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Theoretical Investigation Non-covalent Interactions of *N*-(diphenylphosphinothioyl)-2-pyrazinecarboxamide

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Supplementary Information

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Table S1. Optimized and experimental geometries of compound **1**.

Parameters	**Experimental**	**Cam-B3LYP/6-311+G***
Bond Lengths (Å)		
P(1)-S(1)	1.923	1.946
P(1)-C(8)	1.809	1.829
P(1)-C(14)	1.799	1.819
P(1)-N(1)	1.703	1.718
Bond angles (°)		
S(1)-P(1)-C(8)	110.57	113.96
S(1)-P(1)-C(14)	115.29	115.11
S(1)-P(1)-N(1)	115.57	116.66
C(8)-P(1)-C(14)	107.30	106.54
N(1)-P(1)-C(8)	101.38	98.59
N(1)-P(1)-C(14)	105.55	104.16