Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Directionality of P···O pnicogen bonding in light of geometry corrected statistical analysis

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Table S1. Data for $X_3P\cdots O$ pnicogen bonding (X is any atom).

Angle range	Sin θ	No of Hits Before Cone Correction (n)	% Of hits Before Cone Correction	No of Hits After Cone Correction = n/Sin θ	% Of hits After Cone Correction
90-100	0.9962	28	10.33	28	2.27
100-110	0.9659	13	4.80	13	1.05
110-120	0.9063	16	5.90	18	1.46
120-130	0.8192	19	7.01	23	1.86
130-140	0.7071	07	2.58	10	0.81
140-150	0.5736	17	6.27	30	2.43
150-160	0.4226	29	10.70	69	5.59
160-170	0.2588	77	28.41	298	24.15
170-180	0.0872	65	23.99	745	60.37

Table S2. Data for $X_3P\cdots O$ pnicogen bonding for which X = oxygen in ∠OPX = 90 – 180°.

Angle range	Sin θ	No of Hits Before Cone Correction (n)	% Of hits Before Cone Correction	No of Hits After Cone Correction = n/Sin θ	% Of hits After Cone Correction
90-100	0.9962	05	10.42	5	1.96
100-110	0.9659	00	0.00	0	0.00
110-120	0.9063	02	4.17	2	0.86
120-130	0.8192	03	6.25	4	1.43
130-140	0.7071	01	2.08	1	0.55
140-150	0.5736	02	4.17	3	1.36
150-160	0.4226	06	12.50	14	5.55
160-170	0.2588	14	29.17	54	21.13
170-180	0.0872	15	31.25	172	67.19

Table S3. Data for $X_3P\cdots O$ pnicogen bonding for which X = carbon in ∠OPX = 90 – 180°.

Angle range	Sin θ	No of Hits Before Cone Correction (n)	% Of hits Before Cone Correction	No of Hits After Cone Correction = n/Sin θ	% Of hits After Cone Correction
90-100	0.9962	09	8.57	9	2.04
100-110	0.9659	07	6.67	7	1.64
110-120	0.9063	10	9.52	11	2.49
120-130	0.8192	09	8.57	11	2.48
130-140	0.7071	02	1.90	3	0.64
140-150	0.5736	06	5.71	10	2.36
150-160	0.4226	10	9.52	24	5.34
160-170	0.2588	30	28.57	116	26.17
170-180	0.0872	22	20.95	252	56.95

Table S4. Data for $X_3P\cdots O$ pnicogen bonding for which X = nitrogen in ∠OPX = 90 – 180°.

Angle range	Sin θ	No of Hits Before Cone Correction (n)	% Of hits Before Cone Correction	No of Hits After Cone Correction = n/Sin θ	% Of hits After Cone Correction
90-100	0.9962	09	14.29	9	3.06
100-110	0.9659	04	6.35	4	1.40
110-120	0.9063	00	0.00	0	0.00
120-130	0.8192	02	3.17	2	0.83
130-140	0.7071	01	1.59	1	0.48
140-150	0.5736	02	3.17	3	1.18
150-160	0.4226	09	14.29	21	7.22
160-170	0.2588	21	33.33	81	27.51
170-180	0.0872	15	23.81	172	58.31

Table S5. Data for $X_4P\cdots O$ pnicogen bonding (X is any atom).

Angle range	Sin θ	No of Hits Before Cone Correction (n)	% Of hits Before Cone Correction	No of Hits After Cone Correction = n/Sin θ	% Of hits After Cone Correction
90-100	0.9962	55	14.51	55	4.35
100-110	0.9659	28	7.39	29	2.29
110-120	0.9063	20	5.28	22	1.74
120-130	0.8192	17	4.49	21	1.64
130-140	0.7071	25	6.60	35	2.79
140-150	0.5736	30	7.92	52	4.12
150-160	0.4226	77	20.32	182	14.37
160-170	0.2588	77	20.32	298	23.46
170-180	0.0872	50	13.19	573	45.22

Table S6. Data for $X_4P\cdots O$ pnicogen bonding for which X = oxygen in ∠OPX = 90 – 180°.

Angle range	Sin θ	No of Hits Before Cone Correction (n)	% Of hits Before Cone Correction	No of Hits After Cone Correction = n/Sin θ	% Of hits After Cone Correction
90-100	0.9962	34	14.66	34	4.60
100-110	0.9659	22	9.48	23	3.07
110-120	0.9063	13	5.60	14	1.93
120-130	0.8192	12	5.17	15	1.97
130-140	0.7071	17	7.33	24	3.24
140-150	0.5736	22	9.48	38	5.17
150-160	0.4226	45	19.40	106	14.35
160-170	0.2588	37	15.95	143	19.27
170-180	0.0872	30	12.93	344	46.37

Table S7. Data for $X_4P\cdots O$ pnicogen bonding for which X = carbon in ∠OPX = 90 – 180°.

Angle range	Sin θ	No of Hits Before Cone Correction (n)	% Of hits Before Cone Correction	No of Hits After Cone Correction = n/Sin θ	% Of hits After Cone Correction
90-100	0.9962	12	11.54	12	3.37
100-110	0.9659	05	4.81	5	1.45
110-120	0.9063	06	5.77	7	1.85
120-130	0.8192	05	4.81	6	1.71
130-140	0.7071	06	5.77	8	2.38
140-150	0.5736	07	6.73	12	3.42
150-160	0.4226	24	23.08	57	15.91
160-170	0.2588	26	25.00	100	28.14
170-180	0.0872	13	12.50	149	41.76