SUPPLEMENTARY MATERIALS

Synthesis and characterization of mononuclear Zn(II), Co(II) and Ni(II) complexes containing a sterically demanding silanethiolate ligand derived from tris(2,6-diisopropylphenoxy)silanethiol

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[c] Institute of Physics, Maria Curie-Skłodowska University, Sq. Maria Curie-Skłodowska 1, 20-031 Lublin, Poland
† anndoleg@pg.gda.pl

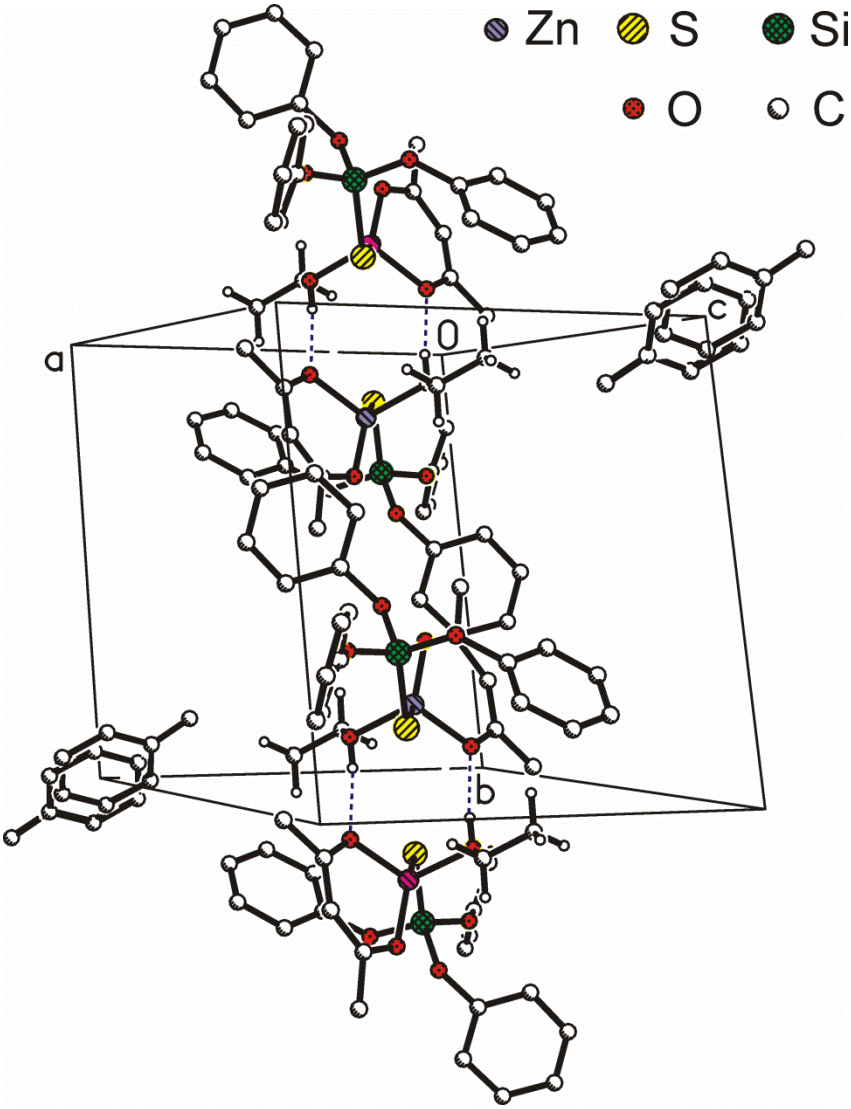

Fig. 1S Crystal packing of **3**. Hydrogen bonds indicated with the dashed lines. Both orientations of disordered toluene molecule are shown.

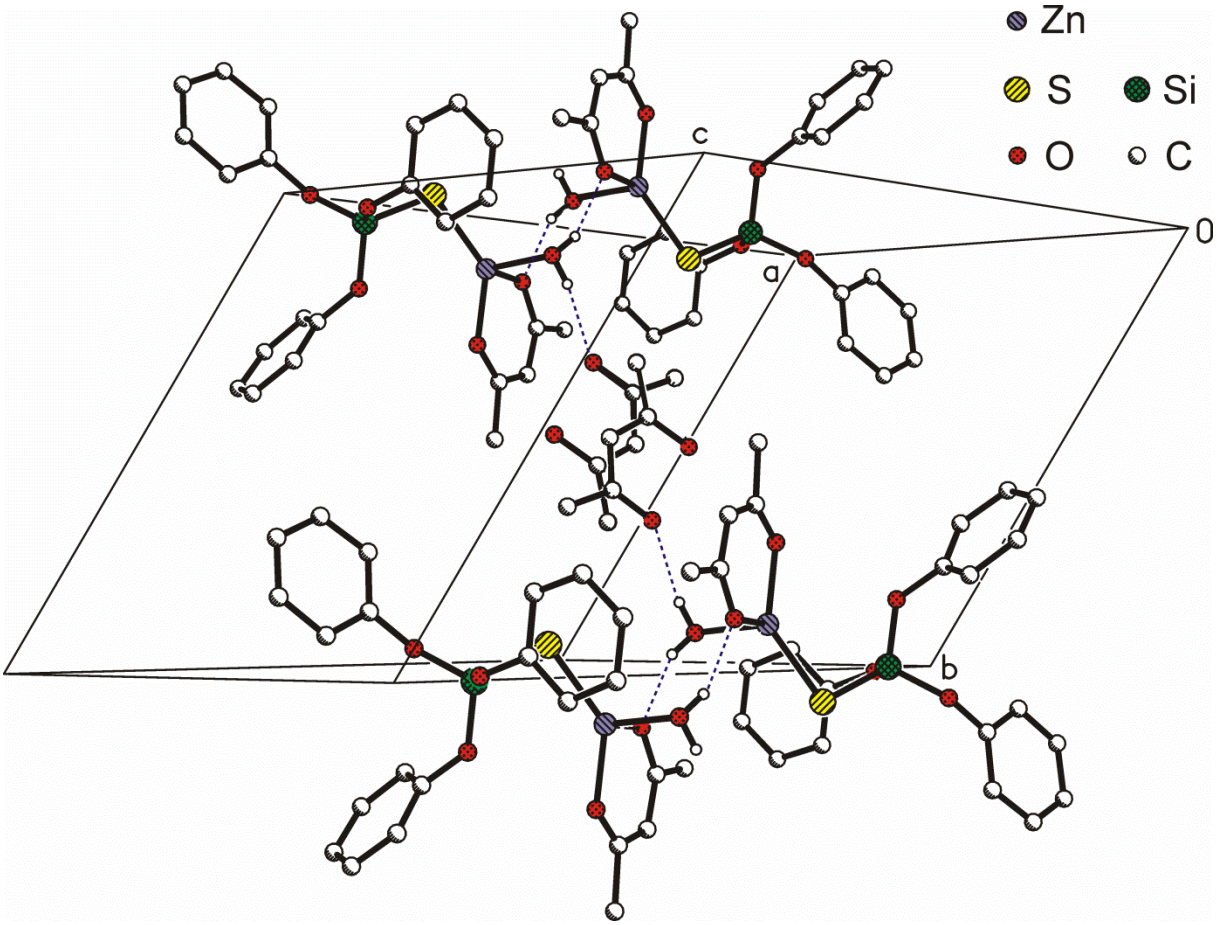

Fig. 2S Crystal packing of **4**. Hydrogen bonds indicated with the dashed lines. Both orientations of disordered acetylacetone molecule are shown.

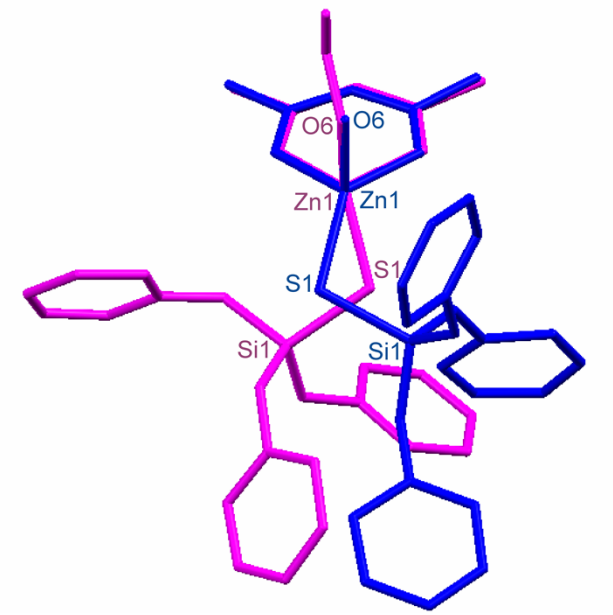

Fig. 3S The overlay of X-ray molecular structures of **3** (magenta) and **4** (blue). Isopropyl groups of 2,6-diisopropylphenoxy substituents and all hydrogen atoms are omitted for clarity.

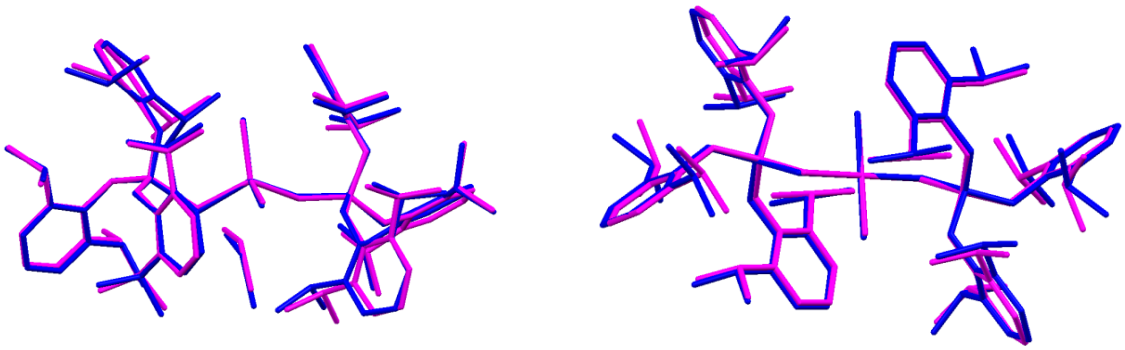

Fig. 4S The overlay of calculated (blue) and experimental (magenta) molecular structures of **1** and **2**. Hydrogen atoms are omitted for clarity.

Table 1S Experimental and calculated bond lengths in **1** and **2**.

Bond \ Compound	**1**		**2**	
	Calculated bond length	Experimental bond length	Calculated bond length	Experimental bond length
M-S	2.202	2.2623(7)	2.307	2.2863(8)
M-N	1.868	1.919(2)	2.098	2.052(4)
Si-S	2.066	2.0771(9)	2.096	2.0599(11)
Si-O	1.631	1.6330(19)	1.657	1.631(2)
Si-O	1.649	1.6499(19)	1.677	1.645(2)
Si-O	1.663	1.6570(19)	1.686	1.652(2)
O-C	1.384	1.396(3)	1.401	1.383(3)
O-C	1.391	1.400(3)	1.407	1.385(4)
O-C	1.391	1.400(3)	1.416	1.400(4)
average aromatic C-C	1.390(5)	1.396(18)	1.405(4)	1.391(12)
average aliphatic C-C	1.511(6)	1.521(13)	1.546(4)	1.528(9)
average arom.-aliph C-C	1.498(3)	1.524(11)	1.527(1)	1.511(3)

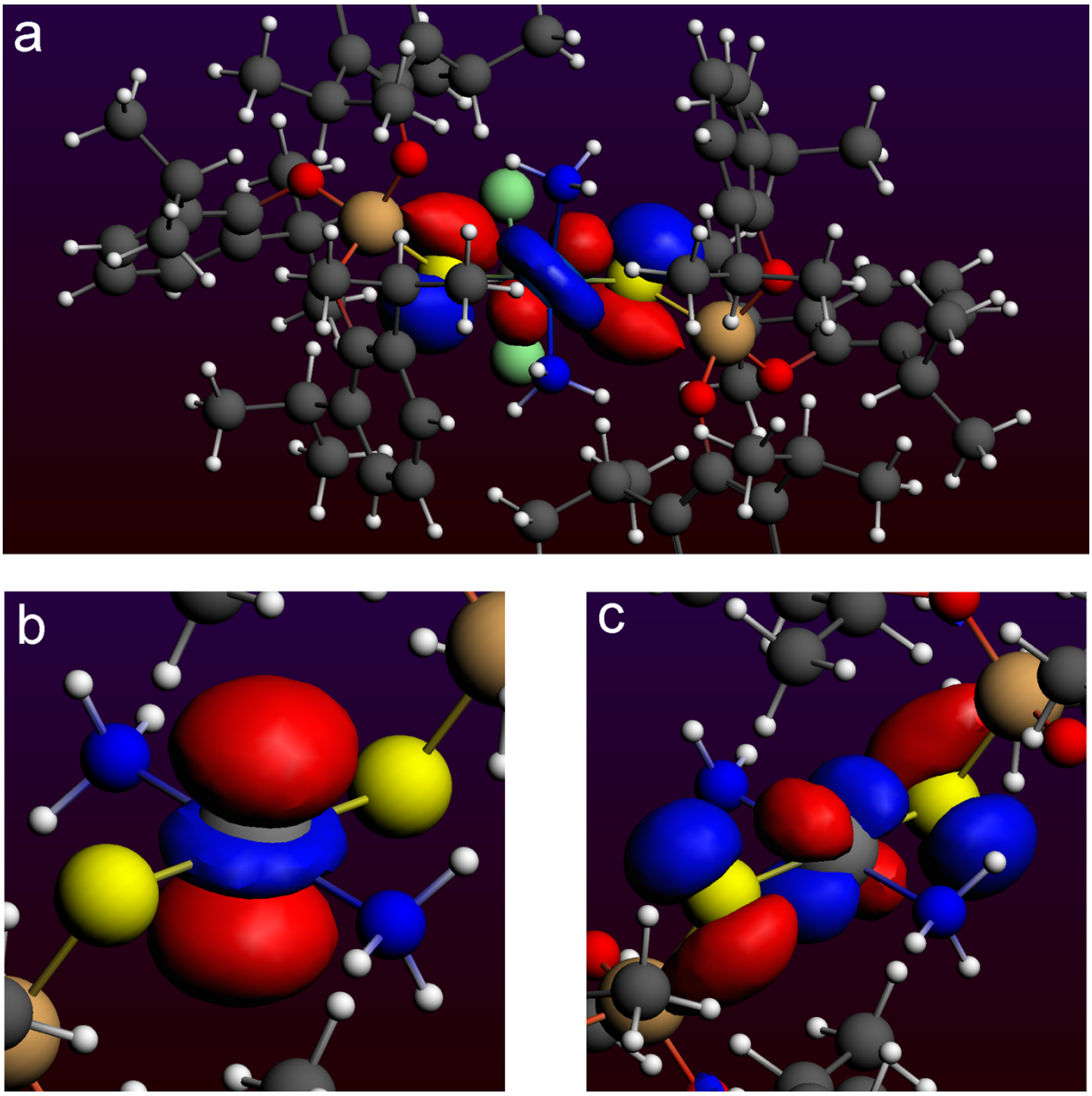

Fig. 5S a) Complex **2**, HOMO; b) complex **1**, HOMO; c) complex **1** HOMO-1

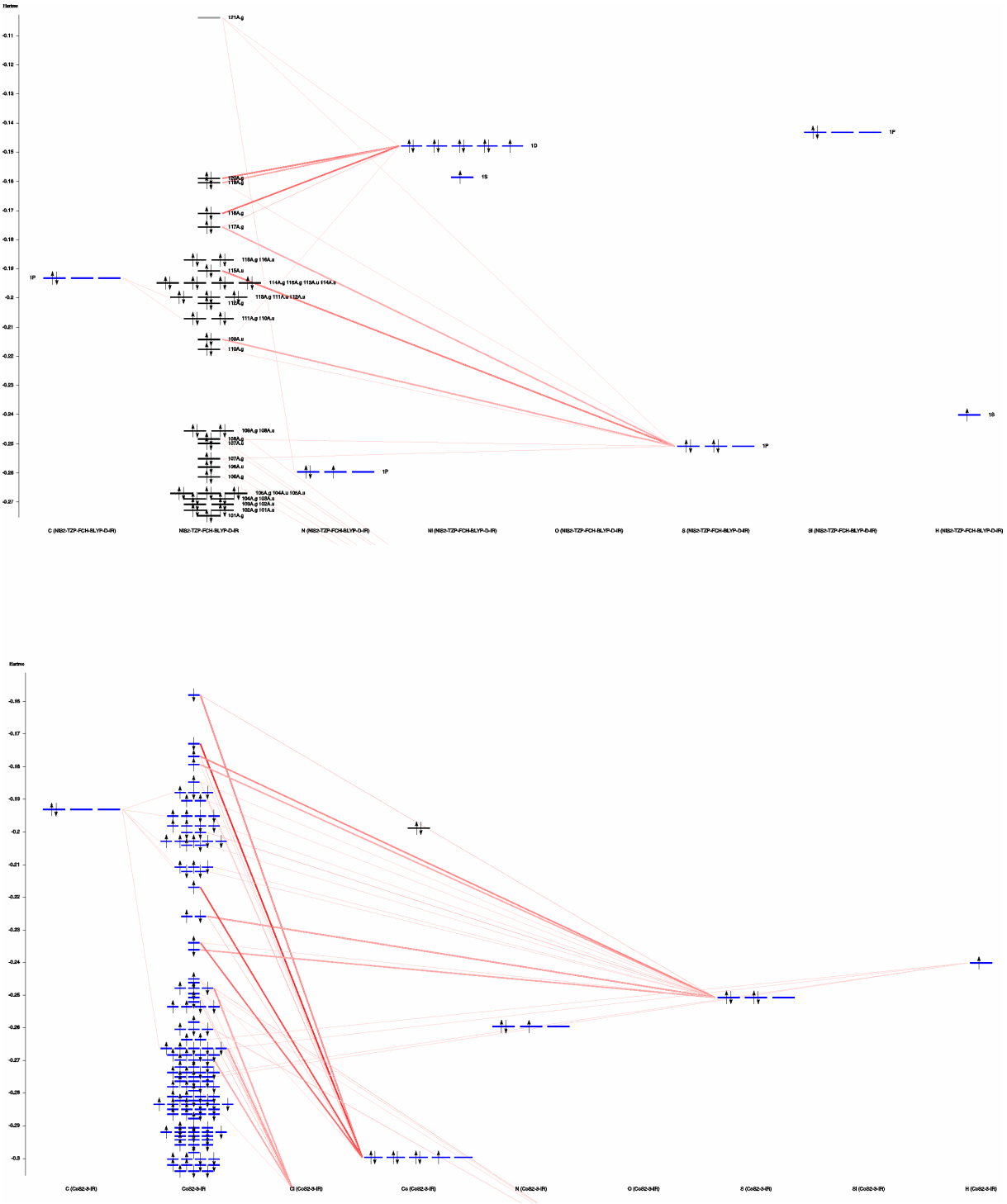

Fig. 6S Partial picture of orbital energy levels in **1** (upper part) ann **2** (lower part)

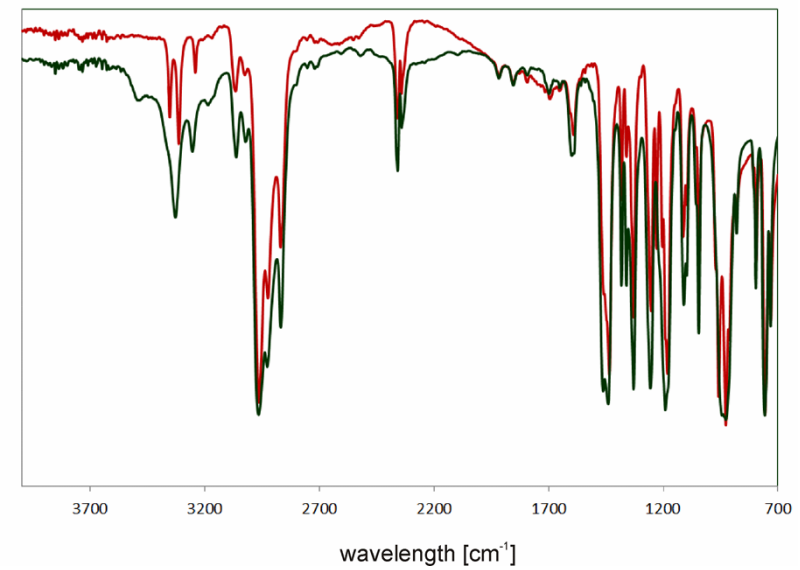

Fig. 7S Experimental FT-IR spectra of **1** (red line) and **2** (green line).

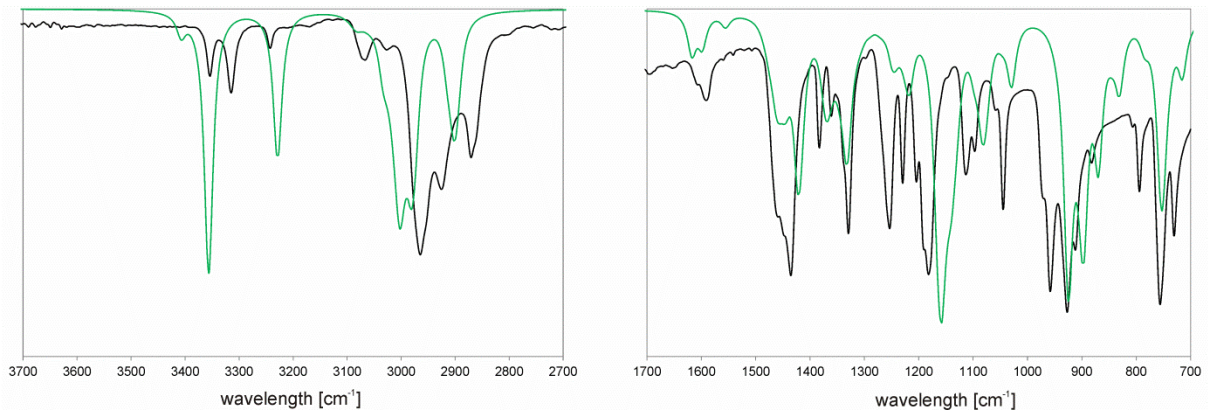

Fig. 8S Experimental (black line) and calculated (green line) FT-IR transmittance spectra of **1**.

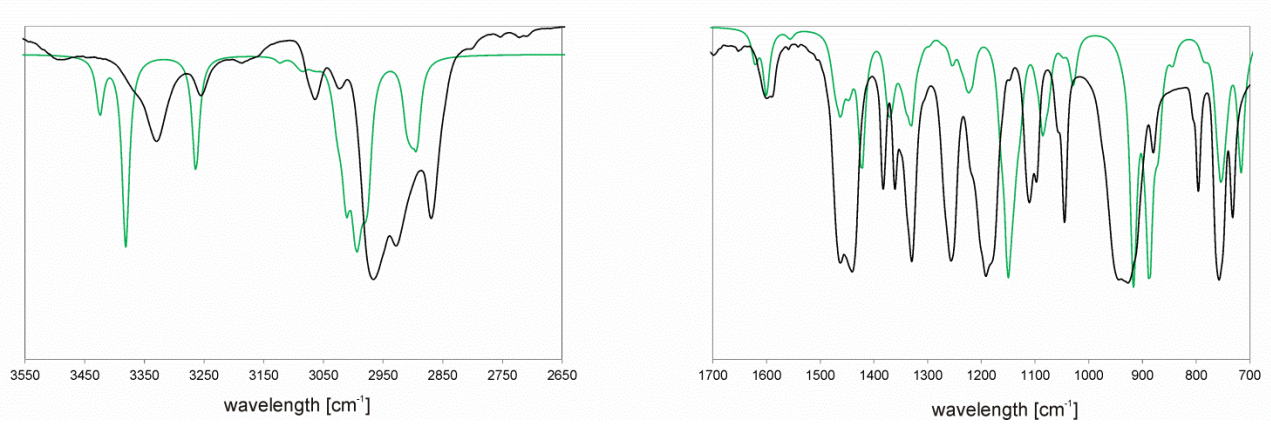

Fig. 9S Experimental (black line) and calculated (green line) FT-IR transmittance spectra of **2**.

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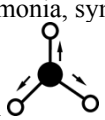
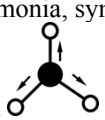
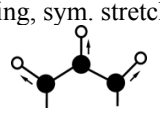
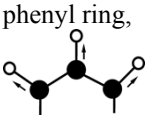
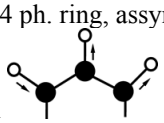
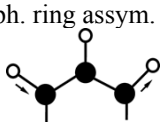
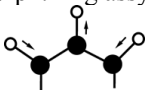
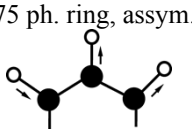
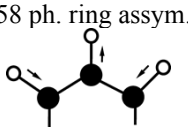
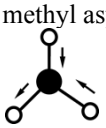
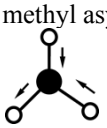
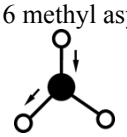
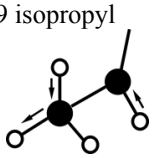
Table 2S Experimental and BLYP-D/6-31G(d) calculated frequencies, and general mode assignments for observed IR bands in the FT-IR spectrum of **1** and **2** (stretching frequencies and fingerprint region). No scaling to the calculated spectrum was applied.

Compound **1**			Compound **2**		
Experimental spectrum [cm^{-1}]	BLYP-D/ 6-31G(d) [cm^{-1}]	Assignment from calculations	Experimental spectrum	BLYP-D/ 6-31G(d)	Assignment from calculations
3355m	3404w	3408, 3356 ammonia, asym. stretch. 	3366w,sh	3423m	3424, 3381 ammonia, asym. stretch. 
3304m	3356s		3333m	3381s	
3245w	3227s	3233 ammonia, sym. stretch 	3259s	3265m	3265 ammonia, sym. stretch 
				3124vw	3124 methylene assymetric stretch in methylene chloride
3087m		3102-3090, 3082 phenyl ring, sym. stretch 	3064w	3085w	3097-3091 phenyl ring, sym. stretch 
3032w	3076w	3088-3074 ph. ring, assym. stretch  3065 ph. ring assym. stretch  3060-3057 ph. ring assym. stretch 	3019w	3064vw	3082-3075 ph. ring, assym. stretch  3067-3058 ph. ring assym. stretch 
2967vs	3028m,sh	3035-3029 methyl asym. stretch 	2975vs	3011s	3039-3029 methyl asym. stretch 
	3002vs				
2908s	2980s		2930vs	2993vs	
		3016 methyl asym.  3027-2971 isopropyl			3024-2989 isopropyl asym. stretch 

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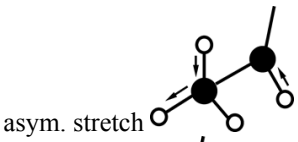
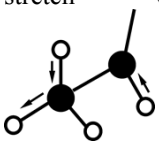
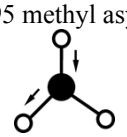
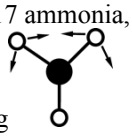
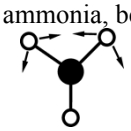
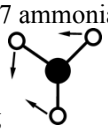
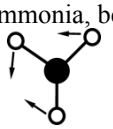
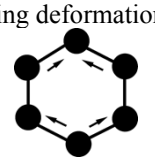
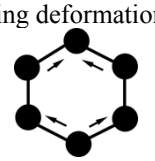
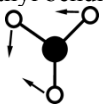
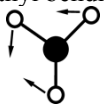
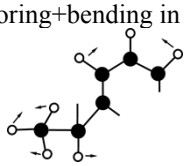
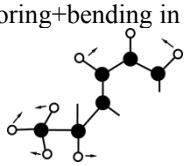
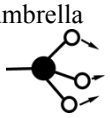
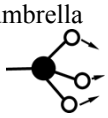
		asym. stretch   2914-2882 methyl sym. 			 3019 methylene symmetric stretch in methylene chloride 2995 methyl asym.  2912-2891 methyl sym. 
1605w,sh	1619w	1619,1617 ammonia, bending 	1600w	1617w	1622 ammonia, bending 
1591w	1598w	1598, 1597 ammonia, bending 	1591w	1604w	1600 ammonia, bending 
	1559-1555	ring deformation 		1557	ring deformation 
1458s,sh	1455m	1485-1436 methyl bending (scissoring) 	1462vs	1463m	1482-1437 methyl bending (scissoring) 
1446s,sh	1448m		1441vs	1446m	
1435vs	1422s	1423-1416 isopropyl and phenyl CH bending (scissoring+bending in plane) 		1427s	1424-1421 isopropyl and phenyl CH bending (scissoring+bending in plane) 
1387m	1367m	1378-1346 methyl wagging (umbrella deformation) 	1383m	1375m	1376-1347 methyl wagging (umbrella deformation) 
1361m			1361m	1340m,sh	
1323s	1334m	1344-1273 methanetriyl wagging (in plane)	1329vs	1329m	1340-1275 methanetriyl wagging (in plane)

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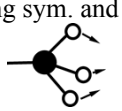
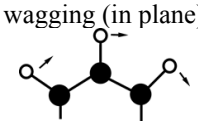
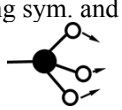
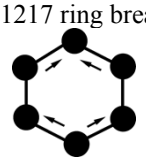
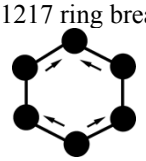
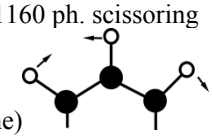
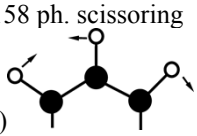
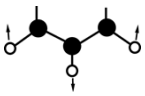
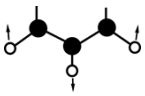
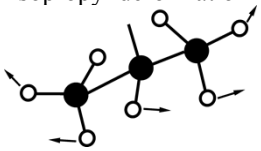
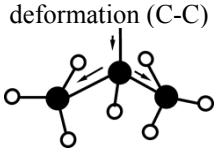
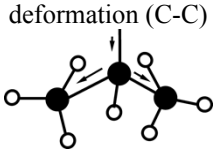
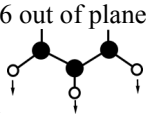
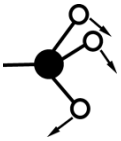
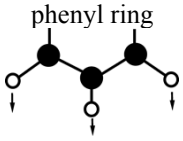
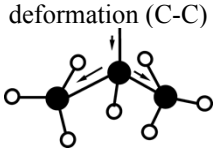
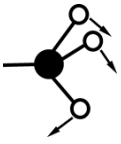
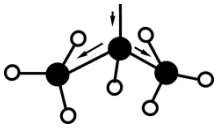
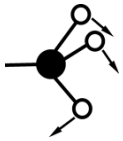
1247s	1246w	1271-1263 ring deformation 1256-1249 ammonia wagging sym. and asym.  1243-1230 ph. ring wagging (in plane) 	1255vs	1255w	1270 - 1263ring deformation 1254 methylene wagging in methylene chloride 1240-1237 phenyl ring wagging (in plane)  1229-1225 ammonia wagging sym. and asym. 
1230m	1216m	1225-1217 ring breathing 	1216m,sh	1220m	1225-1217 ring breathing 
1205m					
1189s,sh		1170-1160 ph. scissoring (in plane) 	1191vs		1167-1158 ph. scissoring (in plane) 
1181vs	1157vs	1158-1129 isopropyl and phenyl deform. - scissoring  1158,1140 – C-O stretch	1183vs,sh	1150vs	1152-1127 isopropyl and phenyl deform. - scissoring 
1113m	1142s,sh		1110m	-	
1098m	1080m	1098-1085 isopropyl deformation 	1098m	1086m	1098-1085 isopropyl deformation 
1057w,sh			1056m,sh		
1045m	1032w	1076-1028 isopropyl rocking 	1044m	1047vw 1030w	1076-1028 isopropyl rocking 
968m,sh		952-947 out of plane			957-951 out of plane

SUPPLEMENTARY MATERIALS

		phenyl ring 			phenyl ring 
957vs	925vs	946-902 isopropyl deformation, rocking	944vs	917vs	941-925, 914-895 isopropyl deformation
926vs	896s	 926, 925 Si-O stretch	928vs	888vs	 918-917 Si-O stretch
911s,sh		898-895, 870-845 Si-O-C deformation	878w	874s,sh	886-868 Si-O-C deformation
887w	870m	Si-O-C deformation			
808w	830		804w,sh	843w	848-846 isopropyl deformation and ring deformation (C-C) 
793m	782w,sh	848-844 isopropyl deformation and ring deformation (C-C) 	795m	783w,sh	789-786 out of plane phenyl 
759vs	752s	831-798 ammonia rocking  787-785 out of plane phenyl ring  780, 756 isopropyl deformation and ring deformation (C-C)  753-736 out of plane phenyl ring  754-752 ammonia rocking 	758vs	755s	781-779 isopropyl deformation  762-739 ring deformation 742-699 ammonia rocking 

731m	716m	718 Si-O stretch + ring deformation	733m	716m	

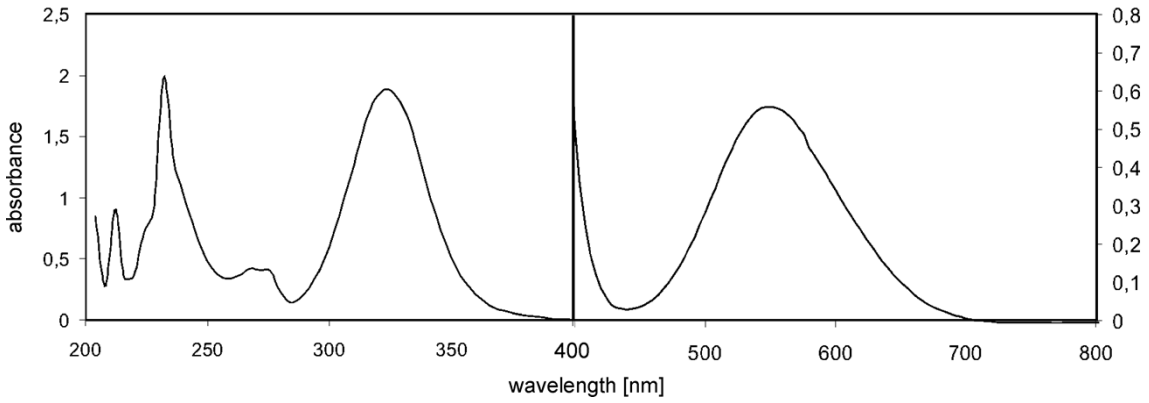


Fig. 10S UV-vis spectra of solutions of **1** in dichloromethane (0.000907 M).

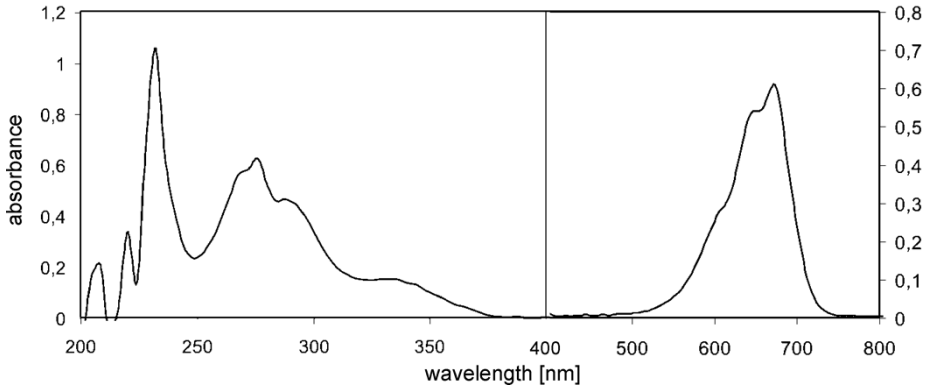


Fig. 11S UV-vis spectra of solutions of **2** in dichloromethane (0.000814 M).