

Table S1: BSSE corrected binding energies (BEs, kcal/mol⁻¹) of ZnX (X = He, Ne, Ar) complexes computed at different levels of theories. D3 is when dispersion is included.

basis sets	6-311++G(d,p)						6-311++G(d,p)	aug-cc-pVDZ			aug-cc-pVTZ		aug-cc-pVDZ		aug-cc-pVTZ		aug-cc-pVTZ(-PP)					
	PBE	PBE+D3	PBE0	PBE0+D3	M05-2X	M05-2X+D3		(R)MP2	(R)MP2	SCS-MP2	(R)MP2	SCS-MP2	(R)CCSD(T)	(R)CCSD	(R)CCSD(T)	(R)CCSD	(R)MP2-F12	(R)CCSD(T)-F12	(R)CCSD-F12	(R)MP2	(R)CCSD(T)	(R)CCSD
ZnHe	-0.055	-0.118	-0.027	-0.084	-0.006	-0.0705	0.018	-0.043	-0.002	-0.029	-0.100	-0.0351	-0.028	-0.020	-0.016	-0.022	-0.013	-0.009	-0.030	-0.025	-0.020	
ZnNe	-0.164	-0.335	-0.073	-0.225	-0.006	-0.162	0.074	-0.117	-0.008	-0.090	-0.024	-0.073	-0.088	-0.097	-0.055	-0.064	-0.098	-0.039	-0.080	-0.112	-0.061	
ZnAr	-0.152	-0.458	-0.090	-0.358	-0.158	-0.466	0.149	-0.360	-0.097	-0.359	-0.161	-0.249	-0.197	-0.216	-0.153	-0.457	-0.276	-0.201	-0.372	-0.230	-0.164	

Table S2: Calculated vibrational stretching frequencies (scaled) for Zn^qIm (q = 0, 1, 2) at the different levels of theories

Basis set	6-311 ⁺⁺ G (d,p)				aug-cc-pVDZ
Method	PBE	PBE0	M05-2X	(R)MP2	(R)MP2
Zn⁰Im I	i 11.4663	18.8118	14.0349	1.26	16.96
	i 6.8682	25.8151	40.5874	13.73	29.45
	38.5878	38.7095	47.532	38.35	47.86
	514.1728	544.5766	552.0092	416.68	560.77
	622.4882	646.9748	652.6995	597.7521	641.73
	658.5848	683.4151	690.6685	656.3161	675.07
	693.9789	739.6538	760.3668	673.8231	717.75
	760.6469	822.2029	856.0938	734.1157	781.82
	821.8328	874.0163	905.2724	776.0605	838.68
	877.7419	912.8522	928.2574	900.7871	890.41
	914.7733	948.9053	960.606	935.1276	926.74
	1048.529	1088.0578	1094.3841	1086.765	1073.34
	1068.4052	1110.4308	1112.9699	1105.827	1095.28
	1114.9415	1158.9874	1162.6031	1155.555	1141.29
	1147.4388	1194.2726	1192.8762	1186.615	1176.79
	1235.4781	1285.5264	1301.8249	1279.928	1258.57
	1331.5792	1392.9844	1400.5212	1373.732	1362.46
	1395.303	1463.1135	1469.8821	1468.346	1461.7
	1457.3787	1525.903	1539.0873	1508.917	1492.67
	1507.4693	1579.1258	1599.0545	1538.755	1524.71
3176.531	3264.616	3291.3925	3284.409	3288.47	
3181.8793	3266.716	3300.7227	3287.321	3290.68	
3207.2501	3296.7416	3328.5978	3311.545	3314.2	
3562.2267	3695.185	3731.9685	3677.366	3658.67	
Zn⁰Im II	32.3936	38.5903	63.1728	57.4513	68.4
	41.0987	48.1598	73.1078	73.9008	80.87
	49.8285	57.9776	85.3542	83.7195	88.09
	515.1714	545.2387	565.9782	478.4243	555.77
	621.1065	645.8377	652.4585	621.5976	634.06
	658.8458	683.0429	688.5247	662.1847	667.63
	699.9191	745.039	765.9596	704.4613	718.24
	766.1941	826.3974	857.2556	773.9568	778.33
	830.9135	882.9311	905.1257	828.1525	839.02
	874.0388	909.3869	925.9267	896.5722	885.58
	913.8179	948.1617	960.4227	933.7507	925.26
	1047.3071	1086.9105	1094.5918	1085.2185	1071.38
	1068.2109	1109.198	1110.7834	1105.2888	1094.23
	1112.9442	1156.6818	1161.3614	1152.295	1137.33
	1148.4011	1195.6156	1194.2851	1189.5542	1180.02
	1235.2201	1284.1698	1300.5192	1278.3576	1256.86
	1328.7786	1391.3699	1398.4001	1371.6207	1359.94
	1391.5992	1459.3994	1466.9104	1464.5361	1457.57
	1452.4874	1520.6441	1535.584	1503.109	1484.59
	1503.1255	1575.4883	1596.2601	1534.5138	1519.36
3175.9789	3264.0418	3290.365	3282.5427	3286.88	
3182.0064	3268.2282	3292.9979	3290.8367	3296.51	
3207.471	3296.9175	3326.1862	3310.1059	3313.12	
3563.9255	3695.5	3736.3238	3673.3381	3654.75	
	109.3218	115.2421	111.9697	104.1672	171.84
	147.2355	150.4366	141.4261	148.1188	199.28

Zn⁺¹Im	242.9724	256.7299	251.3139	258.0019	239.06
	602.7606	628.8742	635.9972	578.5787	639.55
	628.6994	657.5082	664.0099	616.3143	659.4
	673.617	706.488	714.6921	685.5693	740.45
	728.1497	772.5844	789.2046	731.6078	830.41
	785.6269	851.0377	884.5063	779.458	868.81
	840.4271	893.0732	918.9782	803.3392	921.78
	902.2778	936.7161	945.7404	927.7139	935.2
	929.9663	967.7553	978.4468	958.1113	970.34
	1061.762	1103.0333	1104.6843	1107.0112	1123.93
	1096.1566	1134.8975	1145.5764	1129.0842	1163.38
	1127.5093	1167.9968	1160.8265	1171.7515	1193.51
	1174.8324	1221.7855	1225.8735	1216.5948	1232.67
	1249.1958	1300.7289	1314.4136	1290.1553	1311.99
	1322.5098	1381.5321	1388.531	1377.1385	1392.82
	1421.4547	1484.6303	1491.2168	1479.1072	1478.55
	1488.2796	1561.2324	1574.4053	1553.5967	1543.67
	1537.0017	1603.9934	1621.2845	1575.7984	1566.89
	3204.4619	3287.3616	3305.0792	3301.4586	3314.79
	3207.9375	3288.795	3310.9722	3305.9235	3327.65
3225.1549	3310.6217	3340.254	3324.1007	3345.24	
3537.1001	3654.3355	3680.7093	3632.2637	3636.34	
Zn⁺²Im	137.4516	113.0222	126.7848	116.5451	122.6
	202.6901	205.7757	196.4812	202.5933	199.33
	324.4337	343.4863	347.1748	347.8672	350.08
	574.9537	581.4278	623.8626	573.0083	600.92
	609.0926	626.3846	635.8827	601.7992	623.83
	706.022	722.8258	765.0427	715.016	735
	765.7556	751.7094	770.9729	738.882	759.67
	800.8158	862.9458	898.8832	797.2633	816.34
	872.8644	894.9447	925.5143	824.7684	853.01
	877.7578	915.329	928.7759	911.5714	903.78
	921.1932	963.5334	978.2126	955.4194	949.09
	1051.9544	1099.6723	1104.5681	1106.1816	1095.19
	1100.6148	1138.2196	1132.0633	1138.162	1128.72
	1106.0537	1151.3794	1159.7917	1153.4907	1145.12
	1189.8322	1237.9412	1245.6903	1232.9364	1220.74
	1242.888	1298.778	1309.665	1282.0925	1268.74
	1282.4408	1342.9628	1353.4492	1351.9604	1342.17
	1419.7155	1486.1408	1495.4853	1465.1248	1456.39
	1465.981	1543.405	1564.4095	1537.0598	1521.29
	1551.7253	1626.2583	1646.0858	1597.4214	1585.29
3181.3742	3273.9714	3294.6259	3290.0531	3291.53	
3196.9727	3276.9916	3296.3089	3293.2178	3294.94	
3208.4918	3294.3254	3315.1817	3308.2234	3310.36	
3460.4084	3576.9557	3600.9424	3555.5947	3538.42	