

Supplementary Info

Syntheses, structural characterizations and biological activities of *spiroansa-spiro-cyclotriphosphazenes*

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Table

- **Table 1S** 2D ^1H - ^{13}C HSQC and HMBC correlations for **9b** and **9c**

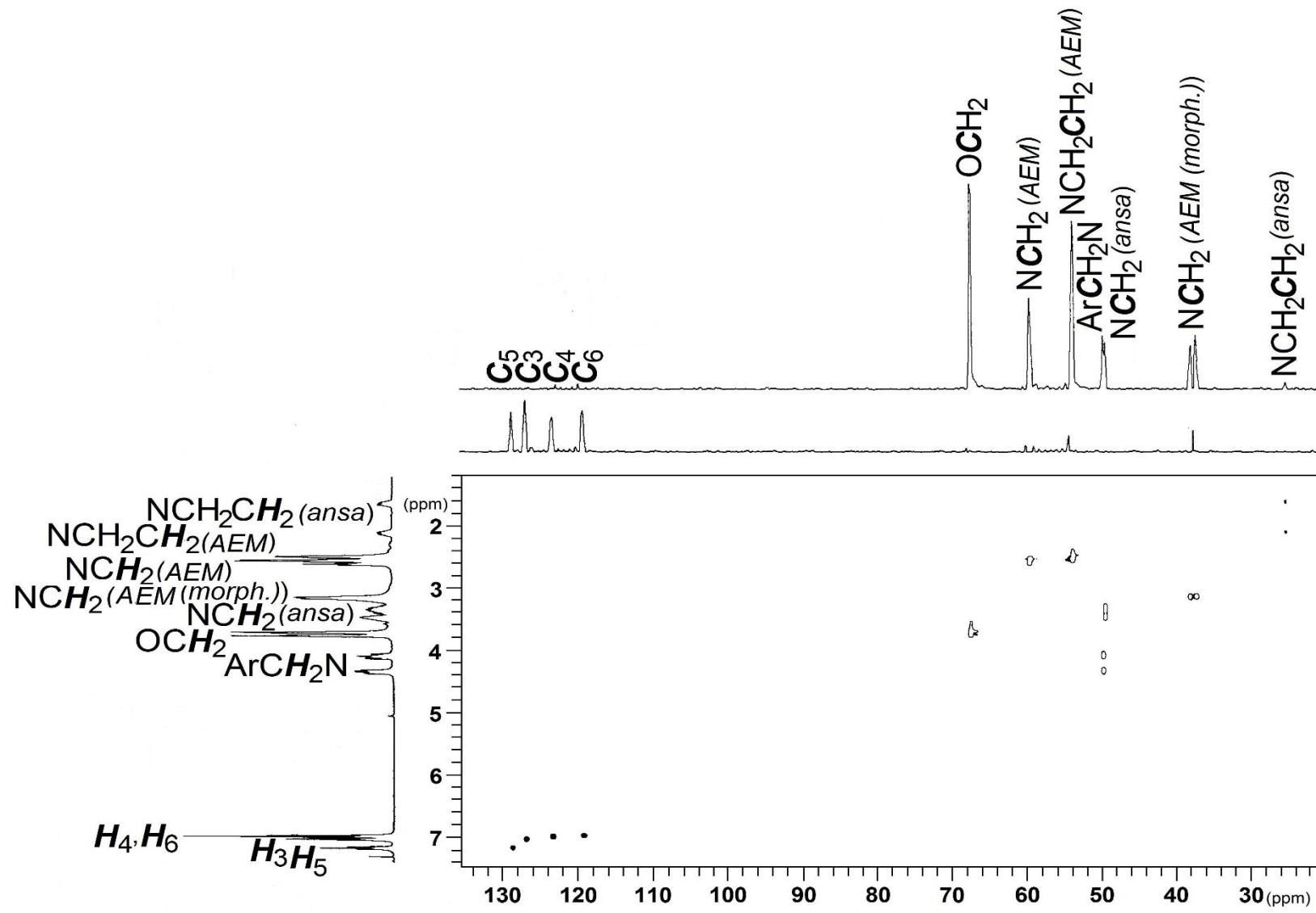


Fig. 1S HSQC spectrum of **9b**.

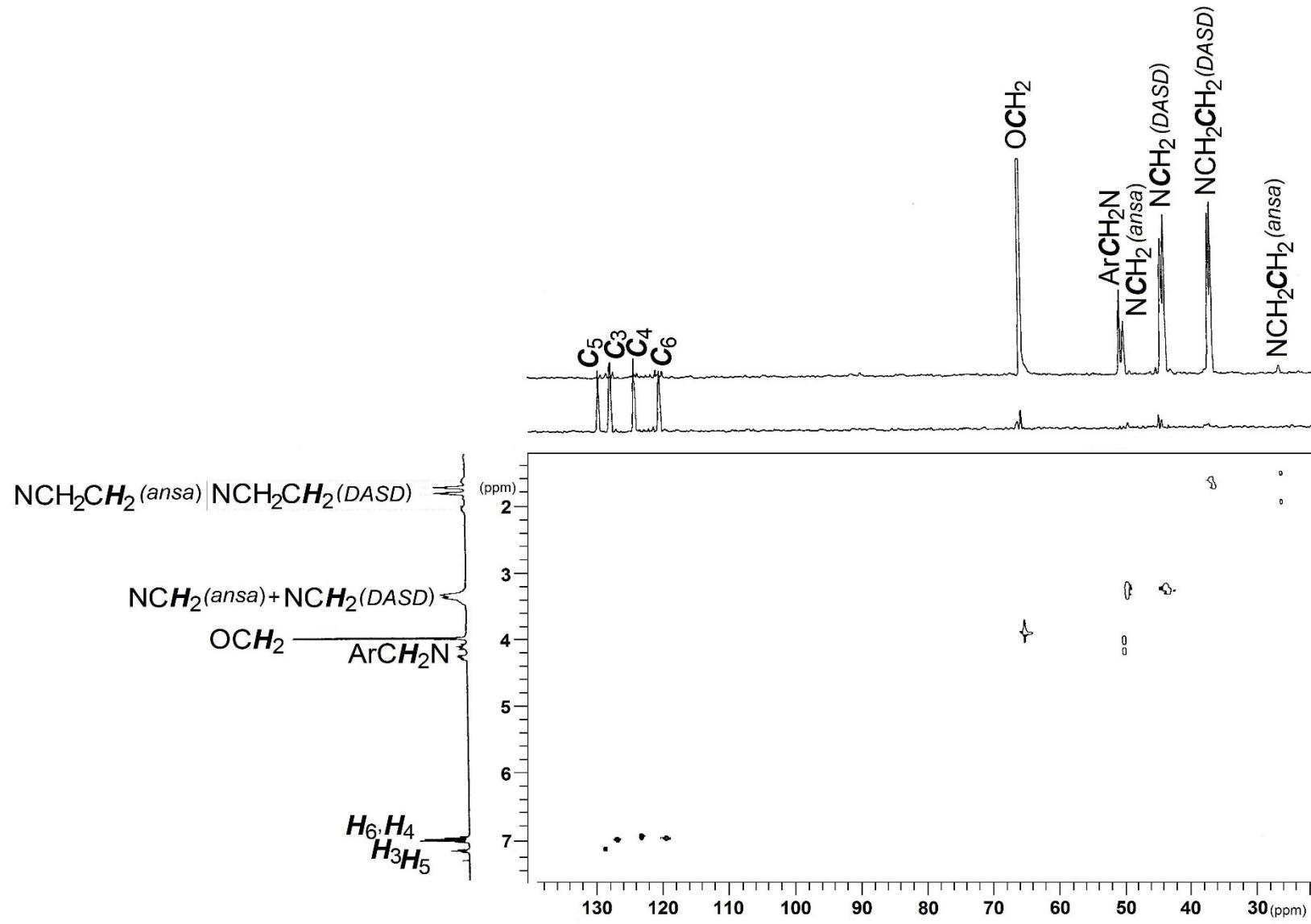


Fig. 2S HSQC spectrum of **9c**.

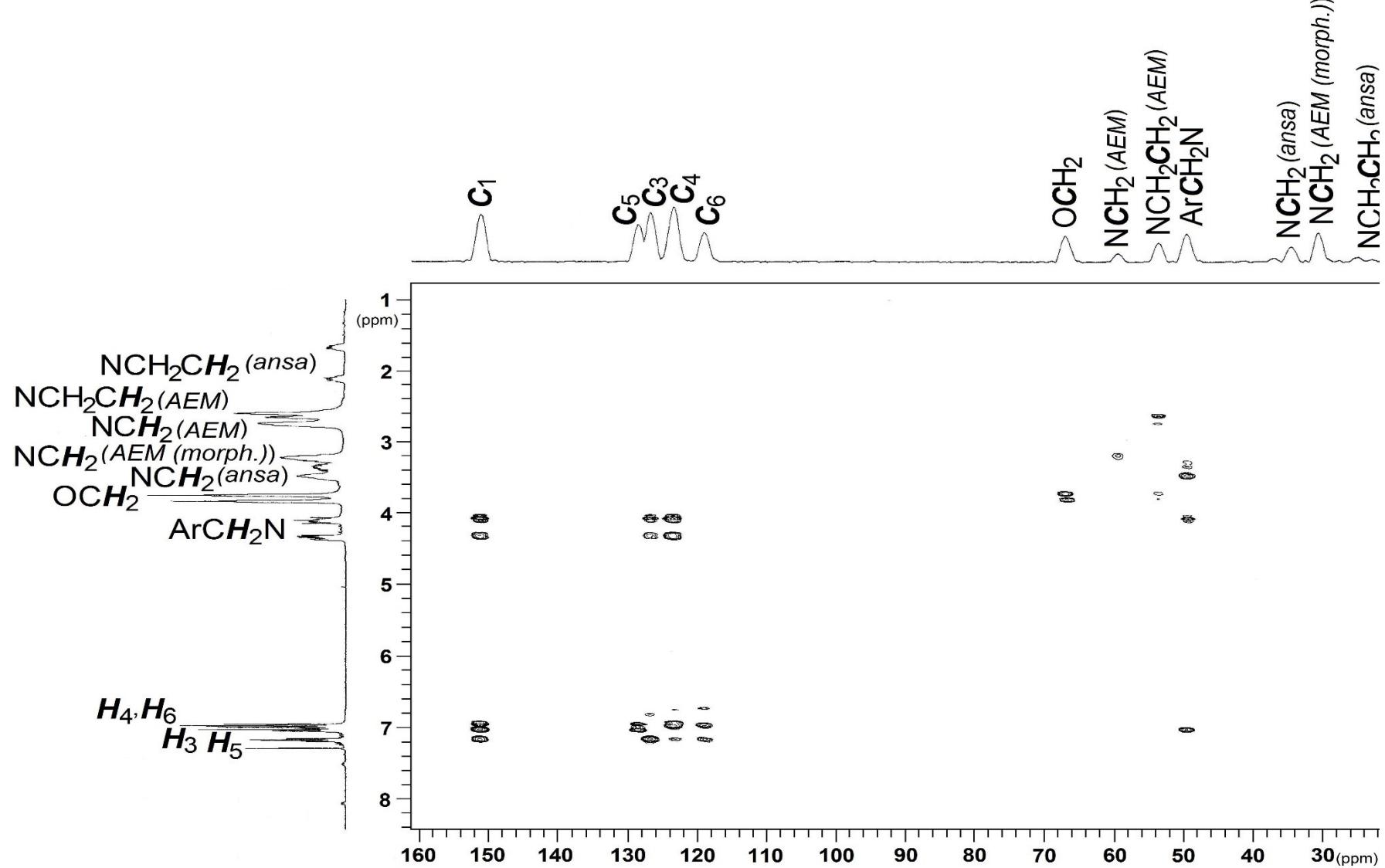


Fig. 3S HMBC spectrum of **9b**.

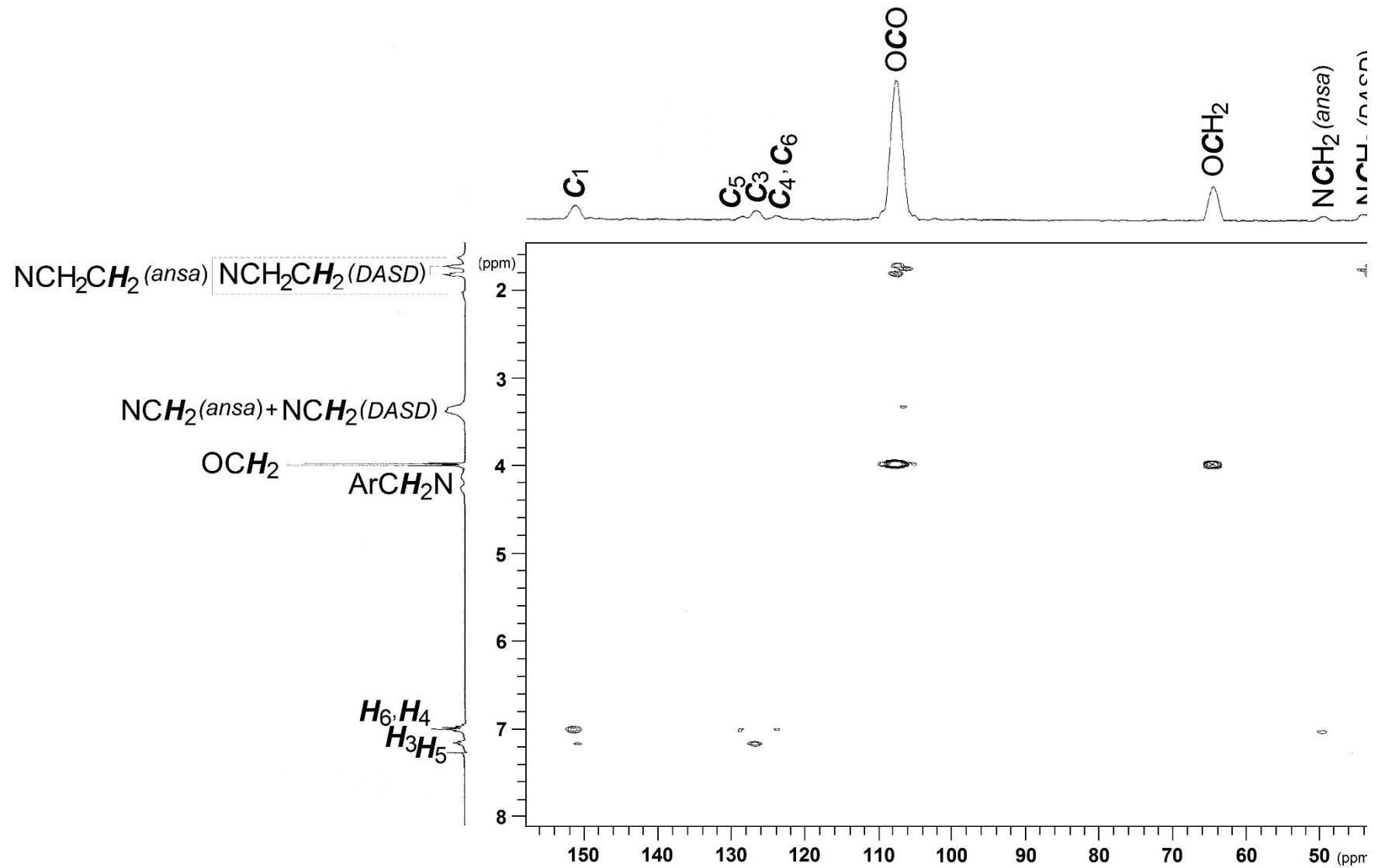


Fig. 4S HMBC spectrum of **9c**.

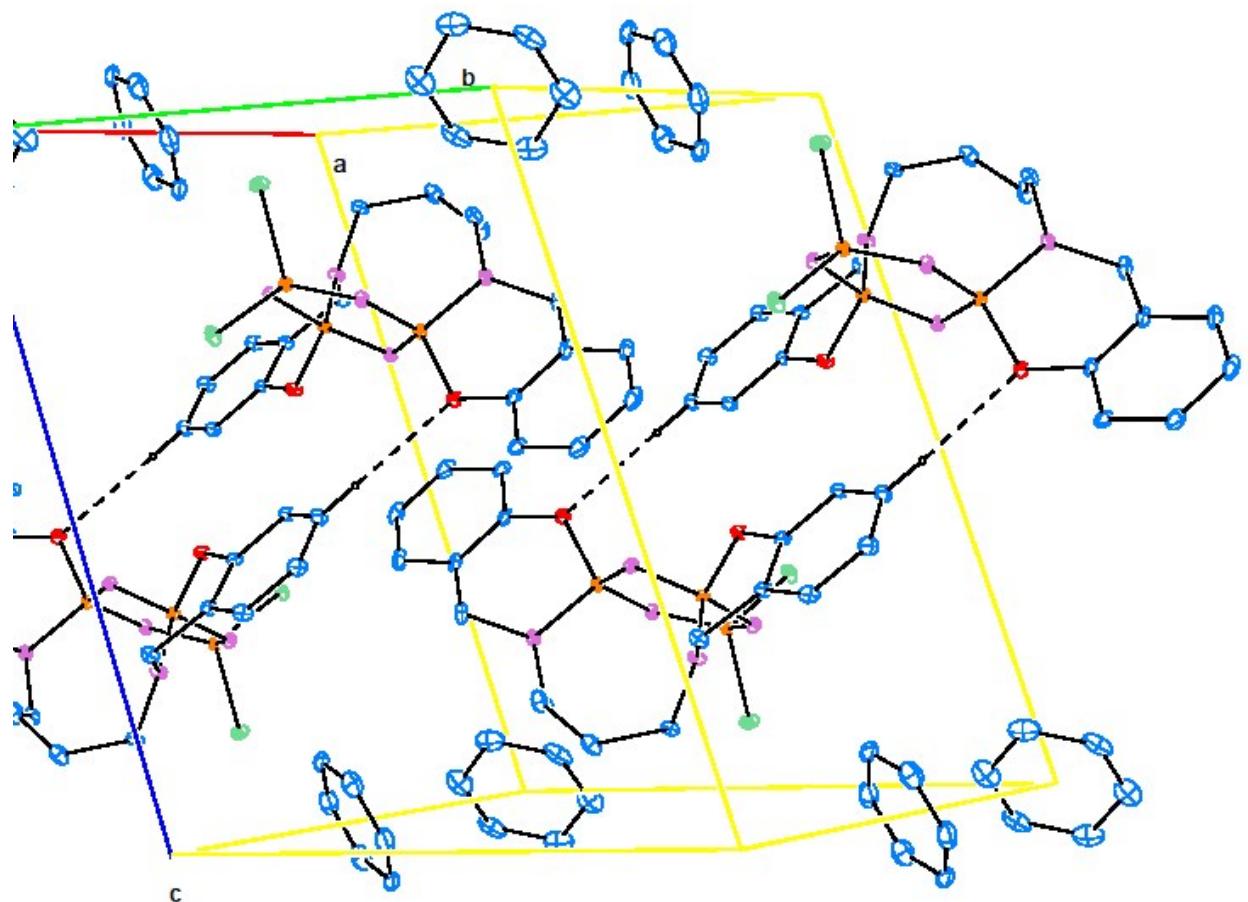


Fig. 5S Packing diagram of **8**.

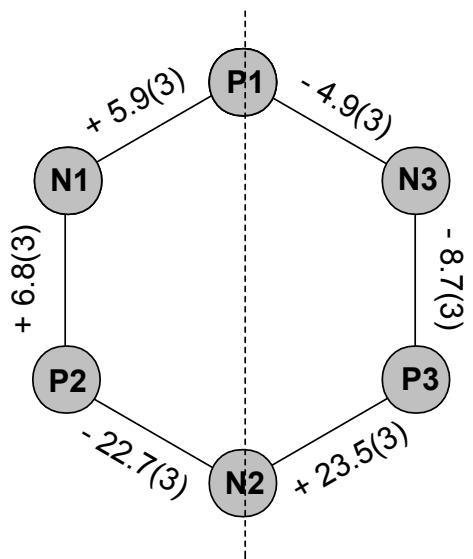


Fig. 6S The shape of the phosphazene ring in **8** with torsion angles (deg) given.

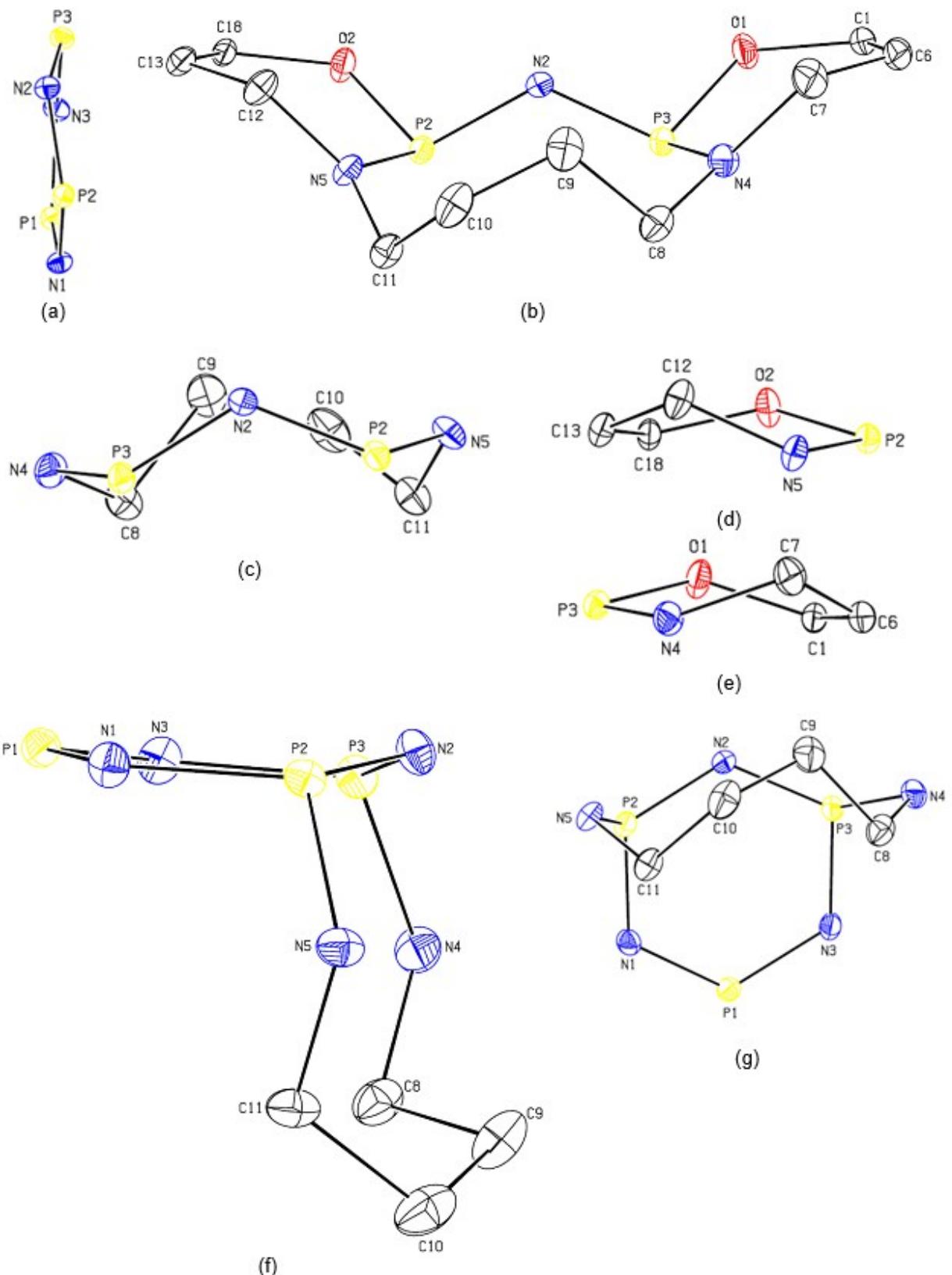


Fig. 7S The conformations of (a) phosphazene, (b) *spiro* and *ansa*, (c) *ansa*, (d) and (e) *spiro* rings, (f) and (g) the bicyclic system made up of phosphazene and the *ansa* rings of **8**.

Table S 2D ^1H - ^{13}C HSQC and HMBC correlations for **9b** and **9c**

Atom	HSQC		HMBC [$J(\text{C},\text{H})$]		
	^1J	^2J	^3J	^4J	Spatial J
9b	NCH ₂ CH ₂ [<i>ansa</i>]	NCH ₂ CH ₂ [<i>ansa</i>]	—	—	—
	NCH ₂ CH ₂ [<i>AEM</i>]	NCH ₂ CH ₂ [<i>AEM</i>]	—	—	—
	NCH ₂ [<i>AEM</i>]	NCH ₂ [<i>AEM</i>]	—	NCH ₂ CH ₂ [<i>AEM</i>]	—
	NCH ₂ [<i>ansa</i>]	NCH ₂ [<i>ansa</i>]	—	ArCH ₂ N	—
	NCH ₂ [<i>AEM (morph.)</i>]	NCH ₂ [<i>AEM (morph.)</i>]	—	NCH ₂ [<i>AEM</i>]	—
	OCH ₂	OCH ₂	—	—	—
	ArCH ₂ N	ArCH ₂ N	—	C ₁ , C ₃	C ₄
	ArH H ₃	C ₃	—	ArCH ₂ N, C ₁ , C ₅	—
	H ₄	C ₄	C ₅	C ₆	—
	H ₅	C ₅	C ₆	C ₁ , C ₃	—
	H ₆	C ₆	C ₁ , C ₅	C ₄	—
9c	NCH ₂ CH ₂ [<i>ansa</i>]	NCH ₂ CH ₂ [<i>ansa</i>]	—	—	—
	NCH ₂ CH ₂ [<i>DASD</i>]	NCH ₂ CH ₂ [<i>DASD</i>]	NCH ₂ [<i>DASD</i>], OCO	—	—
	NCH ₂ [<i>ansa</i>]	NCH ₂ [<i>ansa</i>]	—	—	—
	NCH ₂ [<i>DASD</i>]	NCH ₂ [<i>DASD</i>]	—	OCO	—
	OCH ₂	OCH ₂	—	OCO	—
	ArCH ₂ N	ArCH ₂ N	—	—	—
	ArH H ₃	C ₃	—	—	NCH ₂ [<i>ansa</i>]
	H ₄	C ₄	—	—	—
	H ₅	C ₅	—	C ₁ , C ₃	—
	H ₆	C ₆	C ₁ , C ₅	C ₄	—