SUPPORTING INFORMATION

Comparative studies of the geometric and electronic properties of 1,1-disubstituted-2,3,4,5-tetraphenylsiloles and 1,1,2,2-tetramethyl-3,4,5,6-tetraphenyl-1,2-disila-3,5-cyclohexadiene

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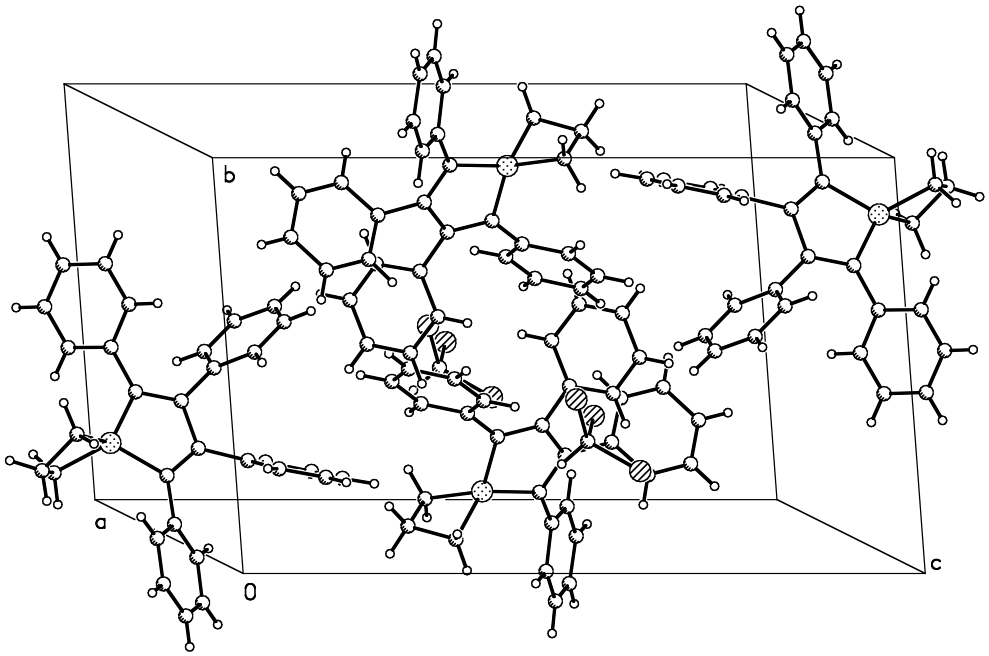

Fig. S1 Crystal packing of **II**.

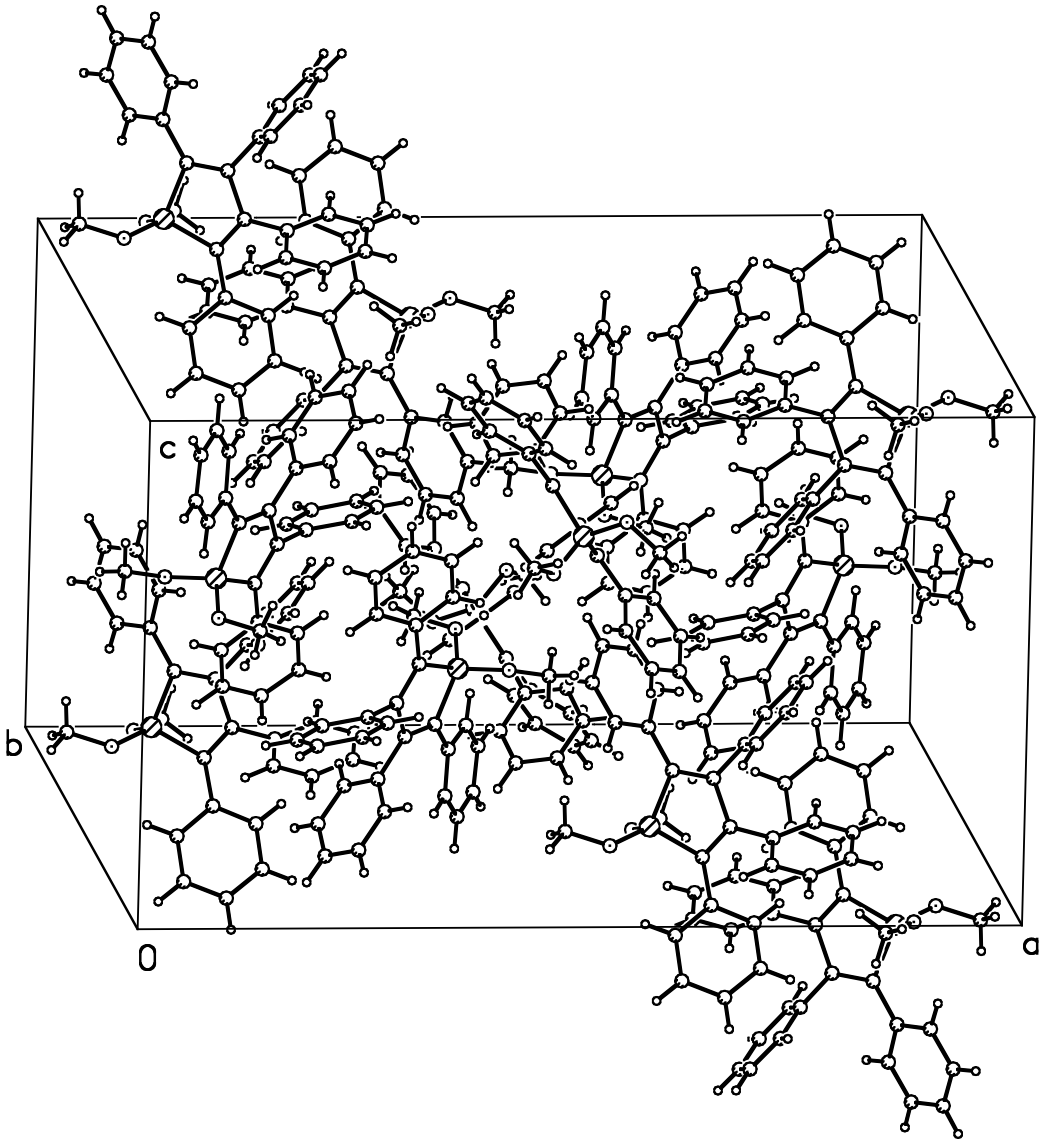

Fig. S2 Crystal packing of **III**.

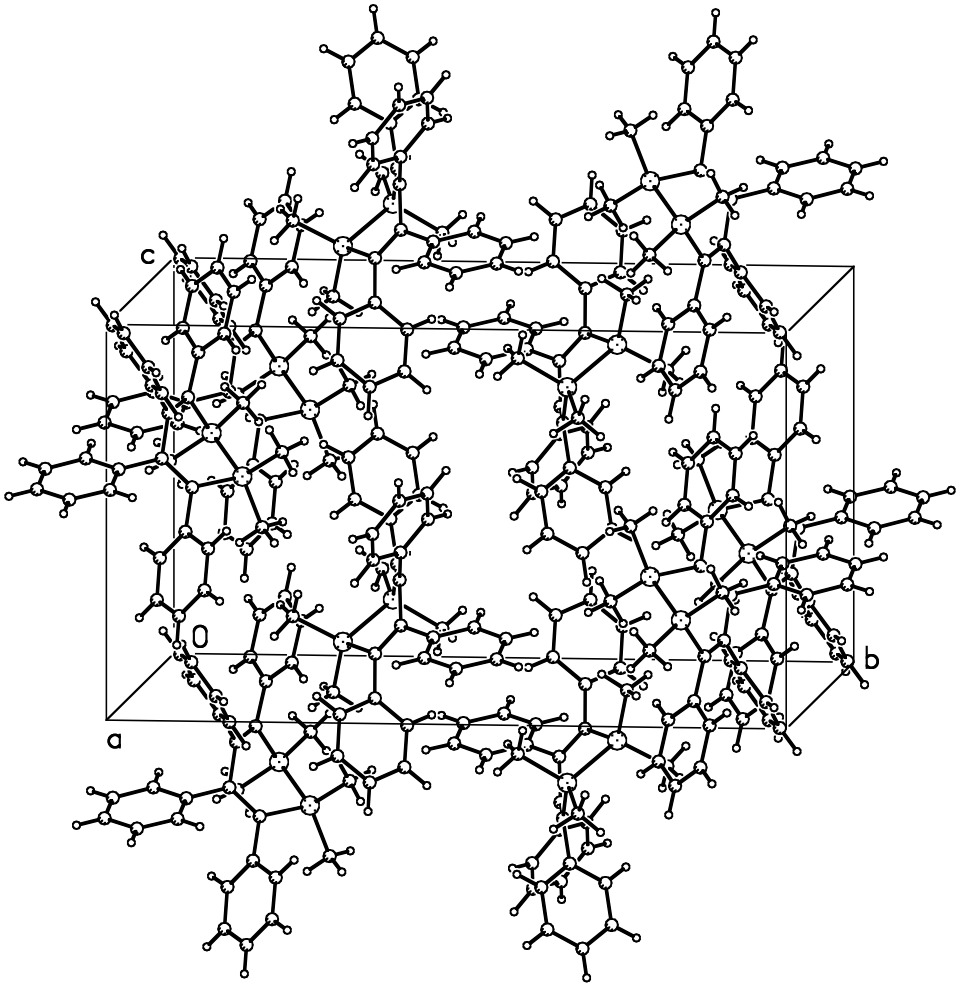

Fig. S3 Crystal packing of **IV**.

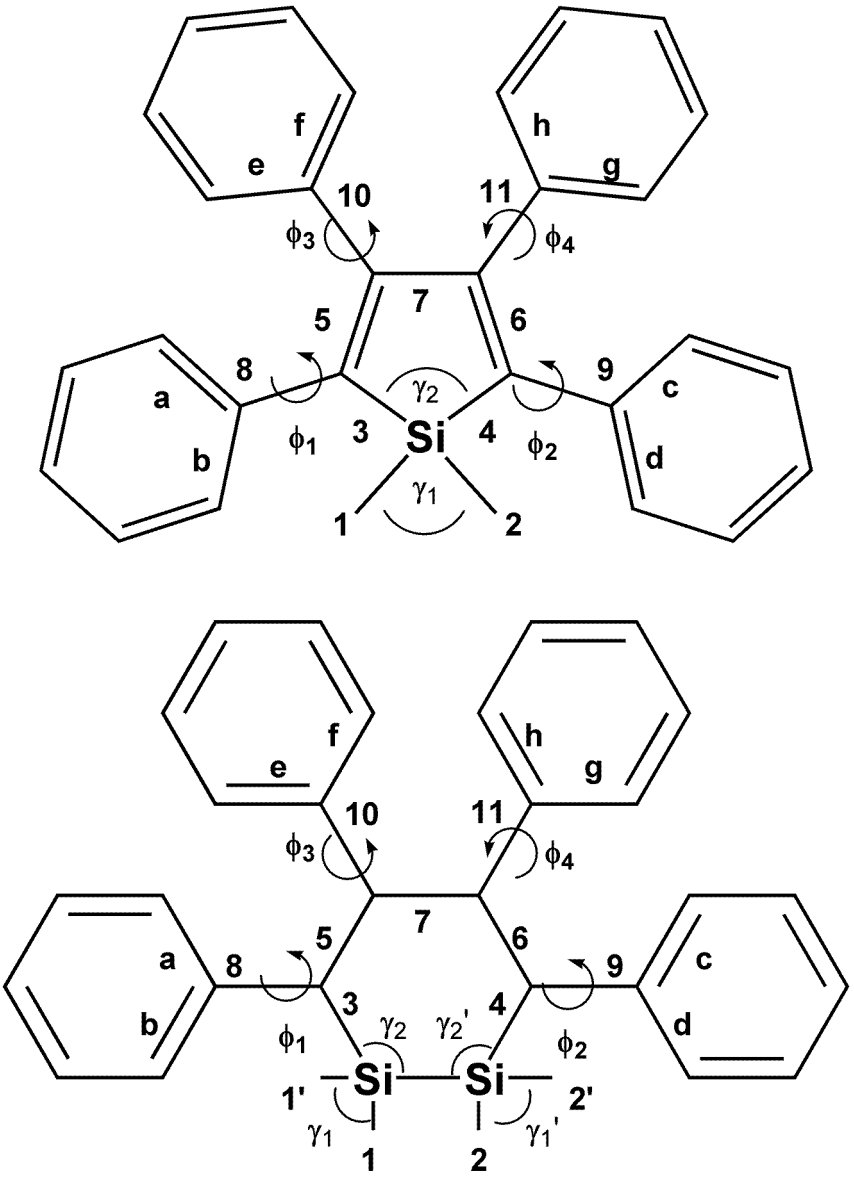

Fig. S4 Bond and angle numbering schemes.

Table S1 Selected X-ray crystallographic and B3LYP/6-31G*-calculated geometric parameters for **I**.

	expt.[a]	calc.				
	neutral	neutral	anion	(a-n)	cation	(c-n)
bond (Å)						
1	1.854	1.893	1.913	0.020	1.885	-0.008
2	1.855	1.893	1.913	0.020	1.885	-0.008
3	1.865	1.886	1.869	-0.017	1.902	0.016
4	1.865	1.886	1.869	-0.017	1.902	0.016
5	1.354	1.367	1.416	0.049	1.409	0.042
6	1.359	1.367	1.416	0.049	1.409	0.042
7	1.513	1.513	1.456	-0.057	1.462	-0.051
8	1.481	1.479	1.458	-0.021	1.450	-0.029
a	-----	1.409	1.422	0.013	1.422	0.013
b	-----	1.408	1.423	0.015	1.421	0.013
9	1.480	1.479	1.458	-0.021	1.450	-0.029
c	-----	1.409	1.422	0.013	1.422	0.013
d	-----	1.408	1.423	0.015	1.421	0.013
10	1.485	1.492	1.487	-0.005	1.485	-0.007
e	-----	1.405	1.410	0.005	1.407	0.002
f	-----	1.404	1.409	0.005	1.406	0.002
11	1.492	1.492	1.487	-0.005	1.485	-0.007
g	-----	1.405	1.410	0.005	1.407	0.002
h	-----	1.404	1.409	0.005	1.406	0.002
angle (°)						
α_1	92.6	92.5	93.3	0.8	90.5	-2.0
α_2	110.0	111.4	105.6	-5.8	112.9	1.5
dihedral angle (°)						
β_1	42.6	50.4	37.6	-12.8	31.6	-18.8
β_2	47.1	50.4	37.6	-12.8	31.6	-18.8
β_3	58.5	57.5	55.4	-2.1	59.2	1.7
β_4	57.1	57.5	55.4	-2.1	59.2	1.7

[a] L. Párkányi, *J. Organomet. Chem.*, 1981, **216**, 9-16.

Table S2 Selected X-ray crystallographic and B3LYP/6-31G*-calculated geometric parameters for **II**.

	expt.	calc.				
	neutral	neutral	anion	(a-n)	cation	(c-n)
bond (Å)						
1	1.855	1.912	1.941	0.029	1.903	-0.009
2	1.858	1.909	1.936	0.027	1.898	-0.011
3	1.854	1.882	1.861	-0.021	1.899	0.017
4	1.849	1.883	1.864	-0.019	1.899	0.016
5	1.340	1.366	1.415	0.049	1.409	0.043
6	1.344	1.366	1.413	0.047	1.408	0.042
7	1.489	1.516	1.457	-0.059	1.464	-0.052
8	1.454	1.478	1.461	-0.017	1.449	-0.029
a	1.382	1.408	1.421	0.013	1.421	0.013
b	1.386	1.408	1.420	0.012	1.422	0.014
9	1.464	1.479	1.462	-0.017	1.451	-0.028
c	1.376	1.408	1.420	0.012	1.420	0.012
d	1.374	1.409	1.419	0.010	1.421	0.012
10	1.479	1.492	1.486	-0.006	1.484	-0.008
e	1.370	1.404	1.410	0.006	1.407	0.003
f	1.379	1.405	1.410	0.005	1.407	0.002
11	1.474	1.492	1.486	-0.006	1.485	-0.007
g	1.383	1.404	1.409	0.005	1.406	0.002
h	1.367	1.405	1.409	0.004	1.407	0.002
angle (°)						
θ_1	79.4	78.5	77.0	-1.5	80.0	1.5
θ_2	92.4	92.7	93.4	0.7	90.8	-1.9
dihedral angle (°)						
τ_1	46.0	51.3	40.1	-11.2	31.6	-19.7
τ_2	55.2	53.1	42.9	-10.2	35.2	-17.9
τ_3	59.8	57.2	53.7	-3.5	58.0	0.8
τ_4	58.8	57.3	54.7	-2.6	58.9	1.6

Table S3 Selected X-ray crystallographic and B3LYP/6-31G*-calculated geometric parameters for **III**.

	expt.	calc.				
	neutral	neutral	anion	(a-n)	cation	(c-n)
bond (Å)						
1	1.628	1.663	1.694	0.031	1.643	-0.020
2	1.619	1.651	1.679	0.028	1.633	-0.018
3	1.856	1.871	1.844	-0.027	1.885	0.014
4	1.875	1.880	1.853	-0.027	1.891	0.011
5	1.352	1.365	1.414	0.049	1.407	0.042
6	1.345	1.365	1.414	0.049	1.406	0.041
7	1.527	1.524	1.463	-0.061	1.471	-0.053
8	1.480	1.476	1.461	-0.015	1.446	-0.030
a	1.402	1.409	1.420	0.011	1.423	0.014
b	1.395	1.410	1.420	0.010	1.423	0.013
9	1.485	1.476	1.460	-0.016	1.448	-0.028
c	1.402	1.410	1.420	0.010	1.422	0.012
d	1.389	1.410	1.421	0.011	1.423	0.013
10	1.489	1.492	1.486	-0.006	1.484	-0.008
e	1.394	1.404	1.410	0.006	1.406	0.002
f	1.382	1.404	1.409	0.005	1.407	0.003
11	1.500	1.492	1.486	-0.006	1.485	-0.007
g	1.388	1.404	1.410	0.006	1.406	0.002
h	1.384	1.404	1.409	0.005	1.407	0.003
angle (°)						
θ_1	107.2	106.1	100.7	-5.4	108.6	2.5
θ_2	93.9	94.0	94.8	0.8	92.1	-1.9
dihedral angle (°)						
τ_1	24.7	40.5	36.4	-4.1	28.1	-12.4
τ_2	26.2	39.3	36.2	-3.1	28.6	-10.7
τ_3	66.6	61.0	55.5	-5.5	59.8	-1.2
τ_4	68.4	61.2	56.2	-5.0	60.8	-0.4

Table S4 Selected X-ray crystallographic and B3LYP/6-31G*-calculated geometric parameters for **IV**.

	expt.	calc.				
	neutral	neutral	anion	(a-n)	cation	(c-n)
bond (Å)						
1	1.869	1.903	1.915	0.012	1.890	-0.013
1’	1.863	1.897	1.912	0.015	1.888	-0.009
2	1.867	1.903	1.915	0.012	1.890	-0.013
2’	1.872	1.897	1.912	0.015	1.888	-0.009
Si-Si	2.317	2.331	2.319	-0.012	2.389	0.058
3	1.893	1.918	1.881	-0.037	1.909	-0.009
4	1.906	1.918	1.881	-0.037	1.909	-0.009
5	1.350	1.363	1.420	0.057	1.393	0.030
6	1.350	1.363	1.420	0.057	1.393	0.030
7	1.507	1.514	1.461	-0.053	1.486	-0.028
8	1.490	1.495	1.480	-0.015	1.475	-0.020
a	1.393	1.405	1.417	0.012	1.413	0.008
b	1.388	1.406	1.416	0.010	1.413	0.007
9	1.496	1.495	1.480	-0.015	1.475	-0.020
c	1.391	1.405	1.417	0.012	1.413	0.008
d	1.387	1.406	1.416	0.010	1.413	0.007
10	1.500	1.504	1.502	-0.002	1.493	-0.011
e	1.388	1.404	1.407	0.003	1.407	0.003
f	1.389	1.402	1.407	0.005	1.406	0.004
11	1.496	1.504	1.502	-0.002	1.493	-0.011
g	1.391	1.404	1.407	0.003	1.407	0.003
h	1.388	1.402	1.407	0.005	1.406	0.004
angle (°)						
θ_1	107.7	109.0	106.4	-2.6	111.1	2.1
θ_1'	110.4	109	106.4	-2.6	111.1	2.1
θ_2	94.3	96.2	97.0	0.8	91.2	-5.0
θ_2'	94.4	96.2	97.0	0.8	91.2	-5.0
dihedral angle (°)						
τ_1	69.3	68.9	55.7	-13.2	55.3	-13.6
τ_2	75.4	68.9	55.6	-13.3	55.3	-13.6
τ_3	50.2	57.2	53.5	-3.7	51.9	-5.3
τ_4	57.2	57.2	53.5	-3.7	52.0	-5.2

Table S5 One-electron molecular orbital energies (eV) as determined at the B3LYP/6-31G* level of theory.

	HOMO-1	HOMO	LUMO	LUMO+1
I	-6.03	-5.29	-1.59	-0.27
II	-6.07	-5.37	-1.76	-0.30
III	-6.12	-5.29	-1.82	-0.34
IV	-5.97	-5.34	-1.24	-0.45