STRUCTURAL CHEMISTRY

Volume 76 (2020)

Supporting information for article:

Conformational flexibility in amidophosphoesters: a CSD analysis completed with two new crystal structures of $(C_6H_5O)_2P(O)X$ [X = NHC_7H_{13} and $N(CH_2C_6H_5)_2$]

Banafsheh Vahdani Alviria, Mehrdad Pourayoubi, Abdul Ajees Abdul Salam, Marek Nečas, Arie van der Lee, Akshara Chithran and Krishnan Damodaran

Supplementary Table S1. Cambridge Structural Database (CSD) study of bond lengths for the molecules containing "$P(O)(OPh)_2N$" skeleton completed with the title compounds (**I**) and (**II**). In the table, if the structures contain more than one molecule in the asymmetric unit, or more than one "$P(O)(OPh)_2$" segment in the compound they are marked as Mol1, Mol2, etc. The average bond length with standard deviation is shown in end of the table.

No.	CSD reference code	O9-P1	P1-O2	O2-C3	C3-C4	C4-C5	C5-C6	C6-C7	C7-C8	C8-C3	P1-O10	O10-C11	C11-C12	C12-C13	C13-C14	C14-C15	C15-C16	C16-C11	P1-N17
1	ABITAG-Mol1	1.454	1.579	1.407	1.366	1.390	1.389	1.381	1.38	1.383	1.567	1.407	1.367	1.388	1.376	1.377	1.381	1.374	1.646
2	ABITAG-Mol2	1.459	1.569	1.411	1.371	1.388	1.382	1.372	1.384	1.367	1.565	1.405	1.376	1.379	1.386	1.382	1.380	1.378	1.642
3	ABITIO-Mol1	1.445	1.572	1.407	1.369	1.389	1.383	1.385	1.389	1.376	1.576	1.401	1.373	1.387	1.386	1.387	1.383	1.378	1.643
4	ABITIO-Mol2	1.463	1.565	1.412	1.369	1.386	1.387	1.382	1.391	1.377	1.574	1.405	1.373	1.386	1.387	1.378	1.383	1.377	1.631
5	AFASIK	1.458	1.588	1.423	1.399	1.389	1.355	1.363	1.409	1.392	1.599	1.425	1.391	1.398	1.359	1.366	1.402	1.397	1.661
6	AKAQEK	1.474	1.616	1.401	1.380	1.393	1.385	1.385	1.393	1.382	1.635	1.389	1.387	1.389	1.384	1.383	1.388	1.383	1.550
7	BACVAD-Mol1	1.466	1.594	1.395	1.392	1.397	1.375	1.374	1.383	1.380	1.589	1.394	1.389	1.389	1.377	1.379	1.382	1.381	1.603
8	BACVAD-Mol2	1.460	1.589	1.394	1.381	1.382	1.379	1.377	1.389	1.389	1.594	1.395	1.380	1.383	1.374	1.375	1.397	1.392	1.603
9	BACVEH-Mol1	1.455	1.585	1.378	1.408	1.376	1.374	1.360	1.412	1.365	1.586	1.389	1.385	1.374	1.376	1.372	1.387	1.375	1.585
10	BACVEH-Mol2	1.459	1.583	1.380	1.399	1.390	1.361	1.378	1.377	1.381	1.586	1.395	1.383	1.407	1.364	1.344	1.365	1.366	1.602
11	BATGUA	1.459	1.565	1.418	1.371	1.371	1.380	1.373	1.381	1.366	1.562	1.419	1.359	1.386	1.365	1.365	1.380	1.367	1.652
12	BILBUV	1.463	1.576	1.419	1.368	1.386	1.369	1.367	1.392	1.365	1.578	1.402	1.365	1.375	1.363	1.361	1.379	1.376	1.628
13	BILCAC	1.456	1.585	1.405	1.368	1.388	1.360	1.355	1.398	1.371	1.593	1.403	1.381	1.386	1.355	1.387	1.381	1.380	1.616
14	BOGPOC	1.457	1.566	1.417	1.367	1.384	1.365	1.366	1.384	1.367	1.574	1.409	1.364	1.382	1.371	1.366	1.387	1.369	1.637
15	BUBNAP	1.470	1.577	1.401	1.386	1.392	1.393	1.391	1.398	1.388	1.591	1.408	1.387	1.393	1.391	1.393	1.396	1.386	1.632
16	CEGGIG	1.464	1.595	1.404	1.386	1.389	1.386	1.386	1.386	1.381	1.587	1.411	1.380	1.390	1.384	1.383	1.385	1.382	1.615
17	CILJAI-Mol1	1.441	1.585	1.415	1.375	1.398	1.365	1.367	1.413	1.371	1.582	1.407	1.369	1.384	1.371	1.384	1.390	1.385	1.652
18	CILJAI-Mol2	1.475	1.569	1.419	1.369	1.400	1.355	1.363	1.389	1.375	1.574	1.416	1.370	1.386	1.380	1.359	1.388	1.363	1.639
19	CILJAI01-Mol1	1.458	1.569	1.413	1.367	1.385	1.367	1.363	1.379	1.367	1.569	1.409	1.369	1.386	1.361	1.361	1.382	1.361	1.632
20	CILJAI01-Mol2	1.446	1.573	1.414	1.358	1.383	1.364	1.361	1.399	1.371	1.575	1.418	1.361	1.384	1.363	1.367	1.388	1.367	1.646

21	CIXSOR	1.453	1.58	1.413	1.349	1.369	1.363	1.361	1.392	1.364	1.585	1.407	1.379	1.379	1.366	1.351	1.382	1.350	1.630
22	DAMPEM	1.456	1.588	1.395	1.367	1.383	1.353	1.352	1.365	1.367	1.595	1.386	1.368	1.384	1.320	1.345	1.376	1.365	1.595
23	DAXGIS	1.470	1.586	1.395	1.413	1.387	1.419	1.344	1.387	1.339	1.600	1.428	1.397	1.390	1.396	1.365	1.389	1.363	1.599
24	ENAWAT	1.472	1.598	1.407	1.373	1.390	1.374	1.384	1.387	1.378	1.602	1.403	1.382	1.389	1.373	1.381	1.391	1.377	1.571
25	EROJAX	1.463	1.583	1.397	1.377	1.383	1.368	1.370	1.381	1.376	1.585	1.408	1.371	1.385	1.372	1.379	1.382	1.372	1.609
26	EXIQIM	1.464	1.582	1.401	1.372	1.382	1.375	1.383	1.392	1.379	1.587	1.416	1.372	1.399	1.370	1.380	1.384	1.369	1.613
27	FACZUG	1.463	1.590	1.401	1.384	1.395	1.382	1.384	1.392	1.388	1.583	1.415	1.386	1.396	1.382	1.377	1.391	1.386	1.621
28	FADBAP	1.462	1.591	1.404	1.382	1.392	1.383	1.394	1.388	1.406	1.588	1.418	1.390	1.376	1.397	1.384	1.403	1.393	1.603
29	FAYNAU-Mol1	1.460	1.603	1.404	1.362	1.403	1.370	1.371	1.383	1.371	1.606	1.397	1.381	1.390	1.374	1.373	1.389	1.373	1.577
30	FAYNAU-Mol2	1.460	1.606	1.397	1.373	1.389	1.373	1.374	1.390	1.381	1.603	1.404	1.371	1.383	1.371	1.370	1.403	1.362	1.577
31	FETWUY	1.449	1.581	1.404	1.371	1.387	1.377	1.339	1.390	1.409	1.579	1.432	1.363	1.460	1.297	1.383	1.411	1.397	1.634
32	FIBROY-Mol1	1.462	1.592	1.392	1.392	1.365	1.376	1.389	1.383	1.391	1.594	1.424	1.382	1.400	1.379	1.380	1.394	1.345	1.609
33	FIBROY-Mol2	1.469	1.582	1.406	1.384	1.387	1.369	1.408	1.378	1.382	1.604	1.394	1.380	1.394	1.377	1.380	1.386	1.377	1.615
34	GUFMID-Mol1	1.453	1.583	1.418	1.383	1.375	1.387	1.388	1.386	1.376	1.584	1.414	1.376	1.388	1.379	1.381	1.392	1.384	1.643
35	GUFMID-Mol2	1.451	1.583	1.420	1.37	1.393	1.377	1.375	1.387	1.379	1.583	1.419	1.374	1.387	1.38	1.379	1.380	1.383	1.634
36	HANTAR	1.460	1.574	1.413	1.378	1.387	1.376	1.38	1.384	1.381	1.565	1.406	1.365	1.383	1.366	1.372	1.382	1.377	1.658
37	HUGJID	1.457	1.584	1.407	1.362	1.381	1.371	1.354	1.378	1.366	1.588	1.407	1.356	1.379	1.353	1.358	1.377	1.37	1.596
38	HUVGIO-Mol1	1.458	1.59	1.388	1.384	1.389	1.377	1.364	1.384	1.38	1.593	1.395	1.388	1.395	1.371	1.373	1.369	1.387	1.595
39	HUVGIO-Mol2	1.458	1.592	1.388	1.384	1.389	1.377	1.364	1.384	1.380	1.593	1.395	1.388	1.395	1.371	1.373	1.369	1.387	1.595
40	HUVGIO-Mol3	1.461	1.586	1.400	1.389	1.393	1.374	1.376	1.386	1.383	1.594	1.398	1.387	1.381	1.367	1.368	1.391	1.392	1.598
41	HUVGIO-Mol4	1.462	1.584	1.400	1.388	1.393	1.374	1.376	1.386	1.383	1.594	1.398	1.388	1.380	1.368	1.368	1.391	1.393	1.598
42	IYALUP-Mol1	1.458	1.588	1.403	1.356	1.396	1.357	1.336	1.395	1.370	1.593	1.397	1.360	1.384	1.350	1.353	1.382	1.349	1.576
43	IYALUP-Mol2	1.469	1.587	1.399	1.368	1.392	1.365	1.376	1.382	1.371	1.597	1.404	1.363	1.391	1.339	1.350	1.382	1.340	1.583
44	IYAMAW-Mol1	1.485	1.575	1.406	1.382	1.388	1.377	1.371	1.370	1.397	1.597	1.405	1.381	1.395	1.377	1.384	1.376	1.397	1.568
45	IYAMAW-Mol2	1.458	1.592	1.401	1.404	1.399	1.368	1.364	1.380	1.356	1.584	1.425	1.376	1.387	1.363	1.369	1.389	1.372	1.611
46	IYAMEA-Mol1	1.465	1.597	1.380	1.399	1.379	1.361	1.383	1.406	1.347	1.596	1.400	1.364	1.397	1.356	1.310	1.416	1.366	1.598

47	IYAMEA-Mol2	1.468	1.617	1.396	1.354	1.41	1.389	1.361	1.421	1.408	1.601	1.382	1.380	1.454	1.371	1.266	1.398	1.306	1.566
48	IYAMEA-Mol3	1.469	1.611	1.401	1.389	1.438	1.470	1.263	1.390	1.313	1.613	1.397	1.346	1.393	1.378	1.348	1.354	1.373	1.568
49	IYAMEA-Mol4	1.455	1.604	1.397	1.386	1.381	1.375	1.340	1.378	1.373	1.591	1.386	1.353	1.380	1.384	1.384	1.382	1.390	1.598
50	JAFFIG	1.462	1.602	1.403	1.374	1.382	1.382	1.377	1.383	1.377	1.608	1.401	1.380	1.378	1.379	1.373	1.387	1.378	1.580
51	JIYLEJ	1.460	1.607	1.409	1.354	1.373	1.369	1.368	1.388	1.368	1.598	1.387	1.364	1.375	1.369	1.377	1.384	1.380	1.581
52	KABZIW	1.449	1.575	1.373	1.394	1.396	1.395	1.395	1.394	1.394	1.577	1.384	1.396	1.395	1.394	1.395	1.395	1.394	1.633
53	KARGAL	1.452	1.591	1.410	1.368	1.375	1.375	1.374	1.384	1.380	1.588	1.406	1.369	1.391	1.389	1.387	1.384	1.388	1.625
54	KAVVAE-Mol1	1.450	1.580	1.408	1.356	1.393	1.357	1.351	1.381	1.353	1.578	1.406	1.365	1.374	1.386	1.349	1.382	1.371	1.635
55	KAVVAE-Mol2	1.450	1.578	1.406	1.371	1.382	1.349	1.386	1.374	1.365	1.580	1.408	1.353	1.381	1.351	1.357	1.393	1.356	1.635
56	KEZTEO	1.463	1.595	1.381	1.414	1.387	1.330	1.389	1.381	1.348	1.607	1.371	1.373	1.388	1.388	1.378	1.397	1.394	1.592
57	KUXNUM	1.455	1.585	1.395	1.393	1.378	1.392	1.402	1.366	1.387	1.592	1.396	1.379	1.388	1.401	1.388	1.378	1.402	1.631
58	KUXNUM01	1.464	1.595	1.401	1.392	1.401	1.394	1.404	1.387	1.391	1.587	1.398	1.388	1.395	1.395	1.394	1.398	1.386	1.630
59	LELVON	1.453	1.587	1.399	1.387	1.376	1.370	1.366	1.406	1.382	1.590	1.412	1.396	1.402	1.372	1.384	1.383	1.37	1.617
60	LEQRIK-Mol1	1.469	1.585	1.400	1.392	1.383	1.388	1.376	1.392	1.374	1.591	1.413	1.382	1.386	1.378	1.385	1.389	1.379	1.609
61	LEQRIK-Mol2	1.469	1.592	1.412	1.378	1.388	1.386	1.378	1.386	1.382	1.586	1.399	1.374	1.392	1.376	1.389	1.383	1.392	1.609
62	LEQRIK01-Mol1	1.467	1.600	1.397	1.384	1.389	1.386	1.381	1.391	1.383	1.587	1.408	1.379	1.387	1.384	1.380	1.393	1.382	1.616
63	LEQRIK01-Mol2	1.468	1.588	1.408	1.382	1.392	1.381	1.385	1.388	1.380	1.600	1.397	1.382	1.392	1.380	1.386	1.389	1.385	1.615
64	LERXUB	1.460	1.588	1.404	1.385	1.380	1.397	1.386	1.387	1.390	1.596	1.419	1.394	1.396	1.390	1.377	1.390	1.377	1.640
65	MOPMIN	1.449	1.579	1.407	1.363	1.376	1.352	1.359	1.387	1.361	1.587	1.408	1.354	1.423	1.340	1.363	1.365	1.383	1.641
66	NACJOR	1.470	1.604	1.398	1.372	1.390	1.357	1.375	1.391	1.369	1.611	1.393	1.381	1.386	1.366	1.389	1.386	1.385	1.581
67	NEWVER	1.473	1.581	1.402	1.376	1.378	1.382	1.390	1.396	1.380	1.593	1.412	1.388	1.382	1.39	1.361	1.404	1.369	1.637
68	NIKLOK	1.462	1.580	1.411	1.382	1.388	1.389	1.384	1.382	1.379	1.568	1.412	1.371	1.387	1.379	1.383	1.391	1.378	1.653
69	NOKHOL	1.487	1.594	1.414	1.371	1.369	1.416	1.401	1.348	1.338	1.644	1.356	1.443	1.328	1.402	1.328	1.403	1.292	1.598
70	OAPHHG-Mol1	1.482	1.581	1.415	1.399	1.379	1.348	1.399	1.390	1.380	1.595	1.392	1.375	1.402	1.380	1.370	1.436	1.368	1.569
71	OAPHHG-Mol2	1.482	1.595	1.392	1.368	1.436	1.370	1.380	1.402	1.375	1.581	1.415	1.380	1.390	1.399	1.348	1.379	1.399	1.569
72	OFESAV-Mol1	1.468	1.596	1.417	1.379	1.395	1.362	1.369	1.400	1.369	1.585	1.417	1.368	1.405	1.359	1.350	1.377	1.370	1.635

73	OFESAV-Mol2	1.468	1.585	1.417	1.37	1.377	1.35	1.36	1.404	1.368	1.596	1.417	1.369	1.400	1.369	1.362	1.395	1.378	1.635
74	OFESEZ-Mol1	1.465	1.564	1.415	1.386	1.378	1.388	1.387	1.381	1.383	1.569	1.411	1.387	1.378	1.389	1.380	1.385	1.376	1.655
75	OFESEZ-Mol2	1.467	1.575	1.417	1.368	1.39	1.394	1.381	1.386	1.383	1.573	1.417	1.383	1.381	1.384	1.377	1.384	1.370	1.643
76	OVUXAF-Mol1	1.458	1.596	1.396	1.348	1.373	1.384	1.347	1.397	1.390	1.614	1.411	1.357	1.380	1.369	1.357	1.392	1.375	1.563
77	OVUXAF-Mol2	1.454	1.604	1.394	1.369	1.387	1.367	1.375	1.375	1.356	1.607	1.401	1.355	1.385	1.383	1.372	1.397	1.374	1.562
78	PABBID	1.458	1.581	1.397	1.388	1.404	1.364	1.366	1.422	1.374	1.587	1.416	1.386	1.398	1.373	1.385	1.394	1.390	1.624
79	PARZOA-Mol1	1.464	1.575	1.414	1.381	1.392	1.385	1.389	1.389	1.376	1.617	1.374	1.382	1.384	1.370	1.373	1.38	1.385	1.613
80	PARZOA-Mol2	1.464	1.583	1.421	1.382	1.383	1.392	1.391	1.391	1.377	1.613	1.380	1.380	1.378	1.373	1.374	1.372	1.382	1.614
81	PECYIH	1.460	1.590	1.405	1.379	1.376	1.381	1.371	1.384	1.367	1.585	1.401	1.374	1.394	1.365	1.367	1.384	1.377	1.604
82	POSBTU10	1.477	1.532	1.408	1.372	1.386	1.367	1.365	1.391	1.365	1.594	1.417	1.375	1.371	1.382	1.375	1.378	1.371	1.660
83	PUGJIL	1.457	1.583	1.401	1.388	1.389	1.383	1.385	1.384	1.381	1.606	1.404	1.372	1.388	1.370	1.365	1.386	1.372	1.616
84	QABZIF	1.465	1.604	1.386	1.384	1.382	1.379	1.386	1.386	1.396	1.59	1.419	1.376	1.393	1.387	1.382	1.396	1.376	1.610
85	QAJJIW	1.469	1.598	1.400	1.389	1.392	1.384	1.389	1.390	1.383	1.587	1.404	1.383	1.390	1.386	1.387	1.390	1.383	1.604
86	QIXMEP-Mol1	1.475	1.601	1.391	1.383	1.386	1.368	1.361	1.391	1.377	1.595	1.403	1.363	1.385	1.349	1.360	1.381	1.340	1.579
87	QIXMEP-Mol2	1.475	1.595	1.403	1.341	1.381	1.361	1.349	1.385	1.364	1.601	1.391	1.376	1.391	1.361	1.369	1.386	1.383	1.578
88	QOQWOI	1.454	1.599	1.393	1.376	1.377	1.368	1.370	1.374	1.371	1.584	1.403	1.378	1.370	1.370	1.371	1.374	1.371	1.604
89	SEYSEU-Mol1	1.446	1.608	1.394	1.393	1.392	1.303	1.419	1.394	1.335	1.580	1.400	1.362	1.372	1.405	1.384	1.405	1.393	1.617
90	SEYSEU-Mol2	1.453	1.601	1.383	1.371	1.426	1.358	1.387	1.391	1.375	1.587	1.404	1.366	1.397	1.390	1.400	1.395	1.374	1.624
91	SIZTUS	1.463	1.591	1.409	1.402	1.367	1.379	1.383	1.388	1.362	1.595	1.424	1.367	1.390	1.380	1.384	1.366	1.381	1.618
92	SOKDUT	1.464	1.583	1.422	1.378	1.394	1.377	1.380	1.401	1.375	1.574	1.389	1.390	1.390	1.390	1.390	1.390	1.390	1.640
93	SOYCUE-Mol1	1.463	1.581	1.385	1.395	1.394	1.396	1.396	1.396	1.394	1.575	1.369	1.394	1.394	1.395	1.395	1.396	1.394	1.646
94	SOYCUE-Mol2	1.460	1.581	1.392	1.396	1.395	1.395	1.394	1.395	1.394	1.579	1.385	1.395	1.395	1.394	1.395	1.395	1.394	1.645
95	TAJXIL	1.450	1.588	1.405	1.371	1.389	1.384	1.369	1.387	1.385	1.591	1.409	1.373	1.379	1.388	1.392	1.391	1.386	1.618
96	TAJXIL01	1.463	1.596	1.402	1.399	1.397	1.403	1.399	1.394	1.385	1.594	1.398	1.387	1.397	1.395	1.393	1.393	1.398	1.621
97	TOTVIH	1.448	1.581	1.378	1.395	1.396	1.396	1.396	1.394	1.396	1.579	1.388	1.395	1.395	1.395	1.395	1.394	1.395	1.578
98	TUDWUL	1.538	1.506	1.581	1.339	1.326	1.361	1.340	1.328	1.351	1.559	1.523	1.372	1.356	1.343	1.359	1.364	1.335	1.578
99	UCIXUB-Mol1	1.479	1.605	1.378	1.383	1.362	1.409	1.374	1.373	1.413	1.588	1.417	1.372	1.387	1.379	1.382	1.386	1.369	1.620
100	UCIXUB-Mol2	1.467	1.594	1.381	1.383	1.375	1.355	1.396	1.386	1.382	1.580	1.418	1.407	1.378	1.383	1.405	1.400	1.338	1.623
101	UCIXUB01-Mol1	1.473	1.605	1.392	1.383	1.376	1.371	1.369	1.39	1.386	1.584	1.437	1.382	1.394	1.388	1.375	1.386	1.363	1.613

102	UCIXUB01-Mol2	1.456	1.595	1.400	1.355	1.387	1.375	1.381	1.379	1.393	1.587	1.422	1.386	1.390	1.390	1.380	1.397	1.367	1.618
103	UCIYAI-Mol1	1.459	1.606	1.380	1.386	1.362	1.373	1.376	1.377	1.373	1.581	1.418	1.379	1.382	1.377	1.387	1.381	1.369	1.609
104	UCIYAI-Mol2	1.459	1.613	1.371	1.39	1.375	1.37	1.368	1.376	1.379	1.577	1.415	1.376	1.380	1.379	1.384	1.385	1.371	1.604
105	UCOFEX	1.469	1.573	1.409	1.366	1.396	1.374	1.373	1.392	1.379	1.573	1.420	1.378	1.390	1.376	1.378	1.394	1.380	1.633
106	UCOFIB	1.474	1.586	1.398	1.373	1.387	1.361	1.388	1.379	1.374	1.570	1.420	1.382	1.389	1.379	1.388	1.378	1.380	1.653
107	UCOFOH-Mol1	1.456	1.569	1.402	1.371	1.388	1.379	1.369	1.378	1.368	1.576	1.404	1.374	1.381	1.382	1.375	1.387	1.375	1.621
108	UCOFOH-Mol2	1.463	1.570	1.395	1.375	1.374	1.382	1.375	1.377	1.377	1.565	1.403	1.375	1.390	1.369	1.369	1.383	1.367	1.621
109	UCOGUO-Mol1	1.465	1.586	1.408	1.378	1.387	1.373	1.386	1.389	1.380	1.592	1.413	1.383	1.392	1.375	1.376	1.388	1.381	1.624
110	UCOGUO-Mol2	1.465	1.592	1.413	1.381	1.388	1.376	1.375	1.392	1.383	1.586	1.408	1.380	1.389	1.386	1.373	1.387	1.378	1.624
111	UCOHAV-Mol1	1.458	1.584	1.389	1.380	1.403	1.355	1.387	1.381	1.373	1.590	1.405	1.368	1.380	1.372	1.367	1.380	1.370	1.608
112	UCOHAV-Mol2	1.458	1.590	1.405	1.370	1.380	1.366	1.372	1.380	1.369	1.584	1.389	1.373	1.381	1.388	1.355	1.403	1.380	1.608
113	UCOHAV-Mol3	1.453	1.587	1.407	1.369	1.384	1.378	1.380	1.384	1.354	1.590	1.414	1.376	1.376	1.395	1.366	1.368	1.385	1.611
114	UCOHAV-Mol4	1.452	1.590	1.414	1.385	1.368	1.366	1.395	1.376	1.376	1.587	1.407	1.369	1.384	1.378	1.380	1.384	1.354	1.611
115	UCOHID	1.458	1.574	1.412	1.370	1.390	1.372	1.366	1.377	1.366	1.574	1.421	1.368	1.390	1.387	1.380	1.391	1.370	1.639
116	UFELIA	1.461	1.581	1.420	1.371	1.389	1.379	1.383	1.386	1.375	1.573	1.407	1.384	1.384	1.380	1.388	1.374	1.385	1.640
117	ULOSOD	1.465	1.590	1.412	1.368	1.389	1.373	1.367	1.390	1.377	1.590	1.412	1.377	1.390	1.367	1.373	1.389	1.368	1.607
118	UREDUR-Mol1	1.463	1.580	1.403	1.382	1.392	1.385	1.385	1.387	1.386	1.591	1.401	1.381	1.393	1.385	1.377	1.388	1.382	1.628
119	UREDUR-Mol2	1.464	1.585	1.404	1.378	1.385	1.378	1.383	1.391	1.377	1.582	1.403	1.386	1.381	1.380	1.383	1.388	1.383	1.629
120	UYESAU	1.465	1.581	1.406	1.375	1.390	1.384	1.382	1.394	1.373	1.596	1.395	1.369	1.369	1.380	1.397	1.392	1.381	1.595
121	UYOLOK	1.451	1.585	1.404	1.373	1.381	1.376	1.382	1.384	1.376	1.578	1.423	1.377	1.388	1.378	1.384	1.374	1.374	1.652

122	VAJVIM	1.466	1.599	1.393	1.354	1.376	1.372	1.358	1.396	1.379	1.606	1.392	1.393	1.387	1.372	1.366	1.413	1.361	1.589
123	VAJVOS	1.466	1.600	1.403	1.373	1.369	1.377	1.377	1.395	1.383	1.611	1.410	1.378	1.386	1.372	1.371	1.386	1.362	1.570
124	VEXPAP	1.453	1.583	1.408	1.367	1.393	1.402	1.383	1.374	1.390	1.636	1.382	1.398	1.364	1.412	1.421	1.428	1.353	1.636
125	VIDGOF	1.446	1.580	1.390	1.361	1.365	1.327	1.384	1.393	1.360	1.574	1.400	1.385	1.383	1.372	1.374	1.394	1.374	1.641
126	VIDYUC	1.463	1.581	1.398	1.381	1.366	1.380	1.363	1.392	1.378	1.576	1.409	1.360	1.386	1.375	1.377	1.380	1.378	1.636
127	VINYEW	1.445	1.573	1.408	1.374	1.372	1.326	1.374	1.443	1.354	1.565	1.403	1.365	1.380	1.358	1.357	1.384	1.363	1.646
128	WAFSUT-Mol1	1.464	1.594	1.407	1.389	1.392	1.392	1.388	1.394	1.384	1.590	1.403	1.386	1.392	1.389	1.385	1.395	1.384	1.628
129	WAFSUT-Mol2	1.464	1.590	1.403	1.384	1.394	1.385	1.389	1.392	1.386	1.595	1.407	1.384	1.394	1.388	1.391	1.392	1.389	1.627
130	WAFTUU	1.469	1.593	1.414	1.377	1.394	1.386	1.386	1.390	1.383	1.579	1.399	1.388	1.387	1.389	1.385	1.394	1.387	1.628
131	WEWVID	1.463	1.588	1.392	1.381	1.386	1.373	1.371	1.382	1.375	1.596	1.404	1.370	1.390	1.371	1.362	1.383	1.375	1.599
132	WEWVOJ	1.449	1.587	1.395	1.380	1.373	1.351	1.374	1.382	1.346	1.594	1.398	1.367	1.381	1.367	1.384	1.365	1.378	1.581
133	WEWVUP	1.452	1.594	1.375	1.384	1.367	1.366	1.361	1.369	1.380	1.589	1.396	1.361	1.371	1.390	1.358	1.407	1.363	1.574
134	WIBKUN-Mol1	1.460	1.586	1.391	1.368	1.390	1.386	1.350	1.413	1.382	1.584	1.398	1.361	1.400	1.373	1.340	1.387	1.364	1.616
135	WIBKUN-Mol2	1.469	1.582	1.408	1.376	1.378	1.346	1.406	1.405	1.379	1.594	1.402	1.373	1.399	1.349	1.358	1.374	1.349	1.622
136	WIHPEI	1.483	1.628	1.429	1.347	1.469	1.333	1.282	1.496	1.348	1.567	1.364	1.296	1.381	1.380	1.330	1.403	1.425	1.570
137	WIHPIM	1.466	1.554	1.434	1.352	1.436	1.296	1.346	1.425	1.420	1.613	1.379	1.413	1.373	1.386	1.440	1.369	1.362	1.633
138	WIVTEB	1.441	1.585	1.402	1.393	1.379	1.371	1.368	1.376	1.375	1.585	1.402	1.375	1.376	1.368	1.371	1.379	1.393	1.596
139	WOBJED	1.403	1.615	1.401	1.407	1.385	1.376	1.373	1.378	1.383	1.614	1.401	1.383	1.378	1.373	1.376	1.385	1.407	1.608
140	XABSEZ	1.450	1.574	1.411	1.370	1.386	1.362	1.373	1.391	1.371	1.586	1.411	1.377	1.388	1.376	1.381	1.381	1.379	1.645
141	XAYKAJ	1.456	1.596	1.403	1.399	1.392	1.362	1.377	1.382	1.387	1.591	1.412	1.387	1.378	1.380	1.385	1.389	1.392	1.586
142	XESCED	1.461	1.573	1.403	1.375	1.388	1.374	1.378	1.388	1.366	1.568	1.407	1.371	1.384	1.381	1.376	1.380	1.378	1.631
143	XOYQIN	1.457	1.604	1.403	1.362	1.384	1.377	1.363	1.383	1.385	1.568	1.407	1.362	1.408	1.352	1.348	1.375	1.375	1.577
144	XOYQIN01-Mol1	1.473	1.615	1.388	1.378	1.436	1.389	1.354	1.376	1.372	1.607	1.411	1.384	1.393	1.380	1.391	1.383	1.378	1.579
145	XOYQIN01-Mol2	1.465	1.601	1.401	1.383	1.390	1.378	1.367	1.397	1.376	1.612	1.400	1.377	1.382	1.376	1.398	1.387	1.367	1.589

146	XOYQIN02-Mol1	1.487	1.596	1.420	1.355	1.418	1.356	1.357	1.361	1.356	1.586	1.416	1.365	1.365	1.350	1.360	1.372	1.333	1.573
147	XOYQIN02-Mol2	1.450	1.600	1.390	1.373	1.417	1.362	1.338	1.378	1.368	1.595	1.424	1.353	1.388	1.337	1.383	1.380	1.356	1.578
148	XOZGAV	1.457	1.595	1.404	1.388	1.392	1.385	1.391	1.385	1.381	1.583	1.403	1.356	1.396	1.342	1.385	1.384	1.370	1.668
149	YEVRIA-Mol1	1.465	1.567	1.413	1.381	1.369	1.365	1.339	1.392	1.382	1.571	1.399	1.381	1.399	1.356	1.385	1.378	1.378	1.641
150	YEVRIA-Mol2	1.453	1.581	1.415	1.378	1.398	1.383	1.373	1.382	1.381	1.575	1.405	1.370	1.390	1.378	1.378	1.386	1.388	1.644
151	YEVROG	1.465	1.578	1.403	1.378	1.380	1.392	1.363	1.386	1.398	1.571	1.409	1.377	1.388	1.376	1.396	1.385	1.404	1.653
152	YEVRUM	1.457	1.568	1.426	1.343	1.384	1.386	1.389	1.399	1.374	1.570	1.409	1.366	1.391	1.374	1.382	1.405	1.372	1.642
153	YEVSAT	1.462	1.565	1.410	1.362	1.386	1.371	1.388	1.375	1.381	1.576	1.419	1.369	1.375	1.386	1.376	1.371	1.368	1.635
154	YIDGOI	1.464	1.623	1.405	1.366	1.376	1.398	1.377	1.381	1.385	1.604	1.411	1.396	1.385	1.357	1.342	1.397	1.339	1.570
155	ZIFYIW-Mol1	1.445	1.580	1.415	1.384	1.371	1.362	1.376	1.379	1.363	1.584	1.417	1.363	1.383	1.363	1.371	1.381	1.377	1.651
156	ZIFYIW-Mol2	1.457	1.570	1.411	1.363	1.387	1.382	1.378	1.391	1.378	1.566	1.407	1.361	1.416	1.346	1.371	1.37	1.369	1.669
157	BIFXIA-Mol1	1.454	1.588	1.399	1.365	1.377	1.359	1.360	1.387	1.370	1.583	1.391	1.313	1.386	1.321	1.294	1.384	1.332	1.597
158	BIFXIA-Mol2	1.456	1.586	1.397	1.329	1.388	1.296	1.322	1.376	1.317	1.588	1.397	1.367	1.388	1.359	1.364	1.384	1.365	1.601
159	GEZHAX	1.474	1.592	1.408	1.385	1.388	1.385	1.388	1.394	1.382	1.602	1.407	1.388	1.394	1.391	1.396	1.391	1.387	1.611
160	GEZHEB	1.470	1.600	1.401	1.387	1.394	1.394	1.387	1.394	1.387	1.590	1.399	1.391	1.393	1.392	1.391	1.397	1.387	1.615
161	BIFYUN	1.457	1.592	1.405	1.370	1.382	1.362	1.364	1.394	1.370	1.591	1.399	1.322	1.383	1.333	1.305	1.384	1.384	1.606
162	QABZIF01	1.465	1.605	1.386	1.384	1.382	1.379	1.386	1.385	1.396	1.590	1.420	1.376	1.392	1.387	1.381	1.397	1.376	1.610
	Average	**1.462**	**1.587**	**1.404**	**1.377**	**1.387**	**1.374**	**1.374**	**1.388**	**1.376**	**1.588**	**1.405**	**1.375**	**1.387**	**1.374**	**1.373**	**1.387**	**1.375**	**1.614**
	Standard deviation	**0.012**	**0.015**	**0.018**	**0.014**	**0.015**	**0.020**	**0.019**	**0.015**	**0.015**	**0.014**	**0.016**	**0.015**	**0.013**	**0.017**	**0.020**	**0.011**	**0.017**	**0.026**
	Bond length	**O9-P1**	**P1-O2**	**O2-C3**	**C3-C4**	**C4-C5**	**C5-C6**	**C6-C7**	**C7-C8**	**C8-C3**	**P1-O10**	**O10-C11**	**C11-C12**	**C12-C13**	**C13-C14**	**C14-C15**	**C15-C16**	**C16-C11**	**P1-N17**
	Title compound-I	**1.464(2)**	**1.601(3)**	**1.405(6)**	**1.394(6)**	**1.371(6)**	**1.385(7)**	**1.369(7)**	**1.394(6)**	**1.341(7)**	**1.581(4)**	**1.399(6)**	**1.409(6)**	**1.377(6)**	**1.377(7)**	**1.370(7)**	**1.409(6)**	**1.351(7)**	**1.607(2)**
	Bond length	**O1-P1**	**P1-O2**	**O2-C1**	**C1-C2**	**C2-C3**	**C3-C4**	**C4-C5**	**C5-C6**	**C6-C1**	**P1-O3**	**O3-C7**	**C7-C8**	**C8-C9**	**C9-C10**	**C10-C11**	**C11-C12**	**C12-C7**	**P1-N1**
	Title compound-II	**1.458(1)**	**1.592(1)**	**1.409(2)**	**1.378(2)**	**1.386(2)**	**1.382(2)**	**1.382(2)**	**1.391(2)**	**1.383(2)**	**1.595(1)**	**1.410(2)**	**1.376(2)**	**1.388(2)**	**1.382(2)**	**1.384(2)**	**1.384(2)**	**1.379(2)**	**1.623(1)**

Supplementary Table S2. Cambridge Structural Database (CSD) study of bond angles for the molecules containing "$P(O)(OPh)_2N$" skeleton completed with the title compounds (**I**) and (**II**). In the table, if the structures contain more than one molecule in the asymmetric unit, or more than one "$P(O)(OPh)_2$" segment in the compound, they are marked as Mol1, Mol2, etc. The average bond angle with standard deviation is shown in end of the table.

No.	CSD reference code	O1-P1-N1	O2-P1-O3	O1-P1-O2	O1-P1-O3	O3-P1-N1	O2-P1-N1
1	ABITAG-Mol1	112.36	94.51	117.75	117.20	107.90	105.20
2	ABITAG-Mol2	109.95	95.85	116.27	115.82	109.27	108.95
3	ABITIO-Mol1	113.98	99.47	117.69	117.14	104.67	101.59
4	ABITIO-Mol2	111.86	101.86	116.52	113.29	109.71	102.67
5	AFASIK	112.66	100.41	118.44	113.51	110.39	100.09
6	AKAQEK	121.50	98.33	111.83	109.02	109.69	103.93
7	BACVAD-Mol1	114.81	101.06	115.89	115.11	106.33	101.88
8	BACVAD-Mol2	114.81	101.06	115.11	115.89	101.88	106.33
9	BACVEH-Mol1	114.01	97.81	115.49	114.75	108.22	104.97
10	BACVEH-Mol2	113.50	97.59	113.79	116.91	103.24	110.32
11	BATGUA	107.85	97.07	116.02	116.44	109.40	109.60
12	BILBUV	110.43	95.42	116.26	115.58	109.63	108.53
13	BILCAC	114.51	98.80	116.49	115.15	106.94	103.11
14	BOGPOC	109.02	95.34	117.83	116.01	111.75	106.03
15	BUBNAP	111.52	99.63	117.94	114.20	107.29	105.00
16	CEGGIG	112.73	93.95	114.41	116.88	106.80	110.47
17	CILJAI-Mol1	113.14	95.11	117.22	117.93	104.28	107.01
18	CILJAI-Mol2	110.45	101.05	116.43	114.17	110.03	103.91
19	CILJAI01-Mol1	113.14	95.11	117.22	117.93	104.28	107.01

20	CILJAI01-Mol2	110.45	101.05	116.43	114.17	110.03	103.91
21	CIXSOR	112.27	94.76	116.39	116.80	107.36	107.62
22	DAMPEM	119.29	104.53	108.57	113.48	103.52	106.26
23	DAXGIS	119.88	100.19	114.39	113.82	102.65	103.42
24	ENAWAT	120.85	105.16	106.88	114.00	105.09	106.35
25	EROJAX	114.24	99.72	114.05	115.93	105.51	105.89
26	EXIQIM	114.72	99.48	113.71	116.72	104.77	105.76
27	FACZUG	113.95	98.73	114.61	114.19	107.93	106.06
28	FADBAP	115.21	95.54	113.09	117.44	103.33	110.22
29	FAYNAU-Mol1	120.41	103.11	107.40	113.08	105.17	106.16
30	FAYNAU-Mol2	120.41	103.11	113.08	107.40	106.16	105.17
31	FETWUY	113.66	99.45	115.76	117.22	103.14	105.77
32	FIBROY-Mol1	111.40	94.03	116.38	115.45	108.22	110.03
33	FIBROY-Mol2	110.52	93.64	115.96	116.10	109.09	110.41
34	GUFMID-Mol1	119.82	106.97	109.85	110.14	104.49	104.75
35	GUFMID-Mol2	120.12	106.61	109.98	109.61	104.79	104.87
36	HANTAR	107.82	96.51	115.94	116.38	110.66	109.09
37	HUGJID	113.69	98.78	114.84	114.65	105.76	107.74
38	HUVGIO-Mol1	113.74	97.65	114.05	115.09	103.41	111.39
39	HUVGIO-Mol2	113.74	97.65	114.05	115.09	103.41	111.39
40	HUVGIO-Mol3	114.10	98.16	115.68	114.12	108.67	104.58
41	HUVGIO-Mol4	114.10	98.16	115.68	114.12	108.67	104.58
42	IYALUP-Mol1	119.66	103.91	106.48	113.68	102.81	109.24
43	IYALUP-Mol2	119.35	103.05	107.52	113.67	103.84	108.14

44	IYAMAW-Mol1	119.83	104.13	110.08	106.03	111.14	104.60
45	IYAMAW-Mol2	115.30	100.93	114.25	115.00	104.27	105.51
46	IYAMEA-Mol1	117.36	99.53	114.81	112.78	108.01	102.44
47	IYAMEA-Mol2	121.71	102.76	113.44	106.52	109.15	101.71
48	IYAMEA-Mol3	122.19	102.86	106.22	113.72	100.65	109.61
49	IYAMEA-Mol4	117.40	98.62	113.15	115.09	102.57	107.93
50	JAFFIG	122.21	103.86	107.65	112.04	104.16	105.33
51	JIYLEJ	116.51	100.31	113.74	111.99	108.83	103.98
52	KABZIW	113.81	99.91	116.38	116.75	103.60	104.49
53	KARGAL	115.68	98.06	115.82	112.15	107.57	105.86
54	KAVVAE-Mol1	112.80	95.01	116.63	116.16	106.50	108.00
55	KAVVAE-Mol2	112.83	95.01	116.16	116.63	107.97	106.48
56	KEZTEO	114.94	97.96	116.58	114.07	108.70	102.77
57	KUXNUM	115.24	95.89	117.76	111.78	108.95	105.31
58	KUXNUM01	116.19	98.22	111.15	117.27	104.58	107.60
59	LELVON	115.88	103.14	114.99	113.89	105.19	102.20
60	LEQRIK-Mol1	114.88	100.28	113.42	115.46	104.83	106.50
61	LEQRIK-Mol2	114.90	100.27	115.46	113.42	106.46	104.86
62	LEQRIK01-Mol1	113.21	93.87	113.78	117.80	106.02	110.42
63	LEQRIK01-Mol2	113.16	93.89	117.80	113.80	110.47	106.00
64	LERXUB	114.83	94.64	116.37	115.83	107.05	105.87
65	MOPMIN	113.00	99.64	116.87	115.58	106.47	103.69
66	NACJOR	120.16	98.05	112.49	112.61	105.23	105.77
67	NEWVER	114.95	94.73	115.43	113.64	107.84	108.26

68	NIKLOK	111.56	101.78	115.06	116.88	102.68	107.63
69	NOKHOL	116.86	99.50	112.68	115.61	107.15	102.97
70	OAPHHG-Mol1	113.24	100.33	117.59	111.16	111.77	101.82
71	OAPHHG-Mol2	113.24	100.33	111.16	117.59	101.82	111.77
72	OFESAV-Mol1	114.22	96.11	115.73	115.24	107.03	106.68
73	OFESAV-Mol2	114.22	96.11	115.28	115.71	106.61	107.08
74	OFESEZ-Mol1	111.41	96.11	118.01	115.66	108.77	105.47
75	OFESEZ-Mol2	110.72	96.72	115.68	118.40	105.94	108.08
76	OVUXAF-Mol1	122.62	105.47	106.38	110.56	104.10	106.51
77	OVUXAF-Mol2	120.09	98.87	112.57	110.50	107.06	105.52
78	PABBID	112.93	99.12	114.36	116.71	103.53	108.83
79	PARZOA-Mol1	116.44	99.37	117.82	111.29	106.14	103.88
80	PARZOA-Mol2	115.14	98.47	117.60	111.44	108.12	104.47
81	PECYIH	114.25	98.16	115.81	114.24	106.56	106.23
82	POSBTU10	112.77	97.37	118.25	113.76	105.61	107.43
83	PUGJIL	116.93	101.10	115.11	110.99	106.72	104.49
84	QABZIF	115.73	98.93	114.13	115.37	105.58	105.27
85	QAJJIW	113.05	98.03	113.95	116.40	103.98	110.08
86	QIXMEP-Mol1	120.04	99.95	112.72	106.48	109.51	106.30
87	QIXMEP-Mol2	120.06	99.96	106.48	112.72	106.31	109.46
88	QOQWOI	115.75	98.52	113.66	115.81	104.51	106.75
89	SEYSEU-Mol1	118.22	103.51	114.26	110.86	104.58	103.96
90	SEYSEU-Mol2	117.95	104.01	112.96	112.19	103.94	104.43
91	SIZTUS	112.05	95.38	115.22	116.86	105.30	110.59

92	SOKDUT	117.40	102.74	114.57	110.06	110.05	100.78
93	SOYCUE-Mol1	109.48	94.66	116.37	116.24	111.55	107.64
94	SOYCUE-Mol2	109.97	94.71	116.38	115.70	111.15	108.00
95	TAJXIL	115.82	97.43	115.78	112.49	106.94	106.52
96	TAJXIL01	116.00	97.49	112.50	115.78	106.10	107.10
97	TOTVIH	119.42	99.20	106.49	114.32	106.24	109.23
98	TUDWUL	114.28	102.59	107.24	109.92	106.40	115.70
99	UCIXUB-Mol1	112.51	93.69	114.26	117.70	106.71	110.37
100	UCIXUB-Mol2	113.37	94.25	115.16	115.37	108.07	108.91
101	UCIXUB01-Mol1	113.09	93.36	114.43	117.82	106.81	109.49
102	UCIXUB01-Mol2	113.60	94.06	115.29	115.72	107.31	109.03
103	UCIYAI-Mol1	115.34	98.46	111.40	117.57	104.47	107.95
104	UCIYAI-Mol2	116.53	99.44	111.36	117.75	103.93	105.91
105	UCOFEX	110.46	97.15	114.27	115.21	107.78	111.22
106	UCOFIB	110.64	97.58	113.85	115.50	107.95	110.58
107	UCOFOH-Mol1	113.48	100.06	115.79	114.49	107.82	103.83
108	UCOFOH-Mol2	110.48	100.37	114.25	115.39	105.77	109.86
109	UCOGUO-Mol1	115.79	100.04	116.51	113.79	106.28	102.59
110	UCOGUO-Mol2	115.79	100.04	113.79	116.51	102.59	106.28
111	UCOHAV-Mol1	115.96	98.89	115.64	114.36	107.03	103.02
112	UCOHAV-Mol2	115.96	98.89	114.36	115.64	103.02	107.03
113	UCOHAV-Mol3	115.71	99.32	115.66	114.03	107.31	103.00
114	UCOHAV-Mol4	115.71	99.32	114.02	115.67	103.00	107.31
115	UCOHID	113.89	100.67	115.71	115.72	104.79	104.43

116	UFELIA	110.47	95.87	115.39	117.03	107.49	109.54
117	ULOSOD	112.40	94.17	115.07	115.07	109.35	106.35
118	UREDUR-Mol1	111.24	93.93	116.88	114.55	110.91	108.11
119	UREDUR-Mol2	111.95	93.98	114.43	116.62	107.74	110.75
120	UYESAU	115.10	97.75	114.57	115.13	106.67	105.84
121	UYOLOK	113.02	100.14	116.02	115.87	103.75	106.50
122	VAJVIM	119.72	97.71	113.00	113.20	102.81	107.76
123	VAJVOS	122.91	104.42	107.59	111.52	103.92	104.91
124	VEXPAP	115.30	92.59	114.16	117.11	106.08	109.12
125	VIDGOF	116.58	100.59	114.00	113.84	103.39	106.72
126	VIDYUC	114.16	100.36	115.36	116.83	103.25	105.08
127	VINYEW	109.89	101.51	115.73	117.31	102.84	108.43
128	WAFSUT-Mol1	114.67	99.05	115.31	115.93	103.87	106.21
129	WAFSUT-Mol2	114.67	99.04	115.93	115.29	106.20	103.91
130	WAFTUU	111.31	94.62	114.33	117.14	107.91	110.33
131	WEWVID	119.38	100.91	112.25	108.22	108.39	106.07
132	WEWVOJ	118.71	99.39	109.89	114.95	104.54	107.43
133	WEWVUP	118.91	99.33	114.48	112.75	105.81	103.32
134	WIBKUN-Mol1	111.28	94.56	115.52	116.02	108.19	110.04
135	WIBKUN-Mol2	111.60	95.61	116.14	114.53	108.78	109.01
136	WIHPEI	116.85	105.50	119.08	110.31	103.63	99.75
137	WIHPIM	112.32	103.96	115.46	114.00	108.49	101.55
138	WIVTEB	116.00	106.62	114.10	114.10	102.28	102.28
139	WOBJED	115.30	104.84	116.48	116.50	100.68	100.67

140	XABSEZ	112.98	99.46	117.21	116.22	105.80	103.41
141	XAYKAJ	117.94	101.84	111.60	114.68	98.62	105.94
142	XESCED	111.56	100.40	113.94	116.47	103.31	110.19
143	XOYQIN	121.64	104.16	111.68	108.08	104.76	105.04
144	XOYQIN01-Mol1	116.64	99.36	112.08	113.94	104.58	108.62
145	XOYQIN01-Mol2	119.60	103.87	107.92	112.76	105.55	105.85
146	XOYQIN02-Mol1	115.93	99.09	111.96	113.64	105.38	109.38
147	XOYQIN02-Mol2	119.83	104.37	107.74	112.68	105.33	105.66
148	XOZGAV	120.24	103.73	108.74	116.20	103.91	101.98
149	YEVRIA-Mol1	110.38	98.43	114.99	116.31	107.95	107.90
150	YEVRIA-Mol2	114.03	100.14	117.05	116.09	101.97	105.54
151	YEVROG	111.49	101.36	113.68	117.20	102.66	109.44
152	YEVRUM	110.33	95.80	115.56	116.03	108.89	109.29
153	YEVSAT	109.99	96.60	116.06	115.66	109.17	108.52
154	YIDGOI	122.33	97.93	111.13	113.23	103.26	105.94
155	ZIFYIW-Mol1	112.72	94.80	117.66	116.77	106.30	106.65
156	ZIFYIW-Mol2	110.44	100.87	116.31	115.99	109.09	102.99
157	BIFXIA-Mol1	112.99	93.33	116.46	114.36	109.44	108.56
158	BIFXIA-Mol2	113.12	96.31	114.18	116.59	108.41	109.48
159	GEZHAX	118.46	100.04	108.58	113.28	104.23	110.69
160	GEZHEB	118.16	99.05	114.17	109.30	109.42	104.99
161	BIFYUN	113.15	93.18	116.63	114.21	109.36	108.52
162	QABZIF01	115.74	98.90	114.15	115.36	105.55	105.28
	Average	**114.93**	**98.94**	**114.19**	**114.50**	**106.23**	**106.49**

	Standard deviation	**3.38**	**3.26**	**2.90**	**2.48**	**2.56**	**2.76**
	Bond angle	**O9-P1-N17**	**O2-P1-O10**	**O9-P1-O2**	**O9-P1-O10**	**O10-P1-N17**	**O2-P1-N17**
	Title compound-I	**113.34(11)**	**93.42(10)**	**114.8(3)**	**115.5(3)**	**109.2(2)**	**108.8(2)**
	Bond angle	**O1-P1-N1**	**O2-P1-O3**	**O1-P1-O2**	**O1-P1-O3**	**O3-P1-N1**	**O2-P1-N1**
	Title compound-II	**113.54(6)**	**97.78(5)**	**115.77(5)**	**116.27(5)**	**107.44(5)**	**104.31(5)**

Supplementary Table S3. Cambridge Structural Database (CSD) study of torsion angles for the molecules containing "$P(O)(OPh)_2N$" skeleton completed with the title compounds (**I**) and (**II**). In the table, if the structures contain more than one molecule in the asymmetric unit, or more than one "$P(O)(OPh)_2$" segment in the compound, they are marked as Mol1, Mol2, etc.

No.	CSD reference code	C3-O2-P1-O10	Conformation	C11-O10-P1-O2	Conformation
1	IYAMEA-Mol2	63.89	sc	62.65	sc
2	SEYSEU-Mol1	68.56	sc	70.47	sc
3	IYAMAW-Mol1	58.06	sc	73.42	sc
4	SEYSEU-Mol2	63.12	sc	81.84	sc
5	WIVTEB	84.00	sc	–84.00	–sc
6	WOBJED	87.02	sc	–87.02	–sc
7	JIYLEJ	57.33	sc	–126.24	–ac
8	AKAQEK	66.73	sc	–138.48	–ac
9	KEZTEO	49.15	sc	–148.82	–ac
10	WEWVUP	88.63	sc	166.86	ap
11	WIHPIM	61.81	sc	169.79	ap
12	UCOHID	68.91	sc	170.68	ap
13	UCOFOH-Mol1	57.14	sc	172.96	ap
14	NOKHOL	52.63	sc	173.80	ap
15	XABSEZ	69.51	sc	174.84	ap
16	OVUXAF-Mol2	81.29	sc	175.32	ap
17	MOPMIN	68.26	sc	176.90	ap
18	UCOHAV-Mol3	61.35	sc	177.56	ap
19	BACVEH-Mol1	53.25	sc	179.16	ap
20	NACJOR	85.39	sc	173.59	ap

21	AFASIK	59.10	sc	–152.86	–ap
22	ABITIO-Mol1	60.99	sc	–156.31	–ap
23	OAPHHG-Mol1	52.99	sc	–161.95	–ap
24	QABZIF	62.78	sc	–162.75	–ap
25	QABZIF01	62.79	sc	–162.75	–ap
26	ABITIO-Mol2	55.98	sc	–165.28	–ap
27	HUVGIO-Mol3	65.49	sc	–166.16	–ap
28	BUBNAP	46.30	sc	–167.02	–ap
29	IYAMEA-Mol1	71.75	sc	–168.35	–ap
30	CILJAI01-Mol1	56.11	sc	–168.64	–ap
31	CILJAI-Mol2	56.22	sc	–168.77	–ap
32	ZIFYIW-Mol2	41.92	sc	–169.56	–ap
33	LEQRIK-Mol1	84.23	sc	–171.65	–ap
34	UYESAU	48.77	sc	–172.06	–ap
35	EROJAX	77.45	sc	–172.56	–ap
36	UCOGUO-Mol1	72.44	sc	–174.26	–ap
37	BILCAC	62.11	sc	–175.19	–ap
38	VIDYUC	83.47	sc	–175.36	–ap
39	WAFSUT-Mol2	62.05	sc	–176.05	–ap
40	KABZIW	80.45	sc	–176.74	–ap
41	UCOHAV-Mol1	56.29	sc	–179.96	–ap
42	GUFMID-Mol2	–81.30	–sc	76.55	sc
43	GUFMID-Mol1	–75.22	–sc	79.98	sc
44	IYAMEA-Mol3	–62.49	–sc	–58.15	–sc

45	IYALUP-Mol1	–58.36	–sc	–60.80	–sc
46	IYALUP-Mol2	–42.42	–sc	–64.54	–sc
47	ENAWAT	–72.84	–sc	–76.64	–sc
48	DAMPEM	–51.84	–sc	–77.93	–sc
49	OVUXAF-Mol1	–75.85	–sc	–85.03	–sc
50	VAJVOS	–73.16	–sc	–87.70	–sc
51	BACVAD-Mol2	–50.72	–sc	110.57	ac
52	JAFFIG	–62.52	–sc	–91.02	–ac
53	XOYQIN02-Mol2	–65.22	–sc	–91.42	–ac
54	XOYQIN01-Mol2	–63.79	–sc	–93.17	–ac
55	FAYNAU-Mol1	–52.50	–sc	–94.64	–ac
56	XOZGAV	–65.55	–sc	–103.62	–ac
57	TOTVIH	–79.23	–sc	160.86	ap
58	QIXMEP-Mol2	–74.69	–sc	165.10	ap
59	TAJXIL01	–85.52	–sc	166.51	ap
60	WEWVOJ	–72.90	–sc	170.55	ap
61	KUXNUM01	–74.85	–sc	170.94	ap
62	GEZHAX	–70.76	–sc	174.63	ap
63	TUDWUL	–52.03	–sc	–162.14	–ap
64	FAYNAU-Mol2	94.64	ac	52.50	sc
65	SOKDUT	148.86	ac	66.37	sc
66	XAYKAJ	148.44	ac	–50.90	–sc
67	IYAMAW-Mol2	132.50	ac	–63.47	–sc
68	XOYQIN02-Mol1	142.55	ac	–66.05	–sc

69	XOYQIN01-Mol1	138.79	ac	–66.57	–sc
70	DAXGIS	141.30	ac	–70.77	–sc
71	XOYQIN	99.54	ac	90.77	ac
72	VIDGOF	129.01	ac	96.15	ac
73	LELVON	95.92	ac	–92.10	–ac
74	YEVRIA-Mol1	120.64	ac	165.39	ap
75	UCIYAI-Mol2	104.72	ac	–167.03	–ap
76	UCIYAI-Mol1	108.13	ac	–170.35	–ap
77	EXIQIM	96.76	ac	–177.55	–ap
78	WEWVID	–128.53	–ac	48.89	sc
79	BACVAD-Mol1	–110.57	–ac	50.72	sc
80	PUGJIL	–120.83	–ac	–86.47	–sc
81	FACZUG	–110.29	–ac	–129.34	–ac
82	XESCED	169.76	ap	–40.30	–sc
83	OAPHHG-Mol2	161.95	ap	–52.99	–sc
84	PECYIH	170.45	ap	–55.33	–sc
85	UCOHAV-Mol2	179.96	ap	–56.29	–sc
86	FETWUY	157.40	ap	–61.03	–sc
87	WAFSUT-Mol1	176.05	ap	–62.05	–sc
88	HUVGIO-Mol1	161.90	ap	–63.51	–sc
89	HUGJID	179.11	ap	–63.99	–sc
90	YEVROG	170.96	ap	–70.00	–sc
91	VAJVIM	177.85	ap	–70.77	–sc
92	IYAMEA-Mol4	163.41	ap	–71.96	–sc

93	UCOGUO-Mol2	174.26	ap	–72.44	–sc
94	QOQWOI	168.98	ap	–73.86	–sc
95	LEQRIK-Mol2	171.65	ap	–84.23	–sc
96	VEXPAP	169.29	ap	104.52	ac
97	HUVGIO-Mol2	161.90	ap	117.08	ac
98	PARZOA-Mol1	166.81	ap	–104.15	–ac
99	PARZOA-Mol2	170.71	ap	–108.00	–ac
100	OFESAV-Mol2	178.12	ap	165.74	ap
101	BATGUA	176.77	ap	167.79	ap
102	KAVVAE-Mol2	176.07	ap	167.94	ap
103	WIBKUN-Mol2	177.39	ap	168.98	ap
104	UFELIA	165.66	ap	169.49	ap
105	NEWVER	159.41	ap	170.29	ap
106	FIBROY-Mol2	172.08	ap	170.97	ap
107	BIFXIA-Mol2	171.41	ap	171.65	ap
108	UREDUR-Mol2	170.49	ap	174.08	ap
109	LEQRIK01-Mol1	166.04	ap	174.81	ap
110	UCOFEX	154.43	ap	176.53	ap
111	SIZTUS	176.62	ap	177.06	ap
112	UCOFIB	153.77	ap	177.44	ap
113	CEGGIG	172.62	ap	178.48	ap
114	OFESEZ-Mol1	174.87	ap	–167.22	–ap
115	ABITAG-Mol1	172.76	ap	–168.40	–ap
116	WAFTUU	173.17	ap	–171.30	–ap

117	ABITAG-Mol2	177.49	ap	–172.42	–ap
118	UCIXUB01-Mol2	169.78	ap	–172.93	–ap
119	UCIXUB-Mol2	167.57	ap	–174.47	–ap
120	POSBTU10	169.70	ap	–175.45	–ap
121	UCIXUB-Mol1	169.96	ap	–178.20	–ap
122	ULOSOD	178.97	ap	–178.97	–ap
123	UCIXUB01-Mol1	167.89	ap	–179.03	–ap
124	BILBUV	175.62	ap	–179.07	–ap
125	GEZHEB	–170.60	–ap	44.03	sc
126	HUVGIO-Mol4	–166.16	–ap	65.49	sc
127	QIXMEP-Mol1	–165.10	–ap	74.69	sc
128	KUXNUM	–167.73	–ap	83.39	sc
129	TAJXIL	–167.58	–ap	85.95	sc
130	UCOFOH-Mol2	–178.53	–ap	–44.34	–sc
131	VINYEW	–175.75	–ap	–48.66	–sc
132	BACVEH-Mol2	–177.57	–ap	–48.92	–sc
133	QAJJIW	–176.56	–ap	–54.17	–sc
134	PABBID	–177.27	–ap	–58.91	–sc
135	UCOHAV-Mol4	–177.56	–ap	–61.35	–sc
136	NIKLOK	–177.84	–ap	–61.68	–sc
137	YIDGOI	–163.82	–ap	–63.85	–sc
138	YEVRIA-Mol2	–164.26	–ap	–63.47	–sc
139	WIHPEI	–172.91	–ap	–83.55	–sc
140	UYOLOK	–163.71	–ap	–88.01	–sc

141	KARGAL	–174.46	–ap	95.87	ac
142	HANTAR	–179.78	–ap	158.36	ap
143	LERXUB	–167.70	–ap	166.29	ap
144	YEVRUM	–179.22	–ap	170.18	ap
145	FADBAP	–156.46	–ap	171.76	ap
146	CIXSOR	–169.38	–ap	173.81	ap
147	CILJAI01-Mol2	–164.35	–ap	178.62	ap
148	CILJAI-Mol1	–164.67	–ap	178.99	ap
149	ZIFYIW-Mol1	–173.41	–ap	–165.93	–ap
150	LEQRIK01-Mol2	–174.81	–ap	–166.04	–ap
151	YEVSAT	–164.61	–ap	–167.24	–ap
152	FIBROY-Mol1	–169.69	–ap	–168.62	–ap
153	OFESEZ-Mol2	–174.40	–ap	–169.37	–ap
154	BIFYUN	–171.90	–ap	–171.46	–ap
155	BIFXIA-Mol1	–171.95	–ap	–171.61	–ap
156	BOGPOC	–177.80	–ap	–173.99	–ap
157	UREDUR-Mol1	–173.14	–ap	–174.20	–ap
158	KAVVAE-Mol1	–167.94	–ap	–176.07	–ap
159	SOYCUE-Mol2	–174.91	–ap	–176.08	–ap
160	SOYCUE-Mol1	–169.43	–ap	–177.34	–ap
161	OFESAV-Mol1	–165.74	–ap	–178.12	–ap
162	WIBKUN-Mol1	–169.03	–ap	–179.34	–ap
	Torsion angle	C3-O2-P1-O10	Conformation	C11-O10-P1-O2	Conformation
	Title compound-I	–178.15°	–ap	–179.71	–ap

	Torsion angle	C1-O2-P1-O3	Conformation	C7-O3-P1-O2	Conformation
	Title compound-II	63.71	sc	178.86	ap

Supplementary Table S4. Distance to ring (Å). The distance between the rings of the title compounds (**I**) and (**II**) are given.

Title Compound (**I**)	Phenyl Ring 1 (C3-C8)	Phenyl Ring 2 (C11-C16)	Seven-Membered Ring (C18-C24)	
Phenyl Ring 1(C3-C8)	-	7.66	5.94	
Phenyl Ring 2(C11-C16)	7.66	-	5.71	
Seven-Membered Ring (C18-C24)	5.94	5.71	-	
Title Compound (**II**)	Phenyl Ring 1 (C1-C6)	Phenyl Ring 2 (C7-C12)	Phenyl Ring 3(C14-C19)	Phenyl Ring 4 (C21-C26)
Phenyl Ring 1(C1-C6)	-	6.52	8.80	7.25
Phenyl Ring 2(C7-C12)	6.52	-	4.84	7.51
Phenyl Ring 3(C14-C19)	8.80	4.84	-	5.72
Phenyl Ring 4(C21-C26)	7.25	7.51	5.72	-

Supplementary Table S5. Molecular pairs and interaction energies (kJ/mole) obtained from energy framework calculations for the title compound (**I**). N is the number of pairs, and R is the distance between molecular centroids (Å). E_{ele}, E_{pol}, E_{disp}, and E_{rep} represent the energy components of electrostatic, polarization, dispersion, and exchange-repulsion respectively, and E_{tot} is calculated as $E_{tot} = k_{ele}E_{ele} + k_{pol}E_{pol} + k_{disp}E_{disp} + k_{rep}E_{rep}$. Total energies are reported only for two benchmarked energy models, are the sum of the four energy components, scaled appropriately. The energy model CE-B3LYP … B3LYP /6-31G(d,p) is used to compare electron densities with the scale factors 1.057 (k_{ele}), 0.740 (k_{pol}), 0.871 (k_{disp}), and 0.618 (k_{rep}).

N	Symmetry Operator	R	E_{ele}	E_{pol}	E_{disp}	E_{rep}	E_{tot}
1	*x*+1/2, –*y*+1/2, *z*	4.68	–51.1	–19.3	–76.0	72.1	–89.9
1	*x*, *y*, *z*	9.79	–2.3	–1.3	–18.4	7.8	–14.6
1	–*x*, –*y*, *z*+1/2	11.16	–1.4	–0.9	–21.5	10.4	–14.4
1	–*x*+1/2, *y*+1/2, *z*+1/2	11.12	–1.8	–0.5	–18.3	8.7	–12.8
1	–*x*+1/2, *y*+1/2, *z*+1/2	11.12	–1.7	–0.4	–15.9	7.3	–11.5
1	–*x*, –*y*, *z*+1/2	10.97	–1.0	–0.4	–16.0	8.3	–10.2
1	*x*+1/2, –*y*+1/2, *z*	10.65	–1.0	–0.3	–14.7	7.6	–9.4

Supplementary Table S6. Molecular pairs and interaction energies (kJ/mole) obtained from energy framework calculations for the title compound (**II**). N is the number of pairs, and R is the distance between molecular centroids (Å). E_{ele}, E_{pol}, E_{disp}, and E_{rep} represent the energy components of electrostatic, polarization, dispersion, and exchange-repulsion respectively, and E_{tot} is calculated as $E_{tot} = k_{ele}E_{ele} + k_{pol}E_{pol} + k_{disp}E_{disp} + k_{rep}E_{rep}$. Total energies are reported only for two benchmarked energy models, are the sum of the four energy components, scaled appropriately. The energy model CE-B3LYP … B3LYP /6-31G(d,p) is used to compare electron densities with the scale factors 1.057 (k_{ele}), 0.740 (k_{pol}), 0.871 (k_{disp}), and 0.618 (k_{rep}).

N	Symmetry Operator	R	E_{ele}	E_{pol}	E_{disp}	E_{rep}	E_{tot}
1	*–x, –y, –z*	7.28	–11.4	–2.1	–63.7	35.2	–47.3
1	*–x, –y, –z*	8.46	–15.3	–5.5	–57.6	38.6	–46.5
1	*x, y, z*	9.53	–8.4	–1.3	–41.2	27.6	–28.6
1	*–x, –y, –z*	9.67	–4.2	–0.8	–28.5	14.1	–21.1
1	*–x, –y, –z*	11.26	–5.6	–0.7	–28.6	19.1	–19.5
1	*x, y, z*	8.34	–1.0	–1.4	–11.3	2.5	–10.4