A computational chemistry investigation of the influence of steric bulk of dithiocarbamato-bound organic substituents upon spodium-bonding in three homoleptic mercury(II) bis(N,N-dialkyldithiocarbamato) compounds for alkyl = ethyl, isobutyl, and cyclohexyl

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***** Supplementary Materials *****

Table S1. QTAIM parameters (a.u.) for the bond critical points that characterize the spodium bonds.

Table S2. Cartesian coordinates for the geometry-optimized monomeric molecules of **1**.

Table S1. QTAIM parameters (a.u.) for the bond critical points that characterize the spodium bonds.[a]

Cmpd	Interaction	ρ	G	V	H	$\nabla^2\rho$
1	Hg···S	0.0226	0.0148	-0.0153	-0.0005	0.0571
2	Hg···S	0.0065	0.0037	-0.0028	0.0009	0.0182

a Abbreviations: electron-density (ρ), total, Lagrangian kinetic and potential energy densities (H, G and V, respectively) and the Laplacian of the electron-density ($\nabla^2\rho$).

Table S2. Cartesian coordinates for the geometry-optimized monomeric molecules of **1**.

1(pseudo-square planar)

Hg	-3.7114620	0.1274194	9.1984201
S	-2.9208632	-0.7087283	11.2855441
S	-4.7143824	-2.5632531	9.7674468
S	-4.5991698	0.9940679	7.1641345
N	-3.6369418	-3.0982518	12.1307912
C	-3.7748224	-2.2316920	11.1263666
C	-2.8056732	-2.8391372	13.2980270
H	-2.3982669	-3.8010732	13.6198175
H	-1.9605539	-2.2198162	12.9947176
C	-3.5726886	-2.1792311	14.4285095
H	-2.9185472	-2.0353375	15.2909750
H	-3.9488036	-1.2038925	14.1167487
H	-4.4194104	-2.7924230	14.7450879
C	-4.3303468	-4.3800402	12.1211337
H	-5.2798270	-4.2448645	11.6031834
H	-4.5438208	-4.6354026	13.1623463
C	-3.5159128	-5.4706850	11.4534467
H	-4.0593839	-6.4172621	11.4870925
H	-3.3343407	-5.2156232	10.4086003
H	-2.5543134	-5.6146380	11.9520092
S	-2.3232815	2.5565208	8.3183298
C	-3.5035029	2.3616223	7.1315702
N	-3.6564879	3.2207932	6.1228647
C	-2.7893761	4.3834620	5.9832762
H	-2.6963720	4.5867433	4.9132062
H	-1.8038494	4.1173363	6.3654645
C	-3.3322304	5.5937629	6.7185002
H	-2.6713732	6.4501943	6.5700329
H	-3.3916835	5.3864525	7.7877469
H	-4.3268531	5.8675469	6.3584253
C	-4.6769328	3.0679080	5.0949974
H	-4.9799122	4.0735029	4.7918247
H	-5.5513004	2.5906177	5.5386764

C	-4.1839267	2.2744586	3.8994155
H	-4.9680502	2.2091900	3.1421098
H	-3.9117803	1.2614791	4.1992737
H	-3.3113564	2.7470735	3.4431871

1(tetrahedral)

Hg	3.8297605	3.0593076	1.3173587
S	4.5580917	2.7325949	3.6889961
S	2.6604491	0.9158904	2.3031776
S	4.6169875	3.5336568	-1.0109354
S	2.3127145	4.9238582	0.2444172
N	3.3647293	0.6714835	4.8485649
N	3.1339143	5.3496088	-2.2422852
C	3.5055158	1.3630118	3.7199603
C	4.0508430	1.0401621	6.0787927
C	5.3981799	0.3580453	6.2191082
C	2.4950922	-0.4945991	4.9282609
C	1.0765362	-0.1276332	5.3200771
C	3.3253368	4.6761333	-1.1103552
C	3.9890557	5.1709319	-3.4074855
C	3.4807373	4.0857964	-4.3376924
C	2.0437990	6.3040897	-2.3913499
C	2.4515809	7.7118933	-2.0017912
H	4.1670955	2.1243171	6.0957425
H	3.3916587	0.7688714	6.9073385
H	5.2966603	-0.7293808	6.2061360
H	2.9373163	-1.1753170	5.6603310
H	2.5059203	-0.9946918	3.9596349
H	0.6340400	0.5239892	4.5653125
H	4.0338167	6.1336112	-3.9232263
H	4.9967971	4.9379100	-3.0620009
H	3.4641139	3.1234451	-3.8244086
H	1.2092881	5.9650176	-1.7771564
H	1.7255139	6.2670235	-3.4364147
H	2.7447897	7.7423965	-0.9515914
H	0.4645638	-1.0285835	5.3986989

H	1.0492979	0.3854304	6.2842007
H	6.0608247	0.6554673	5.4053072
H	5.8660893	0.6423702	7.1639203
H	2.4721804	4.3073195	-4.6940419
H	4.1350757	4.0001786	-5.2076379
H	3.2875936	8.0682290	-2.6082225
H	1.6140585	8.3978102	-2.1449424