Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Dynamic and Static Behavior of Hydrogen Bonds of the X–H---π Type (X = F, Cl, Br, I, RO and RR'N; R, R' = H or Me) in Benzene π-System, Elucidated by QTAIM Dual Functional Analysis

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Table S1 Structural parameters for X–H---π(C_6H_6) optimized at the MP2 level with BSS-F

Species (symmetry)	R_{SL} (Å)	r_{BP1} (Å)	r_{BP1} (Å)	r_{BP} (Å)	type
F–H---π(C_6H_6) (C_s)	2.3215	0.8561	1.4998	2.3559	I_{Bzn}
Cl–H---π(C_6H_6) (C_s)	2.6867	1.0266	1.6875	2.7141	I_{Bzn}
Br–H---π(C_6H_6) (C_{6v})	2.7062	1.0451	1.6850	2.7301	I_{Bzn}
I–H---π(C_6H_6) (C_s)	2.5780	0.9943	1.6038	2.5981	I_{Bzn}
HO–H---π(C_6H_6) (C_s)	2.4862	0.9491	1.5640	2.5131	Ia_{Bzn}
MeO–H---π(C_6H_6) (C_s)	2.4312	0.9339	1.5244	2.4583	II_{Bzn}
H_2N–H---π(C_6H_6) (C_s)	2.6999	1.0445	1.6853	2.7298	Ia_{Bzn}
MeHN–H---π(C_6H_6) (C_1)	2.6380	1.0123	2.1875	3.1998	Iaa_{Bzn}
Me_2N–H---π(C_6H_6) (C_1)	2.5744	0.9820	2.1708	3.1528	Iaa_{Bzn}

Optimized structures given by Cartesian coordinates

Structures were optimized employing the Gaussian 09 program.[S1] Several types of basis set systems (BSSs: BSS-A, BSS-B, BSS-C, BSS-D, BSS-E and BSS-F) were examined for the evaluation. Table 1 summarizes the BSSs. The basis set for I of the 6-311G* type[S2] was obtained from EMSL Basis Set Exchange Library.[S3,S4] Higher basis set for I of the (7433211/743111/7411/2 + 1s1p1d1f) type was from Sapporo Basis Set Factory.[S5] The diffusion functions of the *sp* parts for I in (7433211/743111/7411/2 + *1s1p*1d1f)[S6] were diverted as those of the *sp* type for the 6-311G* basis set of I, since the diffusion functions could not be found for 6-311G* of I. The Møller-Plesset second order energy correlation (MP2) level is applied to the calculations.[S7] The optimized structures were confirmed by the frequency analysis. The abbreviated notation of MP2/BSS-X (X = A, B, C, D, E and F) will also be used to describe the calculation methods employing BSS-X at the MP2 level, if suitable.

Table S2 Basis set systems employed for the calculations

Method	C, H	F, Cl, Br	I
BSS-A	6-311G(d, p)	6-311G(d)	(5211111111/411111111/31111)[a]
BSS-B	6-311G(d, p)	6-311+G(d)	(5211111111/411111111/31111 + 1s1p)[b]
BSS-C	6-311G(d, p)	6-311G(3d)	(7433211/743111/7411/2 + 1s1p1d1f)[c]
BSS-D	6-311G(d, p)	6-311G(3df)	(7433211/743111/7411/2 + 1s1p1d1f)[c]
BSS-E	6-311G(d, p)	6-311+G(3df)	(7433211/743111/7411/2 + 1s1p1d1f)[c]
BSS-F	6-311++G(d, p)	6-311+G(3df)	(7433211/743111/7411/2 + 1s1p1d1f)[c]

[a] The basis set of the 6-311G* type for I was obtained through EMSL Basis Set Exchange Library.[S3,S4] [b] Diffusion functions of the 1s1p parts in (7433211/743111/7411/2 + 1s1p1d1f)[S5] being employed as the diffusion functions of the 1s1p type for (5211111111/411111111/31111). [c] The higher basis set of the (7433211/743111/7411/2 + 1s1p1d1f) type for I was obtained from Sapporo Basis Set Factory.[S5]

References

S1 *Gaussian 09 (Revision D.01)*, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian, Inc.: Wallingford CT, 2009.

S2 For the 6-311G(3d) basis sets, see: (a) R. C. Binning Jr. and L. A. Curtiss, *J. Comput. Chem.*, 1990, **11**, 1206-1216; (b) L. A. Curtiss, M. P. McGrath, J.-P. Blaudeau, N. E. Davis, R. C.

Binning Jr. and L. Radom, *J. Chem. Phys.*, 1995, **103**, 6104-6113; (c) M. P. McGrath and L. Radom, *J. Chem. Phys.*, 1991, **94**, 511-516. For the diffuse functions (+ and ++), see: T. Clark, J. Chandrasekhar, G. W. Spitznagel and P. v. R. Schleyer, *J. Comput. Chem.*, 1983, **4**, 294-301.

S3 D. Feller, *J. Comp. Chem.*, 1996, **17**, 1571-1586.

S4 K. L. Schuchardt, B. T. Didier, T. Elsethagen, L. Sun, V. Gurumoorthi, J. Chase, J. Li and T. L. Windus, *J. Chem. Inf. Model.*, 2007, **47**, 1045-1052.

S5 T. Noro, M. Sekiya and T. Koga, *Theoret. Chem. Acc.*, 2012, **131**, 1124.

S6 (a) For inner and valence shells: T. Koga, S. Yamamoto, T. Shimazaki and H. Tatewaki, *Theor. Chem. Acc.*, 2002, **108**, 41-45; (b) For valence correlated set: M. Sekiya, T. Noro, Y. Osanai and T. Koga, *Theor. Chem. Acc.*, 2001, **106**, 297-300.

S7 C. Møller and M. S. Plesset, *Phys. Rev.*, 1934, **46**, 618-622; J. Gauss, *J. Chem. Phys.*, 1993, **99**, 3629-3643; J. Gauss, Ber. Bunsen-Ges. *Phys. Chem.*, 1995, **99**, 1001-1008.

MP2/BSS-A C, H, F: 6-311G(d,p)
Adduct F–H---π(C_6H_6)
Symmetry C_s
Energy E = -331.8536911 au
Standard orientation

6	0	-0.572264	1.148568	0.700839
6	0	-0.572264	1.148568	-0.700839
6	0	-0.569996	-0.064980	1.400451
6	0	-0.569996	-0.064980	-1.400451
6	0	-0.569996	-1.276241	0.699692
6	0	-0.569996	-1.276241	-0.699692
1	0	-0.567869	2.089374	1.243568
1	0	-0.567869	2.089374	-1.243568
1	0	-0.561650	-0.064535	2.486289
1	0	-0.561650	-0.064535	-2.486289
1	0	-0.561092	-2.216595	1.242598
1	0	-0.561092	-2.216595	-1.242598
1	0	1.584590	0.436348	0.000000
9	0	2.482633	0.250998	0.000000

MP2/BSS-A C, H, Cl: 6-311G(d,p)
Adduct Cl–H---π(C_6H_6)
Symmetry C_1
Energy E = -691.8288301 au
Standard orientation

6	0	-0.980686	-1.038018	0.967214
6	0	-0.941018	0.295455	1.394261
6	0	-1.106749	-1.332841	-0.395757
6	0	-1.027863	1.333209	0.457707
6	0	-1.193380	-0.295204	-1.331225
6	0	-1.153838	1.037396	-0.904805
1	0	-0.911816	-1.842904	1.693422
1	0	-0.842293	0.524508	2.451558
1	0	-1.134500	-2.366879	-0.726970
1	0	-0.994966	2.367214	0.788756
1	0	-1.287554	-0.524278	-2.388719
1	0	-1.217782	1.842335	-1.631195

1	0	1.300770	0.000089	0.139003
17	0	2.559373	-0.000004	-0.085307

MP2/BSS-A C, H, Br: 6-311G(d,p)
Adduct Br–H---π(C_6H_6)
Symmetry C_1
Energy E = -2804.6746855 au
Standard orientation

6	0	-1.726673	1.190654	-0.732944
6	0	-1.734373	-0.042475	-1.395728
6	0	-1.710424	1.233256	0.666390
6	0	-1.725835	-1.233136	-0.659377
6	0	-1.701870	0.042487	1.402957
6	0	-1.709585	-1.190776	0.739971
1	0	-1.730391	2.114447	-1.304318
1	0	-1.743968	-0.075433	-2.481395
1	0	-1.701750	2.189998	1.180683
1	0	-1.728914	-2.189887	-1.173668
1	0	-1.686689	0.075444	2.488610
1	0	-1.700273	-2.114560	1.311345
1	0	0.628138	0.000058	0.044873
35	0	2.043326	-0.000004	-0.005535

MP2/BSS-A C, H: 6-311G(d,p), I: 5211111111/411111111/31111
Adduct I–H---π(C_6H_6)
Symmetry C_s
Energy E = -7149.1980749 au
Standard orientation

6	0	-2.220508	1.200812	0.700104
6	0	-2.220508	1.200812	-0.700104
6	0	-2.220508	-0.011771	1.399991
6	0	-2.220508	-0.011771	-1.399991
6	0	-2.220391	-1.223987	0.699896
6	0	-2.220391	-1.223987	-0.699896
1	0	-2.219299	2.141646	1.243253
1	0	-2.219299	2.141646	-1.243253
1	0	-2.218754	-0.011723	2.486298
1	0	-2.218754	-0.011723	-2.486298
1	0	-2.218184	-2.164717	1.243035
1	0	-2.218184	-2.164717	-1.243035
1	0	0.151585	0.113527	0.000000
53	0	1.756562	0.007083	0.000000

MP2/BSS-B C, H: 6-311G(d,p), F: 6-311+G(d)
Adduct F–H---π(C_6H_6)
Symmetry C_s
Energy E = -331.8654946 au
Standard orientation

6	0	-0.592254	1.083374	0.700969
6	0	-0.592254	1.083374	-0.700969
6	0	-0.591076	-0.130401	1.400746
6	0	-0.591076	-0.130401	-1.400746

6	0	-0.591076	-1.341942	0.699887
6	0	-0.591076	-1.341942	-0.699887
1	0	-0.590982	2.024403	1.243640
1	0	-0.590982	2.024403	-1.243640
1	0	-0.587528	-0.129796	2.486792
1	0	-0.587528	-0.129796	-2.486792
1	0	-0.586871	-2.282445	1.242948
1	0	-0.586871	-2.282445	-1.242948
1	0	1.653054	0.519876	0.000000
9	0	2.574510	0.547047	0.000000

MP2/BSS-B C, H: 6-311G(d,p), Cl: 6-311+G(d)
Adduct Cl–H---π(C_6H_6)
Symmetry C_1
Energy E = -691.830449 au
Standard orientation

6	0	-1.014100	0.245508	1.389357
6	0	-1.044538	1.316754	0.487760
6	0	-1.030202	-1.071342	0.912741
6	0	-1.090935	1.071071	-0.889980
6	0	-1.076636	-1.316578	-0.465164
6	0	-1.106966	-0.245414	-1.366294
1	0	-0.976011	0.435898	2.458119
1	0	-1.029514	2.338051	0.857348
1	0	-1.004290	-1.902232	1.611924
1	0	-1.111300	1.901991	-1.589217
1	0	-1.086081	-2.337894	-0.834788
1	0	-1.139572	-0.435814	-2.435140
1	0	1.270800	0.000004	0.063947
17	0	2.544484	0.000000	-0.031924

MP2/BSS-B C, H: 6-311G(d,p), Br: 6-311+G(d)
Adduct Br–H---π(C_6H_6)
Symmetry C_s
Energy E = -2804.8285695 au
Standard orientation

6	0	-1.708536	1.189073	0.700229
6	0	-1.708536	1.189073	-0.700229
6	0	-1.708536	-0.023736	1.400258
6	0	-1.708536	-0.023736	-1.400258
6	0	-1.708470	-1.236203	0.700032
6	0	-1.708470	-1.236203	-0.700032
1	0	-1.706834	2.129847	1.243339
1	0	-1.706834	2.129847	-1.243339
1	0	-1.706368	-0.023677	2.486505
1	0	-1.706368	-0.023677	-2.486505
1	0	-1.705861	-2.176881	1.243156
1	0	-1.705861	-2.176881	-1.243156
1	0	0.621310	0.083531	0.000000
35	0	2.032095	0.025951	0.000000

MP2/BSS-B C, H: 6-311G(d,p), I: 5211111111/411111111/31111 + 1s1p

Adduct I–H---π(C_6H_6)
Symmetry C_1
Energy E = -7149.198852 au
Standard orientation

6	0	-2.208281	1.398928	-0.066896
6	0	-2.212834	0.641539	-1.244714
6	0	-2.212147	0.757399	1.177852
6	0	-2.220884	-0.756841	-1.177556
6	0	-2.220226	-0.641035	1.244452
6	0	-2.224500	-1.397910	0.066866
1	0	-2.201980	2.484081	-0.118785
1	0	-2.209457	1.139216	-2.210367
1	0	-2.208314	1.344956	2.091611
1	0	-2.223015	-1.344284	-2.091298
1	0	-2.221902	-1.138601	2.210089
1	0	-2.229091	-2.482923	0.118754
1	0	0.152588	0.153813	-0.000048
53	0	1.753479	-0.003184	0.000000

MP2/BSS-B C, H: 6-311G(d,p), O: 6-311+G(d)
Adduct HO–H---π(C_6H_6)
Symmetry C_s
Energy E = -307.8593517 au
Standard orientation

6	0	-0.623285	-1.260642	0.700133
6	0	-0.623285	-1.260642	-0.700133
6	0	-0.623714	-0.048569	1.400398
6	0	-0.623714	-0.048569	-1.400398
6	0	-0.623714	1.164234	0.700327
6	0	-0.623714	1.164234	-0.700327
1	0	-0.626113	-2.201319	1.243630
1	0	-0.626113	-2.201319	-1.243630
1	0	-0.621430	-0.047824	2.486536
1	0	-0.621430	-0.047824	-2.486536
1	0	-0.620914	2.104992	1.243279
1	0	-0.620914	2.104992	-1.243279
1	0	1.747705	0.395170	0.000000
8	0	2.703549	0.287374	0.000000
1	0	2.809381	-0.666137	0.000000

MP2/BSS-B C, H: 6-311G(d,p), O: 6-311+G(d)
Adduct OH_2---π(C_6H_6)
Symmetry C_2
Energy E = -307.8588854 au
Standard orientation

6	0	0.000000	1.399966	-0.610391
6	0	-1.212805	0.699290	-0.610391
6	0	1.212674	0.700600	-0.609313
6	0	-1.212674	-0.700600	-0.609313
6	0	1.212805	-0.699290	-0.610391
6	0	0.000000	-1.399966	-0.610391
1	0	-0.000012	2.486457	-0.616319
1	0	-2.154038	1.242008	-0.616329

1	0	2.153105	1.243917	-0.608874
1	0	-2.153105	-1.243917	-0.608874
1	0	2.154038	-1.242008	-0.616329
1	0	0.000012	-2.486457	-0.616319
1	0	0.372593	-0.644214	2.078014
8	0	0.000000	0.000000	2.686020
1	0	-0.372593	0.644214	2.078014
8	0	2.703549	0.287374	0.000000
1	0	2.809381	-0.666137	0.000000

MP2/BSS-B C, H: 6-311G(d,p), O: 6-311+G(d)
Adduct MeO–H---π(C_6H_6)
Symmetry C_1
Energy E = -347.0310345 au
Standard orientation

6	0	-0.686813	1.296784	-0.700298
6	0	-1.010020	0.128359	-1.400317
6	0	-0.686779	1.296886	0.700116
6	0	-1.335610	-1.040329	-0.700200
6	0	-1.009951	0.128562	1.400320
6	0	-1.335575	-1.040227	0.700389
1	0	-0.437149	2.203849	-1.243667
1	0	-1.006933	0.126654	-2.486514
1	0	-0.437088	2.204030	1.243341
1	0	-1.583070	-1.947923	-1.243144
1	0	-1.006811	0.127015	2.486517
1	0	-1.583008	-1.947743	1.243477
1	0	1.104624	-0.812004	-0.000005
8	0	2.048935	-0.991469	-0.000007
6	0	2.707258	0.264238	-0.000002
1	0	3.779029	0.061280	-0.000004
1	0	2.461935	0.855481	-0.890598
1	0	2.461937	0.855472	0.890601

MP2/BSS-B C, H: 6-311G(d,p), N: 6-311+G(d)
Adduct H_2N–H---π(C_6H_6)
Symmetry C_s
Energy E = -287.9983609 au
Standard orientation

6	0	-0.659887	-0.658671	1.212129
6	0	-0.659887	0.741311	1.212103
6	0	-0.659532	-1.358756	0.000000
6	0	-0.660463	1.441423	0.000000
6	0	-0.659887	-0.658671	-1.212129
6	0	-0.659887	0.741311	-1.212103
1	0	-0.657563	-1.202444	2.152583
1	0	-0.661474	1.284386	2.153139
1	0	-0.652632	-2.444829	0.000000
1	0	-0.661496	2.527874	0.000000
1	0	-0.657563	-1.202444	-2.152583
1	0	-0.661474	1.284386	-2.153139
1	0	1.794897	-0.234883	0.000000
7	0	2.808187	-0.280221	0.000000

1	0	3.128627	0.230911	-0.814787
1	0	3.128627	0.230911	0.814787

MP2/BSS-B C, H: 6-311G(d,p), N: 6-311+G(d)
Adduct MeHN–H---π(C_6H_6)
Symmetry C_1
Energy E = -327.1779792 au
Standard orientation

6	0	1.533133	-1.110003	0.359395
6	0	1.469719	-0.718110	-0.983287
6	0	1.108667	-0.233056	1.365043
6	0	0.982877	0.550781	-1.320286
6	0	0.621843	1.035295	1.027589
6	0	0.560176	1.427825	-0.314834
1	0	1.909608	-2.094802	0.621286
1	0	1.799859	-1.398365	-1.763550
1	0	1.152637	-0.539068	2.406329
1	0	0.935167	0.855134	-2.362235
1	0	0.293157	1.715690	1.808264
1	0	0.183864	2.413077	-0.575880
1	0	-1.105282	-0.900620	0.052417
7	0	-2.106859	-1.051641	0.001367
1	0	-2.280896	-1.553802	-0.862683
6	0	-2.801114	0.236667	-0.020611
1	0	-3.878850	0.064062	-0.080731
1	0	-2.601012	0.761825	0.916432
1	0	-2.512038	0.901956	-0.847276

MP2/BSS-B C, H: 6-311G(d,p), N: 6-311+G(d)
Adduct Me_2N–H---π(C_6H_6)
Symmetry C_1
Energy E = -366.3646689 au
Standard orientation

6	0	1.021577	-0.699911	1.278174
6	0	1.021586	0.699760	1.278257
6	0	1.335733	-1.400042	0.106823
6	0	1.335734	1.400028	0.106985
6	0	1.649057	-0.700330	-1.064690
6	0	1.649064	0.700451	-1.064607
1	0	0.779851	-1.243485	2.187405
1	0	0.779856	1.243230	2.187551
1	0	1.336430	-2.486594	0.107055
1	0	1.336449	2.486579	0.107349
1	0	1.890642	-1.243068	-1.974241
1	0	1.890633	1.243295	-1.974100
1	0	-0.835196	0.000000	-0.704815
7	0	-1.848958	0.000006	-0.683570
6	0	-2.306716	1.201881	-0.001336
1	0	-3.398222	1.257573	-0.067987
1	0	-1.887955	2.085223	-0.490183
1	0	-2.029679	1.228459	1.067681
6	0	-2.306733	-1.201853	-0.001321
1	0	-3.398240	-1.257531	-0.067970

1	0	-1.887986	-2.085208	-0.490157
1	0	-2.029696	-1.228422	1.067696

MP2/BSS-D C, H: 6-311G(d,p), F: 6-311G(3df)
Adduct F–H---π(C_6H_6)
Symmetry C_1
Energy E = -331.9027395 au
Standard orientation

6	0	-0.006534	-0.002212	1.452682
6	0	-0.273699	1.212422	0.806332
6	0	-0.275166	-1.214629	0.802792
6	0	-0.809603	1.213325	-0.486937
6	0	-0.811075	-1.211112	-0.490465
6	0	-1.079826	0.002208	-1.133547
1	0	0.415223	-0.003924	2.453631
1	0	-0.055742	2.151661	1.305977
1	0	-0.058341	-2.155582	1.299695
1	0	-1.008466	2.154615	-0.990373
1	0	-1.011080	-2.150690	-0.996642
1	0	-1.487585	0.003923	-2.139949
1	0	1.592055	-0.000010	-0.194910
9	0	2.349927	-0.000002	-0.715840

MP2/BSS-D C, H: 6-311G(d,p), Cl: 6-311G(3df)
Adduct Cl–H---π(C_6H_6)
Symmetry C_1
Energy E = -691.8824335 au
Standard orientation

6	0	-0.918585	-0.803599	1.177605
6	0	-0.905076	0.592393	1.298869
6	0	-1.057896	-1.395058	-0.084242
6	0	-1.031231	1.395235	0.157997
6	0	-1.183224	-0.591676	-1.223486
6	0	-1.169861	0.802715	-1.102507
1	0	-0.819048	-1.426327	2.062157
1	0	-0.795541	1.051405	2.277390
1	0	-1.064570	-2.477094	-0.178372
1	0	-1.017346	2.477250	0.251874
1	0	-1.286192	-1.050768	-2.202383
1	0	-1.262653	1.425545	-1.987425
1	0	1.265528	0.000191	0.229522
17	0	2.504415	-0.000016	-0.105775

MP2/BSS-D C, H: 6-311G(d,p), Br: 6-311G(3df)
Adduct Br–H---π(C_6H_6)
Symmetry C_1
Energy E = -2804.8964197 au
Standard orientation

6	0	-1.752596	0.755424	-1.160940
6	0	-1.755974	-0.642855	-1.225798
6	0	-1.688070	1.398877	0.080605
6	0	-1.694827	-1.398810	-0.049216

6	0	-1.626359	0.643417	1.258310
6	0	-1.629794	-0.756052	1.193341
1	0	-1.796198	1.341596	-2.074318
1	0	-1.802137	-1.141685	-2.189537
1	0	-1.682157	2.483922	0.131010
1	0	-1.694118	-2.483864	-0.099550
1	0	-1.573573	1.142169	2.221974
1	0	-1.579561	-1.342137	2.106658
1	0	0.611610	0.000018	0.213443
35	0	2.011482	-0.000001	-0.025357

MP2/BSS-D C, H: 6-311G(d,p), I: 7433211/743111/7411/2 + 1s1p1d1f
Adduct I–H---π(C_6H_6)
Symmetry C_1
Energy E = -7150.2553657 au
Standard orientation

6	0	-2.151882	-0.719878	-1.194661
6	0	-2.165681	-1.388676	0.036625
6	0	-2.120502	0.679568	-1.230531
6	0	-2.150507	-0.656477	1.231239
6	0	-2.103332	1.410353	-0.036577
6	0	-2.119011	0.742884	1.193922
1	0	-2.163277	-1.287637	-2.120941
1	0	-2.189440	-2.474645	0.065004
1	0	-2.106231	1.197842	-2.185204
1	0	-2.160730	-1.175074	2.185917
1	0	-2.075052	2.495976	-0.064955
1	0	-2.103539	1.310319	2.120196
1	0	0.118340	-0.379295	-0.000041
53	0	1.689536	-0.001776	-0.000001

MP2/BSS-F C, H: 6-311++G(d,p), F: 6-311+G(3df)
Adduct F–H---π(C_6H_6)
Symmetry C_s
Energy E = -331.9201056 au
Standard orientation

6	0	-0.588536	1.111726	0.701399
6	0	-0.588536	1.111726	-0.701399
6	0	-0.587877	-0.102877	1.401678
6	0	-0.587877	-0.102877	-1.401678
6	0	-0.587877	-1.315490	0.700407
6	0	-0.587877	-1.315490	-0.700407
1	0	-0.587365	2.052905	1.244360
1	0	-0.587365	2.052905	-1.244360
1	0	-0.583858	-0.102345	2.488071
1	0	-0.583858	-0.102345	-2.488071
1	0	-0.582929	-2.256262	1.243677
1	0	-0.582929	-2.256262	-1.243677
1	0	1.635472	0.445989	0.000000
9	0	2.560479	0.427234	0.000000

MP2/BSS-F C, H: 6-311++G(d,p), Cl: 6-311+G(3df)

Adduct Cl–H---π(C_6H_6)
Symmetry C_s
Energy E = -691.89065 au
Standard orientation

6	0	-1.051144	-1.401365	0.000000
6	0	-1.051130	-0.700659	1.213657
6	0	-1.051130	-0.700659	-1.213657
6	0	-1.051130	0.700751	1.213656
6	0	-1.051130	0.700751	-1.213656
6	0	-1.051145	1.401456	0.000000
1	0	-1.048088	-2.487916	0.000000
1	0	-1.048079	-1.243934	2.154638
1	0	-1.048079	-1.243934	-2.154638
1	0	-1.048078	1.244025	2.154638
1	0	-1.048078	1.244025	-2.154638
1	0	-1.048086	2.488007	0.000000
1	0	1.241240	-0.000195	0.000000
17	0	2.522830	-0.000101	0.000000

MP2/BSS-F C, H: 6-311++G(d,p), Br: 6-311+G(3df)
Adduct Br–H---π(C_6H_6)
Symmetry C_{6v}
Energy E = -2804.9037959 au
Standard orientation

6	0	0.000000	1.401287	-1.705664
6	0	1.213550	0.700644	-1.705664
6	0	-1.213550	0.700644	-1.705664
6	0	1.213550	-0.700644	-1.705664
6	0	-1.213550	-0.700644	-1.705664
6	0	0.000000	-1.401287	-1.705664
1	0	0.000000	2.487902	-1.702107
1	0	2.154586	1.243951	-1.702107
1	0	-2.154586	1.243951	-1.702107
1	0	2.154586	-1.243951	-1.702107
1	0	-2.154586	-1.243951	-1.702107
1	0	0.000000	-2.487902	-1.702107
1	0	0.000000	0.000000	0.609459
35	0	0.000000	0.000000	2.028774

MP2/BSS-F C, H: 6-311++G(d,p), I: 7433211/743111/7411/2 + 1s1p1d1f
Adduct I–H---π(C_6H_6)
Symmetry C_s
Energy E = -7150.2615906 au
Standard orientation

6	0	2.167621	1.411205	0.000000
6	0	2.167981	0.710192	1.213835
6	0	2.167981	0.710192	-1.213835
6	0	2.167981	-0.691037	1.213411
6	0	2.167981	-0.691037	-1.213411
6	0	2.167806	-1.391307	0.000000
1	0	2.165856	2.498011	0.000000
1	0	2.165856	1.253685	2.154937
1	0	2.165856	1.253685	-2.154937

1	0	2.165335	-1.234374	2.154541
1	0	2.165335	-1.234374	-2.154541
1	0	2.164798	-2.478005	0.000000
1	0	-0.116252	0.215346	0.000000
53	0	-1.715488	-0.011759	0.000000

MP2/BSS-F C, H: 6-311++G(d,p), O: 6-311+G(3df)
Adduct HO–H---π(C_6H_6)
Symmetry C_s
Energy E = -307.906387 au
Standard orientation

6	0	-0.621401	-1.260462	0.700630
6	0	-0.621401	-1.260462	-0.700630
6	0	-0.621401	-0.047508	1.401382
6	0	-0.621401	-0.047508	-1.401382
6	0	-0.621751	1.166072	0.700808
6	0	-0.621751	1.166072	-0.700808
1	0	-0.623998	-2.201468	1.244318
1	0	-0.623998	-2.201468	-1.244318
1	0	-0.618592	-0.046843	2.487893
1	0	-0.618592	-0.046843	-2.487893
1	0	-0.618596	2.107113	1.243924
1	0	-0.618596	2.107113	-1.243924
1	0	1.727273	0.351651	0.000000
8	0	2.688595	0.286512	0.000000
1	0	2.860984	-0.658572	0.000000

MP2/BSS-F C, H: 6-311++G(d,p), O:6-311+G(3df)
Adduct OH_2---π(C_6H_6)
Symmetry C_2
Energy E = -307.9057564 au
Standard orientation

6	0	-1.212893	0.700779	-0.614927
6	0	-1.212893	-0.700777	-0.614927
6	0	0.000000	1.401519	-0.614481
6	0	0.000000	-1.401519	-0.614481
6	0	1.212893	0.700777	-0.614927
6	0	1.212893	-0.700779	-0.614927
1	0	-2.154038	1.244433	-0.621935
1	0	-2.154039	-1.244431	-0.621944
1	0	0.000000	2.488040	-0.614444
1	0	0.000000	-2.488040	-0.614444
1	0	2.154039	1.244431	-0.621944
1	0	2.154038	-1.244433	-0.621935
1	0	0.752922	0.000348	2.105478
8	0	0.000000	0.000000	2.704714
1	0	-0.752922	-0.000348	2.105478

MP2/BSS-F C, H: 6-311++G(d,p), O: 6-311+G(3df)
Adduct MeO–H---π(C_6H_6)
Symmetry C_s
Energy E = -347.0806409 au

Standard orientation

6	0	1.003580	1.057064	0.700671
6	0	1.003580	-0.155905	1.401385
6	0	1.003580	1.057064	-0.700671
6	0	1.003430	-1.369945	0.700761
6	0	1.003580	-0.155905	-1.401385
6	0	1.003430	-1.369945	-0.700761
1	0	1.005565	1.998304	1.244024
1	0	0.999243	-0.156513	2.487950
1	0	1.005565	1.998304	-1.244024
1	0	0.998251	-2.310922	1.243930
1	0	0.999243	-0.156513	-2.487950
1	0	0.998251	-2.310922	-1.243930
1	0	-1.252682	-0.464062	0.000000
8	0	-2.211944	-0.381300	0.000000
6	0	-2.540676	1.000102	0.000000
1	0	-3.630587	1.061500	0.000000
1	0	-2.155166	1.508021	0.892861
1	0	-2.155166	1.508021	-0.892861

MP2/BSS-F C, H: 6-311++G(d,p), N: 6-311+G(3df)
Adduct H_2N–H---π(C_6H_6)
Symmetry C_s
Energy E = -288.0364155 au
Standard orientation

6	0	-0.654897	-0.664448	1.212943
6	0	-0.654897	0.736581	1.212974
6	0	-0.654910	-1.365044	0.000000
6	0	-0.655067	1.437204	0.000000
6	0	-0.654897	-0.664448	-1.212943
6	0	-0.654897	0.736581	-1.212974
1	0	-0.652936	-1.208291	2.153764
1	0	-0.656646	1.279840	2.154304
1	0	-0.648313	-2.451476	0.000000
1	0	-0.656194	2.523987	0.000000
1	0	-0.652936	-1.208291	-2.153764
1	0	-0.656646	1.279840	-2.154304
1	0	1.772689	-0.183485	0.000000
7	0	2.785036	-0.260613	0.000000
1	0	3.116563	0.246802	-0.813514
1	0	3.116563	0.246802	0.813514

MP2/BSS-F C, H: 6-311++G(d,p), N: 6-311+G(3df)
Adduct MeHN–H---π(C_6H_6)
Symmetry C_1
Energy E = -327.2181585 au
Standard orientation

6	0	1.498542	-1.008897	0.630123
6	0	1.518873	-0.896630	-0.766270
6	0	1.019703	0.051609	1.410890
6	0	1.061295	0.276150	-1.381916
6	0	0.562727	1.223835	0.795021
6	0	0.584086	1.336478	-0.601246

1	0	1.851042	-1.919009	1.107863
1	0	1.891184	-1.718829	-1.371765
1	0	0.999185	-0.037403	2.493661
1	0	1.078540	0.363483	-2.465145
1	0	0.191881	2.046496	1.400810
1	0	0.230308	2.246762	-1.078210
1	0	-1.079677	-0.874982	0.088076
7	0	-2.077588	-1.050420	0.039180
1	0	-2.230783	-1.584350	-0.809632
6	0	-2.805276	0.215527	-0.019989
1	0	-3.877987	0.009955	-0.083523
1	0	-2.626142	0.768014	0.906809
1	0	-2.524136	0.864376	-0.862888

MP2/BSS-F C, H: 6-311++G(d,p), N: 6-311+G(3df)
Adduct Me_2N–H---π(C_6H_6)
Symmetry C_1
Energy E = -366.407443 au
Standard orientation

6	0	-1.022056	0.704142	1.277439
6	0	-1.020947	-0.696417	1.281751
6	0	-1.328159	1.400955	0.100831
6	0	-1.325963	-1.400939	0.109461
6	0	-1.632619	0.697074	-1.071717
6	0	-1.631527	-0.704773	-1.067395
1	0	-0.786223	1.250838	2.186738
1	0	-0.784272	-1.237131	2.194404
1	0	-1.329177	2.487873	0.097727
1	0	-1.325255	-2.487857	0.113051
1	0	-1.867069	1.237133	-1.985126
1	0	-1.865144	-1.250815	-1.977456
1	0	0.813927	-0.000081	-0.676919
7	0	1.827785	-0.000079	-0.669112
6	0	2.295430	-1.203042	-0.002694
1	0	3.384847	-1.269994	-0.102067
1	0	1.852838	-2.082105	-0.480030
1	0	2.047937	-1.224847	1.074416
6	0	2.295424	1.203066	-0.003017
1	0	3.384841	1.269996	-0.102405
1	0	1.852828	2.082001	-0.480586
1	0	2.047928	1.225150	1.074087