850.322	-154886.147	-154926.159
140	-154850.636	-154886.502	-154926.538
150	-154850.820	-154886.728	-154926.738
160	-154850.904	-154886.924	-154926.926
170	-154850.852	-154886.905	-154926.896
180	-154850.759	-154886.588	-154926.615
opt	-154850.987	-154886.870	-154926.879
10C			
120	-154850.119	-154885.794	-154925.886
130	-154850.327	-154886.087	-154926.102
140	-154850.649	-154886.576	-154926.583
150	-154850.829	-154886.750	-154926.787
160	-154850.896	-154886.912	-154926.929
170	-154850.813	-154886.798	-154926.791
180	-154850.757	-154886.568	-154926.581
opt	-154850.963	-154886.847	-154926.856
10D			
120	-154850.127	-154885.762	-154925.836
130	-154850.316	-154886.052	-154926.086
140	-154850.649	-154886.566	-154926.596
150	-154850.831	-154886.755	-154926.779
160	-154850.891	-154886.908	-154926.930
170	-154850.809	-154886.777	-154926.760
180	-154850.755	-154886.601	-154926.642
opt	-154850.949	-154886.887	-154926.904
10			
120	-154849.736	-154885.131	-154925.221
130	-154850.157	-154885.747	-154925.760
140	-154850.677	-154886.635	-154926.634
150	-154850.928	-154886.866	-154926.873
160	-154850.945	-154887.008	-154926.995
170	-154850.807	-154886.921	-154926.892
180	-154850.676	-154886.416	-154926.472
opt	-154850.896	-154886.890	-154926.871