

Supplementary Information  
For

# Metal– $\pi$ Interactions in Light of Geometry –Corrected Statistical Analysis

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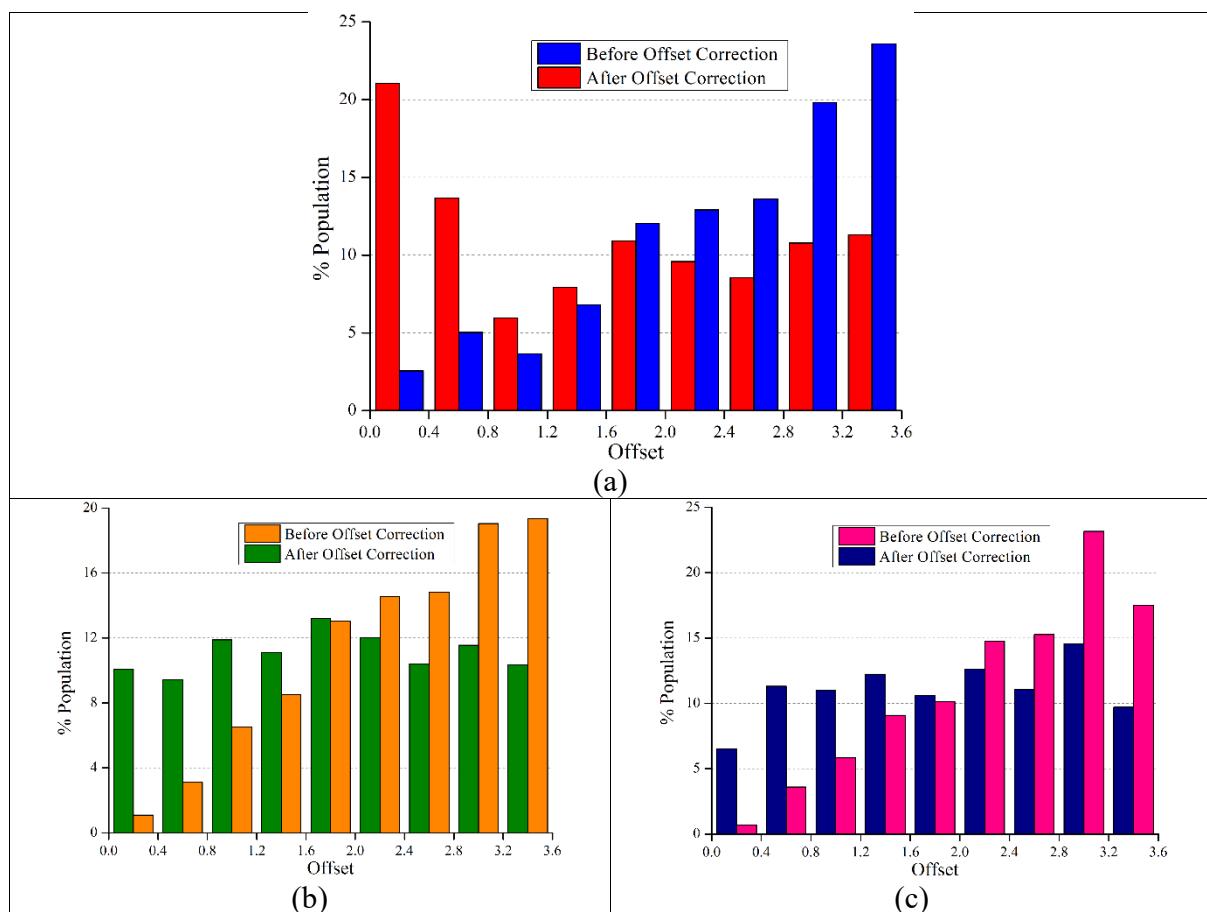
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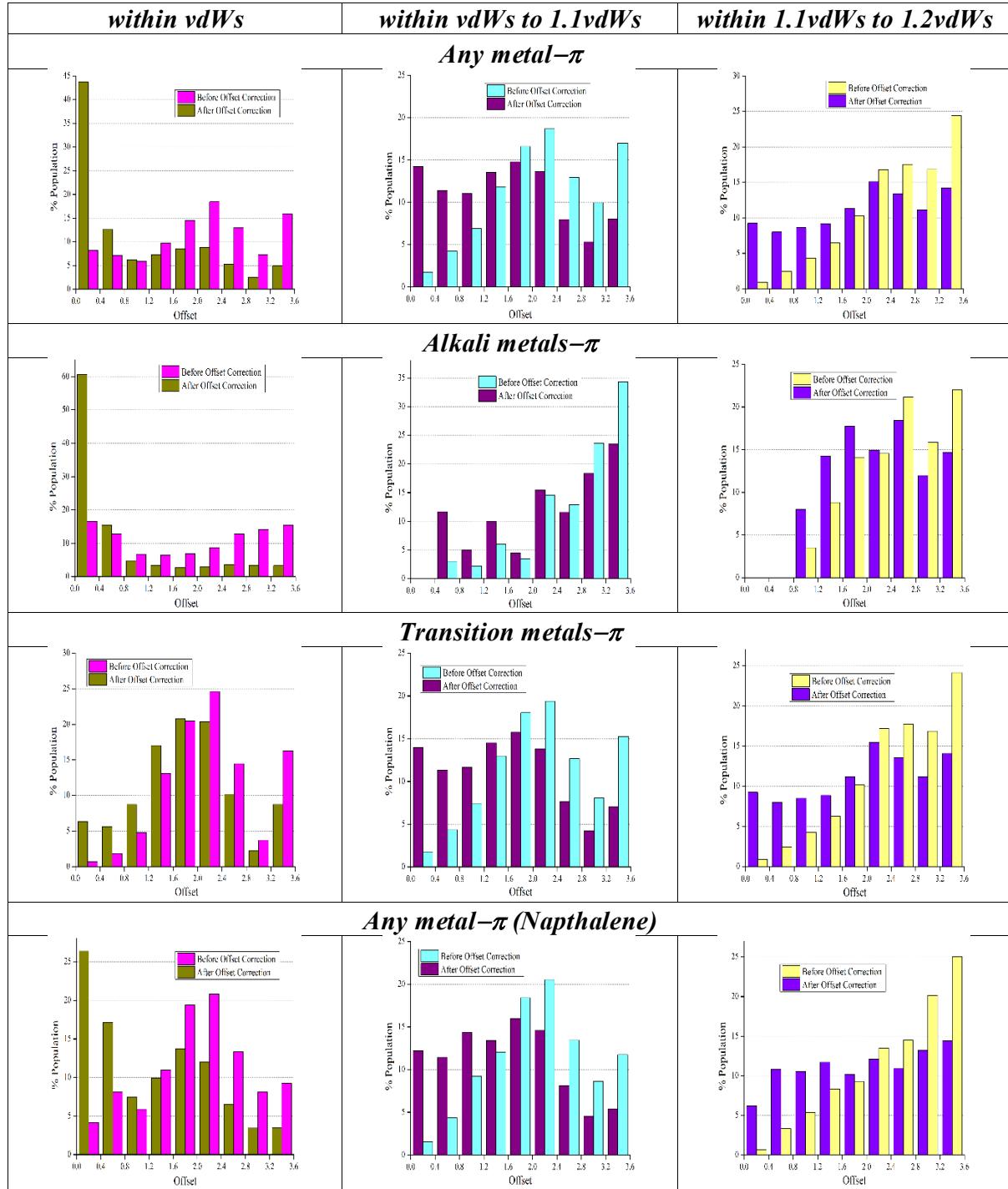
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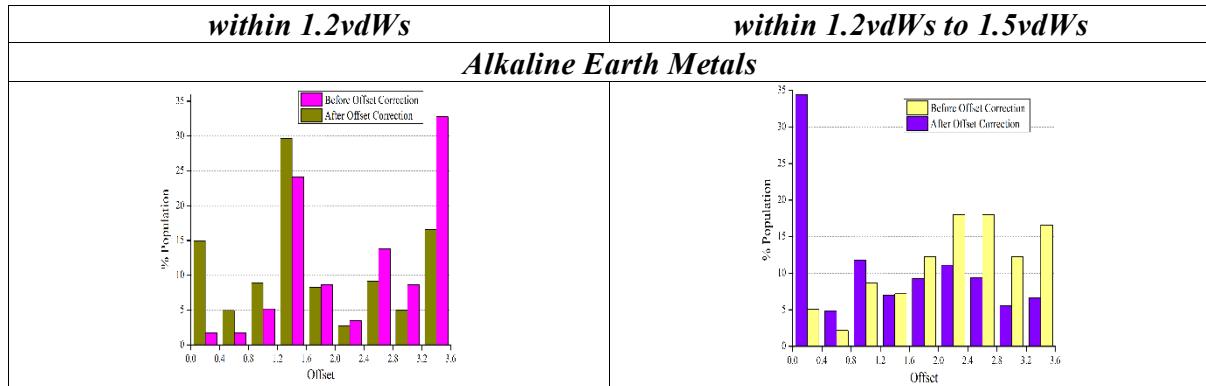
**Figure 1.** Offset uncorrected and corrected 2D plots of % population of any metal- $\pi$  (naphthalene) interactions vs offset for (a) within vdWs, (b) within vdWs to 1.1vdWs and (c) within 1.1vdWs to 1.2vdWs.



**Figure 2.** Offset uncorrected and corrected 2D plots of % population of metal– $\pi$  interactions vs offset for (a) within vdWs, (b) within vdWs to 1.1vdWs and (c) within 1.1vdWs to 1.2vdWs radii of carbon and hydrogen atom of benzene and the metal. Here for the benzene plane the van der Waals radius considered is 1.7 Å (radius of C atom) for the offset of 0 to 2.6 Å and 1.2 Å (radius of H atom) for the offset of 2.6 to 3.6 Å. Though this is an approximate way to treat the thickness of the benzene plane, it is good enough to understand the change in population distribution at least qualitatively due to change in thickness of the plane.



**Figure 3.** Offset uncorrected and corrected 2D plots of % population of alkaline earth metal– $\pi$  interactions vs offset for (a) within 1.2vdWs, (b) within 1.2vdWs to 1.5vdWs radii of carbon and hydrogen atom of benzene and the metal. Here for the benzene plane the van der Waals radius considered is 1.7 Å (radius of C atom) for the offset of 0 to 2.6 Å and 1.2 Å (radius of H atom) for the offset of 2.6 to 3.6 Å. Though this is an approximate way to treat the thickness of the benzene plane, it is good enough to understand the change in population distribution at least qualitatively due to change in thickness of the plane.



**Table S1.** Any metal– $\pi$  interactions at different offset ( $r$ ) within vdWs radii of carbon atom of benzene and the metal.

<i>Offset (Å)</i>	No of hits before correction	% before correction	Offset Correction factor	After offset correction	% after correction
<b>3.2-3.6</b>	3745	33.64	8.55	438	15.17
<b>2.8-3.2</b>	2237	20.10	7.54	297	10.27
<b>2.4-2.8</b>	1360	12.22	6.53	208	7.21
<b>2.0-2.4</b>	1094	9.83	5.53	198	6.85
<b>1.6-2.0</b>	862	7.74	4.52	191	6.60
<b>1.2-1.6</b>	575	5.17	3.52	163	5.66
<b>0.8-1.2</b>	347	3.12	2.51	138	4.79
<b>0.4-0.8</b>	424	3.81	1.51	281	9.72
<b>0.0-0.4</b>	487	4.38	0.5	974	33.73

**Table S2.** Any metal– $\pi$  interactions at different offset ( $r$ ) within vdWs to 1.1vdWs radii of carbon atom of benzene and the metal.

<i>Offset (Å)</i>	No of hits before correction	% before correction	Offset Correction factor	After offset correction	% after correction
<b>3.2-3.6</b>	3364	27.27	8.55	393	15.61
<b>2.8-3.2</b>	2574	20.87	7.54	341	13.54
<b>2.4-2.8</b>	1707	13.84	6.53	261	10.37
<b>2.0-2.4</b>	1458	11.82	5.53	264	10.46
<b>1.6-2.0</b>	1296	10.51	4.52	287	11.37
<b>1.2-1.6</b>	926	7.51	3.52	263	10.44
<b>0.8-1.2</b>	539	4.37	2.51	215	8.52
<b>0.4-0.8</b>	333	2.70	1.51	221	8.75
<b>0.0-0.4</b>	138	1.12	0.50	276	10.95

**Table S3.** Any metal- $\pi$  interactions at different offset (r) within 1.1vdWs to 1.2vdWs radii of carbon atom of benzene and the metal.

<b>Offset (Å)</b>	No of hits before correction	% before correction	Offset Correction factor	After offset correction	% after correction
<b>3.2-3.6</b>	3784	28.20	8.55	443	18.16
<b>2.8-3.2</b>	3231	24.08	7.54	429	17.58
<b>2.4-2.8</b>	2401	17.89	6.53	368	15.09
<b>2.0-2.4</b>	1630	12.15	5.53	295	12.10
<b>1.6-2.0</b>	997	7.43	4.52	221	9.05
<b>1.2-1.6</b>	629	4.69	3.52	179	7.33
<b>0.8-1.2</b>	422	3.14	2.51	168	6.90
<b>0.4-0.8</b>	236	1.76	1.51	156	6.41
<b>0.0-0.4</b>	90	0.67	0.50	180	7.39

**Table S4.** Alkali metal- $\pi$  interactions at different offset (r) within vdWs radii of carbon atom of benzene and the metal.

<b>Offset (Å)</b>	No of hits before correction	% before correction	Offset Correction factor	After offset correction	% after correction
<b>3.2-3.6</b>	355	19.21	8.55	41.52	4.49
<b>2.8-3.2</b>	302	16.34	7.54	40.05	4.33
<b>2.4-2.8</b>	242	13.10	6.53	37.06	4.01
<b>2.0-2.4</b>	142	7.68	5.53	25.68	2.78
<b>1.6-2.0</b>	113	6.11	4.52	25.00	2.70
<b>1.2-1.6</b>	105	5.68	3.52	29.83	3.23
<b>0.8-1.2</b>	108	5.84	2.51	43.03	4.65
<b>0.4-0.8</b>	209	11.31	1.51	138.41	14.97
<b>0.0-0.4</b>	272	14.72	0.5	544.00	58.84

**Table S5.** Alkali metal- $\pi$  interactions at different offset (r) within vdWs to 1.1vdWs radii of carbon atom of benzene and the metal.

<b>Offset (Å)</b>	No of hits before correction	% before correction	Offset Correction factor	After offset correction	% after correction
<b>3.2-3.6</b>	59	29.21	8.55	6.90	19.21
<b>2.8-3.2</b>	48	23.76	7.54	6.37	17.72
<b>2.4-2.8</b>	27	13.37	6.53	4.13	11.51
<b>2.0-2.4</b>	34	16.83	5.53	6.15	17.12
<b>1.6-2.0</b>	08	3.96	4.52	1.77	4.93
<b>1.2-1.6</b>	14	6.93	3.52	3.98	11.07
<b>0.8-1.2</b>	05	2.48	2.51	1.99	5.55
<b>0.4-0.8</b>	07	3.47	1.51	4.64	12.91
<b>0.0-0.4</b>	00	0.00	0.50	0.00	0.00

**Table S6.** Alkali metal- $\pi$  interactions at different offset (r) within 1.1vdWs to 1.2vdWs radii of carbon atom of benzene and the metal.

<b>Offset (Å)</b>	No of hits before correction	% before correction	Offset Correction factor	After offset correction	% after correction
<b>3.2-3.6</b>	103	31.89	8.55	12.05	23.34
<b>2.8-3.2</b>	88	27.24	7.54	11.67	22.61
<b>2.4-2.8</b>	39	12.07	6.53	5.97	11.57
<b>2.0-2.4</b>	33	10.22	5.53	5.97	11.56
<b>1.6-2.0</b>	32	9.91	4.52	7.08	13.72
<b>1.2-1.6</b>	20	6.19	3.52	5.68	11.01
<b>0.8-1.2</b>	08	2.48	2.51	3.19	6.18
<b>0.4-0.8</b>	00	0.00	1.51	0.00	0.00
<b>0.0-0.4</b>	00	0.00	0.50	0.00	0.00

**Table S7.** Transition metal- $\pi$  interactions at different offset (r) within vdWs radii of carbon atom of benzene and the metal.

<b>Offset (Å)</b>	No of hits before correction	% before correction	Offset Correction factor	After offset correction	% after correction
<b>3.2-3.6</b>	2769	38.60	8.55	324	27.33
<b>2.8-3.2</b>	1526	21.27	7.54	202	17.08
<b>2.4-2.8</b>	892	12.44	6.53	137	11.53
<b>2.0-2.4</b>	746	10.40	5.53	135	11.38
<b>1.6-2.0</b>	621	8.66	4.52	137	11.59
<b>1.2-1.6</b>	397	5.53	3.52	113	9.52
<b>0.8-1.2</b>	145	2.02	2.51	58	4.88
<b>0.4-0.8</b>	56	0.78	1.51	37	3.13
<b>0.0-0.4</b>	21	0.29	0.5	42	3.54

**Table S8.** Transition metal- $\pi$  interactions at different offset (r) within vdWs to 1.1vdWs radii of carbon atom of benzene and the metal.

<b>Offset (Å)</b>	No of hits before correction	% before correction	Offset Correction factor	After offset correction	% after correction
<b>3.2-3.6</b>	2858	26.49	8.55	334	15.06
<b>2.8-3.2</b>	2216	20.54	7.54	294	13.24
<b>2.4-2.8</b>	1469	13.61	6.53	225	10.13
<b>2.0-2.4</b>	1288	11.94	5.53	233	10.49
<b>1.6-2.0</b>	1198	11.10	4.52	265	11.94
<b>1.2-1.6</b>	862	7.99	3.52	245	11.03
<b>0.8-1.2</b>	493	4.57	2.51	196	8.85
<b>0.4-0.8</b>	289	2.68	1.51	191	8.62
<b>0.0-0.4</b>	118	1.09	0.50	236	10.63

**Table S9.** Transition metal- $\pi$  interactions at different offset (r) within 1.1vdWs to 1.2vdWs radii of carbon atom of benzene and the metal.

<b>Offset (Å)</b>	No of hits before correction	% before correction	Offset Correction factor	After offset correction	% after correction
<b>3.2-3.6</b>	3102	27.79	8.55	363	17.91
<b>2.8-3.2</b>	2666	23.88	7.54	354	17.45
<b>2.4-2.8</b>	2063	18.48	6.53	316	15.59
<b>2.0-2.4</b>	1388	12.44	5.53	251	12.39
<b>1.6-2.0</b>	820	7.35	4.52	181	8.95
<b>1.2-1.6</b>	506	4.53	3.52	144	7.10
<b>0.8-1.2</b>	346	3.10	2.51	138	6.80
<b>0.4-0.8</b>	196	1.76	1.51	130	6.41
<b>0.0-0.4</b>	75	0.67	0.50	150	7.40

**Table S10.** Alkaline earth metal- $\pi$  interactions at different offset (r) within 1.2vdWs radii of carbon atom of benzene and the metal.

<b>Offset (Å)</b>	No of hits before correction	% before correction	Offset Correction factor	After offset correction	% after correction
<b>3.2-3.6</b>	34	41.98	8.55	3.98	24.44
<b>2.8-3.2</b>	11	13.58	7.54	1.46	8.97
<b>2.4-2.8</b>	10	12.35	6.53	1.53	9.41
<b>2.0-2.4</b>	02	2.47	5.53	0.36	2.22
<b>1.6-2.0</b>	05	6.17	4.52	1.11	6.80
<b>1.2-1.6</b>	14	17.28	3.52	3.98	24.45
<b>0.8-1.2</b>	03	3.70	2.51	1.20	7.35
<b>0.4-0.8</b>	01	1.23	1.51	0.66	4.07
<b>0.0-0.4</b>	01	1.23	0.50	2.00	12.29

**Table S11.** Alkaline earth metal- $\pi$  interactions at different offset (r) within 1.2vdWs to 1.5vdWs radii of carbon atom of benzene and the metal.

<b>Offset (Å)</b>	No of hits before correction	% before correction	Offset Correction factor	After offset correction	% after correction
<b>3.2-3.6</b>	73	28.52	8.55	8.54	15.28
<b>2.8-3.2</b>	60	23.44	7.54	7.96	14.24
<b>2.4-2.8</b>	49	19.14	6.53	7.50	13.43
<b>2.0-2.4</b>	25	9.77	5.53	4.52	8.09
<b>1.6-2.0</b>	17	6.64	4.52	3.76	6.73
<b>1.2-1.6</b>	10	3.91	3.52	2.84	5.08
<b>0.8-1.2</b>	12	4.69	2.51	4.78	8.55
<b>0.4-0.8</b>	3	1.17	1.51	1.99	3.55
<b>0.0-0.4</b>	7	2.73	0.5	14.00	25.05

**Table S12.** Metal- $\pi$  interactions with naphthalene moiety at different offset (r) within vdWs radii of carbon atom of benzene and the metal.

<b>Offset (Å)</b>	No of hits before correction	% before correction	Offset Correction factor	After offset correction	% after correction
<b>3.2-3.6</b>	239	23.57	8.55	28	11.32
<b>2.8-3.2</b>	201	19.82	7.54	27	10.79
<b>2.4-2.8</b>	138	13.61	6.53	21	8.56
<b>2.0-2.4</b>	131	12.92	5.53	24	9.59
<b>1.6-2.0</b>	122	12.03	4.52	27	10.93
<b>1.2-1.6</b>	69	6.80	3.52	20	7.94
<b>0.8-1.2</b>	37	3.65	2.51	15	5.97
<b>0.4-0.8</b>	51	5.03	1.51	34	13.67
<b>0.0-0.4</b>	26	2.56	0.50	52	21.05

**Table S13.** Metal- $\pi$  interactions with naphthalene moiety at different offset (r) within vdWs to 1.1vdWs radii of carbon atom of benzene and the metal.

<b>Offset (Å)</b>	No of hits before correction	% before correction	Offset Correction factor	After offset correction	% after correction
<b>3.2-3.6</b>	193	19.34	8.55	23	10.35
<b>2.8-3.2</b>	190	19.04	7.54	25	11.56
<b>2.4-2.8</b>	148	14.83	6.53	23	10.40
<b>2.0-2.4</b>	145	14.53	5.53	26	12.03
<b>1.6-2.0</b>	130	13.03	4.52	29	13.19
<b>1.2-1.6</b>	85	8.52	3.52	24	11.08
<b>0.8-1.2</b>	65	6.51	2.51	26	11.88
<b>0.4-0.8</b>	31	3.11	1.51	21	9.42
<b>0.0-0.4</b>	11	1.10	0.50	22	10.09

**Table S14.** Metal- $\pi$  interactions with naphthalene moiety at different offset (r) within 1.1vdWs to 1.2vdWs radii of carbon atom of benzene and the metal.

<b>Offset (Å)</b>	No of hits before correction	% before correction	Offset Correction factor	After offset correction	% after correction
<b>3.2-3.6</b>	102	17.50	8.55	12	9.70
<b>2.8-3.2</b>	135	23.16	7.54	18	14.56
<b>2.4-2.8</b>	89	15.27	6.53	14	11.08
<b>2.0-2.4</b>	86	14.75	5.53	16	12.64
<b>1.6-2.0</b>	59	10.12	4.52	13	10.61
<b>1.2-1.6</b>	53	9.09	3.52	15	12.24
<b>0.8-1.2</b>	34	5.83	2.51	14	11.01
<b>0.4-0.8</b>	21	3.60	1.51	14	11.31
<b>0.0-0.4</b>	04	0.69	0.50	8	6.50

**Table S15.** Any metal- $\pi$  interactions at different offset (r) within vdWs radii of carbon (offset 0 to 2.6Å) and hydrogen atom (offset 2.6 to 3.6Å) of benzene and the metal.

<i>Offset</i> (Å)	No of hits before correction	% before correction	Offset Correction factor	After offset correction	% after correction
<b>3.2-3.6</b>	941	15.86	8.55	110	4.94
<b>2.8-3.2</b>	433	7.30	7.54	57	2.58
<b>2.4-2.8</b>	771	12.99	6.53	118	5.29
<b>2.0-2.4</b>	1094	18.44	5.53	198	8.87
<b>1.6-2.0</b>	862	14.53	4.52	191	8.55
<b>1.2-1.6</b>	575	9.69	3.52	163	7.33
<b>0.8-1.2</b>	347	5.85	2.51	138	6.20
<b>0.4-0.8</b>	424	7.15	1.51	281	12.59
<b>0.0-0.4</b>	487	8.21	0.5	974	43.68

**Table S16.** Any metal- $\pi$  interactions at different offset (r) within vdWs to 1.1vdWs radii of carbon (offset 0 to 2.6Å) and hydrogen atom (offset 2.6 to 3.6Å) of benzene and the metal.

<i>Offset</i> (Å)	No of hits before correction	% before correction	Offset Correction factor	After offset correction	% after correction
<b>3.2-3.6</b>	1328	17.01	8.55	155	8.01
<b>2.8-3.2</b>	778	9.97	7.54	103	5.32
<b>2.4-2.8</b>	1010	12.94	6.53	155	7.98
<b>2.0-2.4</b>	1458	18.68	5.53	264	13.60
<b>1.6-2.0</b>	1296	16.60	4.52	287	14.79
<b>1.2-1.6</b>	926	11.86	3.52	263	13.57
<b>0.8-1.2</b>	539	6.90	2.51	215	11.08
<b>0.4-0.8</b>	333	4.27	1.51	221	11.38
<b>0.0-0.4</b>	138	1.77	0.50	276	14.24

**Table S17.** Any metal- $\pi$  interactions at different offset (r) within 1.1vdWs to 1.2vdWs radii of carbon (offset 0 to 2.6Å) and hydrogen atom (offset 2.6 to 3.6Å) of benzene and the metal.

<i>Offset</i> (Å)	No of hits before correction	% before correction	Offset Correction factor	After offset correction	% after correction
<b>3.2-3.6</b>	2370	24.40	8.55	277	14.19
<b>2.8-3.2</b>	1635	16.83	7.54	217	11.10
<b>2.4-2.8</b>	1704	17.54	6.53	261	13.36
<b>2.0-2.4</b>	1630	16.78	5.53	295	15.09
<b>1.6-2.0</b>	997	10.26	4.52	221	11.29
<b>1.2-1.6</b>	629	6.48	3.52	179	9.15
<b>0.8-1.2</b>	422	4.34	2.51	168	8.61
<b>0.4-0.8</b>	236	2.43	1.51	156	8.00
<b>0.0-0.4</b>	90	0.93	0.50	180	9.22

**Table S18.** Alkali metal- $\pi$  interactions at different offset (r) within vdWs radii of carbon (offset 0 to 2.6Å) and hydrogen atom (offset 2.6 to 3.6Å) of benzene and the metal.

<b>Offset (Å)</b>	No of hits before correction	% before correction	Offset Correction factor	After offset correction	% after correction
<b>3.2-3.6</b>	253	15.40	8.55	29.59	3.29
<b>2.8-3.2</b>	232	14.12	7.54	30.77	3.43
<b>2.4-2.8</b>	209	12.72	6.53	32.01	3.56
<b>2.0-2.4</b>	142	8.64	5.53	25.68	2.86
<b>1.6-2.0</b>	113	6.88	4.52	25.00	2.78
<b>1.2-1.6</b>	105	6.39	3.52	29.83	3.32
<b>0.8-1.2</b>	108	6.57	2.51	43.03	4.79
<b>0.4-0.8</b>	209	12.72	1.51	138.41	15.41
<b>0.0-0.4</b>	272	16.56	0.5	544.00	60.56

**Table S19.** Alkali metal- $\pi$  interactions at different offset (r) within vdWs to 1.1vdWs radii of carbon (offset 0 to 2.6Å) and hydrogen atom (offset 2.6 to 3.6Å) of benzene and the metal.

<b>Offset (Å)</b>	No of hits before correction	% before correction	Offset Correction factor	After offset correction	% after correction
<b>3.2-3.6</b>	80	34.33	8.55	9.36	23.53
<b>2.8-3.2</b>	55	23.61	7.54	7.29	18.34
<b>2.4-2.8</b>	30	12.88	6.53	4.59	11.55
<b>2.0-2.4</b>	34	14.59	5.53	6.15	15.46
<b>1.6-2.0</b>	08	3.43	4.52	1.77	4.45
<b>1.2-1.6</b>	14	6.01	3.52	3.98	10.00
<b>0.8-1.2</b>	05	2.15	2.51	1.99	5.01
<b>0.4-0.8</b>	07	3.00	1.51	4.64	11.66
<b>0.0-0.4</b>	00	0.00	0.50	0.00	0.00

**Table S20.** Alkali metal- $\pi$  interactions at different offset (r) within 1.1vdWs to 1.2vdWs radii of carbon (offset 0 to 2.6Å) and hydrogen atom (offset 2.6 to 3.6Å) of benzene and the metal.

<b>Offset (Å)</b>	No of hits before correction	% before correction	Offset Correction factor	After offset correction	% after correction
<b>3.2-3.6</b>	50	22.03	8.55	5.85	14.66
<b>2.8-3.2</b>	36	15.86	7.54	4.77	11.97
<b>2.4-2.8</b>	48	21.15	6.53	7.35	18.43
<b>2.0-2.4</b>	33	14.54	5.53	5.97	14.96
<b>1.6-2.0</b>	32	14.10	4.52	7.08	17.75
<b>1.2-1.6</b>	20	8.81	3.52	5.68	14.24
<b>0.8-1.2</b>	08	3.52	2.51	3.19	7.99
<b>0.4-0.8</b>	00	0.00	1.51	0.00	0.00
<b>0.0-0.4</b>	00	0.00	0.50	0.00	0.00

**Table S21.** Transition metal- $\pi$  interactions at different offset (r) within vdWs radii of carbon (offset 0 to 2.6Å) and hydrogen atom (offset 2.6 to 3.6Å) of benzene and the metal.

<b>Offset (Å)</b>	No of hits before correction	% before correction	Offset Correction factor	After offset correction	% after correction
<b>3.2-3.6</b>	494	16.30	8.55	58	8.73
<b>2.8-3.2</b>	112	3.70	7.54	15	2.24
<b>2.4-2.8</b>	439	14.48	6.53	67	10.16
<b>2.0-2.4</b>	746	24.61	5.53	135	20.38
<b>1.6-2.0</b>	621	20.49	4.52	137	20.75
<b>1.2-1.6</b>	397	13.10	3.52	113	17.04
<b>0.8-1.2</b>	145	4.78	2.51	58	8.73
<b>0.4-0.8</b>	56	1.85	1.51	37	5.60
<b>0.0-0.4</b>	21	0.69	0.50	42	6.34

**Table S22.** Transition metal- $\pi$  interactions at different offset (r) within vdWs to 1.1vdWs radii of carbon (offset 0 to 2.6Å) and hydrogen atom (offset 2.6 to 3.6Å) of benzene and the metal.

<b>Offset (Å)</b>	No of hits before correction	% before correction	Offset Correction factor	After offset correction	% after correction
<b>3.2-3.6</b>	1012	15.25	8.55	118	7.02
<b>2.8-3.2</b>	537	8.09	7.54	71	4.23
<b>2.4-2.8</b>	841	12.67	6.53	129	7.64
<b>2.0-2.4</b>	1288	19.40	5.53	233	13.82
<b>1.6-2.0</b>	1198	18.05	4.52	265	15.73
<b>1.2-1.6</b>	862	12.99	3.52	245	14.53
<b>0.8-1.2</b>	493	7.43	2.51	196	11.66
<b>0.4-0.8</b>	289	4.35	1.51	191	11.36
<b>0.0-0.4</b>	118	1.78	0.50	236	14.01

**Table S23.** Transition metal- $\pi$  interactions at different offset (r) within 1.1vdWs to 1.2vdWs radii of carbon (offset 0 to 2.6Å) and hydrogen atom (offset 2.6 to 3.6Å) of benzene and the metal.

<b>Offset (Å)</b>	No of hits before correction	% before correction	Offset Correction factor	After offset correction	% after correction
<b>3.2-3.6</b>	1951	24.15	8.55	228	14.06
<b>2.8-3.2</b>	1363	16.87	7.54	181	11.14
<b>2.4-2.8</b>	1435	17.76	6.53	220	13.54
<b>2.0-2.4</b>	1388	17.18	5.53	251	15.46
<b>1.6-2.0</b>	820	10.15	4.52	181	11.18
<b>1.2-1.6</b>	506	6.26	3.52	144	8.86
<b>0.8-1.2</b>	346	4.28	2.51	138	8.49
<b>0.4-0.8</b>	196	2.43	1.51	130	8.00
<b>0.0-0.4</b>	75	0.93	0.50	150	9.24

**Table S24.** Alkaline earth metal- $\pi$  interactions at different offset (r) within 1.2vdWs radii of carbon (offset 0 to 2.6Å) and hydrogen atom (offset 2.6 to 3.6Å) of benzene and the metal.

<b>Offset (Å)</b>	No of hits before correction	% before correction	Offset Correction factor	After offset correction	% after correction
<b>3.2-3.6</b>	19	32.76	8.55	2.22	16.57
<b>2.8-3.2</b>	05	8.62	7.54	0.66	4.95
<b>2.4-2.8</b>	08	13.79	6.53	1.23	9.14
<b>2.0-2.4</b>	02	3.45	5.53	0.36	2.70
<b>1.6-2.0</b>	05	8.62	4.52	1.11	8.25
<b>1.2-1.6</b>	14	24.14	3.52	3.98	29.66
<b>0.8-1.2</b>	03	5.17	2.51	1.20	8.91
<b>0.4-0.8</b>	01	1.72	1.51	0.66	4.94
<b>0.0-0.4</b>	01	1.72	0.50	2.00	14.91

**Table S25.** Alkaline earth metal- $\pi$  interactions at different offset (r) within 1.2vdWs to 1.5vdWs radii of carbon (offset 0 to 2.6Å) and hydrogen atom (offset 2.6 to 3.6Å) of benzene and the metal.

<b>Offset (Å)</b>	No of hits before correction	% before correction	Offset Correction factor	After offset correction	% after correction
<b>3.2-3.6</b>	23	16.55	8.55	2.69	6.62
<b>2.8-3.2</b>	17	12.23	7.54	2.25	5.55
<b>2.4-2.8</b>	25	17.99	6.53	3.83	9.42
<b>2.0-2.4</b>	25	17.99	5.53	4.52	11.12
<b>1.6-2.0</b>	17	12.23	4.52	3.76	9.25
<b>1.2-1.6</b>	10	7.19	3.52	2.84	6.99
<b>0.8-1.2</b>	12	8.63	2.51	4.78	11.76
<b>0.4-0.8</b>	3	2.16	1.51	1.99	4.89
<b>0.0-0.4</b>	7	5.04	0.5	14.00	34.43

**Table S26.** Metal- $\pi$  interactions of naphthalene at different offset (r) within vdWs radii of carbon (offset 0 to 2.6Å) and hydrogen atom (offset 2.6 to 3.6Å) of benzene and the metal.

<b>Offset (Å)</b>	No of hits before correction	% before correction	Offset Correction factor	After offset correction	% after correction
<b>3.2-3.6</b>	58	9.22	8.55	6.78	3.44
<b>2.8-3.2</b>	51	8.11	7.54	6.76	3.43
<b>2.4-2.8</b>	84	13.35	6.53	12.86	6.52
<b>2.0-2.4</b>	131	20.83	5.53	23.69	12.01
<b>1.6-2.0</b>	122	19.40	4.52	26.99	13.69
<b>1.2-1.6</b>	69	10.97	3.52	19.60	9.94
<b>0.8-1.2</b>	37	5.88	2.51	14.74	7.47
<b>0.4-0.8</b>	51	8.11	1.51	33.77	17.13
<b>0.0-0.4</b>	26	4.13	0.50	52.00	26.37

**Table S27.** Metal- $\pi$  interactions of naphthalene at different offset (r) within vdWs to 1.1vdWs radii of carbon (offset 0 to 2.6Å) and hydrogen atom (offset 2.6 to 3.6Å) of benzene and the metal.

<b>Offset (Å)</b>	No of hits before correction	% before correction	Offset Correction factor	After offset correction	% after correction
<b>3.2-3.6</b>	83	11.76	8.55	9.71	5.40
<b>2.8-3.2</b>	61	8.64	7.54	8.09	4.50
<b>2.4-2.8</b>	95	13.46	6.53	14.55	8.09
<b>2.0-2.4</b>	145	20.54	5.53	26.22	14.58
<b>1.6-2.0</b>	130	18.41	4.52	28.76	15.99
<b>1.2-1.6</b>	85	12.04	3.52	24.15	13.42
<b>0.8-1.2</b>	65	9.21	2.51	25.90	14.39
<b>0.4-0.8</b>	31	4.39	1.51	20.53	11.41
<b>0.0-0.4</b>	11	1.56	0.50	22.00	12.23

**Table S28.** Metal- $\pi$  interactions with naphthalene moiety at different offset (r) within 1.1vdWs to 1.2vdWs radii of carbon (offset 0 to 2.6Å) and hydrogen atom (offset 2.6 to 3.6Å) of benzene and the metal.

<b>Offset (Å)</b>	No of hits before correction	% before correction	Offset Correction factor	After offset correction	% after correction
<b>3.2-3.6</b>	159	25.00	8.55	18.60	14.44
<b>2.8-3.2</b>	128	20.13	7.54	16.98	13.18
<b>2.4-2.8</b>	92	14.47	6.53	14.09	10.94
<b>2.0-2.4</b>	86	13.52	5.53	15.55	12.08
<b>1.6-2.0</b>	59	9.28	4.52	13.05	10.14
<b>1.2-1.6</b>	53	8.33	3.52	15.06	11.69
<b>0.8-1.2</b>	34	5.35	2.51	13.55	10.52
<b>0.4-0.8</b>	21	3.30	1.51	13.91	10.80
<b>0.0-0.4</b>	04	0.63	0.50	8.00	6.21