



STRUCTURAL  
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**Supporting information for article:**

**The synergistic co-operation of N—H···O&dbnd;P hydrogen bonds and C—H···OX weak intermolecular interactions ( $X$  is &dbnd;P or —C) in the  $(\text{CH}_3\text{O})_2\text{P}(\text{O})(\text{NH}-\text{NHC}_6\text{F}_5)$  amidophospho-ester: a combined X-ray crystallographic and theoretical study**

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**Table S1:** The calculated N—H···O hydrogen bonds geometry

Clusters	N—H (Å)	H···O	N···O	N—H···O (°)
Cluster I	N1B—H1B: 1.037	H1B···O1B: 1.679	N1B···O1B: 2.714	175.040
	N2B—H2B: 1.025	H1B···O1A: 1.807	N2B···O1A: 2.784	157.967
Cluster II	N1B—H1B: 1.023	H1B···O1B: 1.765	N1B···O1B: 2.733	156.184
	N1B—H1B: 1.023	H1B···O1B: 1.765	N1B···O1B: 2.733	156.187
Cluster III	N2B—H2B: 1.021	H2B···O1A: 1.904	N2B···O1A: 2.836	159.841

**Table S2:** The calculated C—H···O intermolecular interactions geometries

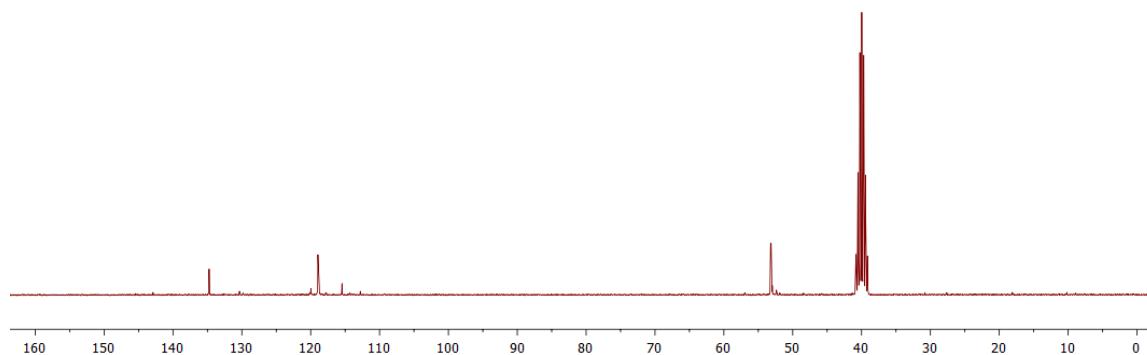
Clusters	C—H (Å)	H···O	C···O	C—H···O (°)
Cluster IV	C7A—H7AC	H7AC···O2A	C7A···O2A	C7A—H7AC···O2A
	1.085	2.717	3.752	159.277
	1.085	2.716	3.751	159.307
Cluster V	C8A—H8AB	H8AB···O1B	C8A···O1B	C8A—H8AB···O1B
	1.088	2.714	3.575	135.71

**Table S3:** NBO analysis results for N—H···O interactions in cluster I at the B3LYP/6-311g(d,p) calculational level

Donor	Occu. No.	E (a.u.)	Acceptor	Occu. No.	E (a.u.)	E <sup>(2)</sup> (kcal.mol <sup>-1</sup> )
LP(1) O1A	1.95625	-0.85844	σ*(N2B—H2B)	0.04340	0.41152	13.08
LP(1) O1B	1.95646	-0.86132	σ*(N1B—H1B)	0.04414	0.43244	14.49

**Table S4:** NBO analysis results for N—H···O interactions in clusters II and III at the B3LYP/6-311g(d,p) calculational level

Donor	Occu. No.	E (a.u.)	Acceptor	Occu. No.	E (a.u.)	E <sup>(2)</sup> (kcal.mol <sup>-1</sup> )
LP(1) O1B	1.96393	-0.85290	σ*(N1B—H1B)	0.03994	0.42905	8.34
LP(2) O1B	1.85980	-0.30377	σ*(N1B—H1B)	0.03994	0.42905	5.70
LP(1) O1A	1.96215	-0.87858	σ*(N2B—H2B)	0.05130	0.42689	9.39



**Figure S1:** The  $^{13}\text{C}\{\text{H}\}$ NMR spectrum of  $(\text{CH}_3\text{O})_2\text{P}(\text{O})(\text{NH-NHC}_6\text{F}_5)$ .