Coriolis Interactions in Benzene-Water and Related Molecular Complexes

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Supplementary Material :

Table S1 : Vibrational frequencies from *ab initio* calculations for benzene-water and rare gas-benzene-water complexes at MP2/6-311++g(d,p) level, including BSSE CP (basis-set superposition error counterpoise) corrections

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Table S1: Vibrational frequencies from *ab initio* calculations for benzene-water and rare gas-benzene-water complexes at MP2/6-311++g(d,p) level, including BSSE CP (basis-set superposition error counterpoise) corrections

	$C_6H_6-H_2O$	$^{13}CC_5H_6-H_2O$	$C_6H_6-H_2^{18}O$	$Ne-C_6H_6-H_2O$	$Ar-C_6H_6-H_2O$	$Kr-C_6H_6-H_2O$
1	12.79	12.81	12.70	9.64	10.92	11.27
2	28.91	28.78	28.41	10.66	15.38	17.50
3	42.66	42.64	42.45	17.45	21.96	25.88
4	77.47	77.14	74.96	20.27	28.60	33.30
5	107.04	107.04	106.23	31.11	34.88	40.12
6	228.69	228.70	227.76	44.52	46.50	49.98
7	388.18	385.11	388.19	78.10	78.61	79.27
8	388.98	388.24	388.98	107.11	106.83	105.71
9	609.34	603.06	609.34	230.74	230.33	229.88
10	609.54	608.18	609.54	388.43	387.25	386.69
11	682.29	681.94	682.29	389.22	388.13	387.56
12	742.74	739.52	742.74	609.31	609.16	609.02
13	856.10	855.21	856.09	609.51	609.37	609.24
14	857.56	856.17	857.56	682.73	682.09	681.89
15	959.94	956.63	959.94	742.91	741.57	740.67
16	960.72	960.70	960.72	856.19	855.30	855.17
17	1007.57	997.19	1007.57	857.92	857.37	857.37
18	1014.36	1011.74	1014.36	960.00	958.36	958.29
19	1059.91	1056.66	1059.91	960.70	958.72	958.86
20	1060.43	1058.13	1060.43	1007.69	1007.66	1007.63
21	1079.41	1077.04	1079.41	1014.13	1013.94	1013.96
22	1173.80	1173.58	1173.80	1059.98	1059.92	1059.88
23	1199.71	1197.69	1199.71	1060.51	1060.46	1060.42
24	1200.28	1200.25	1200.28	1078.81	1077.24	1076.17
25	1374.58	1372.20	1374.58	1173.86	1173.78	1173.77
26	1447.13	1436.28	1447.13	1199.74	1199.64	1199.59
27	1505.39	1498.75	1505.39	1200.34	1200.24	1200.18
28	1505.76	1502.44	1505.76	1374.53	1374.38	1374.25
29	1634.11	1620.42	1634.09	1447.53	1448.38	1449.78
30	1634.89	1631.85	1634.83	1505.49	1505.39	1505.28
31	1644.33	1644.31	1637.76	1505.86	1505.76	1505.66
32	3198.11	3195.48	3198.11	1634.25	1634.06	1633.83
33	3207.66	3203.97	3207.66	1635.04	1634.85	1634.60
34	3209.19	3209.15	3209.19	1644.96	1644.80	1644.71
35	3223.53	3220.78	3223.53	3197.80	3197.83	3197.71
36	3225.07	3225.00	3225.07	3207.33	3207.34	3207.18
37	3233.65	3232.40	3233.65	3208.95	3208.96	3208.82
38	3868.32	3868.32	3859.58	3223.24	3223.23	3223.05
39	3980.51	3980.51	3964.87	3224.80	3224.80	3224.64
40				3233.38	3233.36	3233.17
41				3868.26	3868.25	3868.32
42				3980.04	3980.04	3980.05

Table S2: *Ab initio* coordinates of the equilibrium structure of $C_6H_6 - H_2O$ complex at MP2/6-311++g(d,p) level, including BSSE CP corrections

Atom	X / Å	Y / Å	Z / Å
C	0.371473	0.950480	-1.084740
C	0.577476	-0.407225	-1.363890
C	0.829698	-1.305537	-0.319368
C	0.941632	-0.836183	0.995915
C	0.734773	0.520684	1.275504
C	0.482993	1.419679	0.231149
H	0.495551	-0.770030	-2.384734
H	0.985673	-2.358969	-0.535599
H	1.147162	-1.531905	1.805139
H	0.815291	0.883828	2.296388
H	0.329060	2.473426	0.446888
H	0.173658	1.647319	-1.894802
H	-2.575221	-0.932310	0.713372
H	-2.040903	0.182337	-0.135352
O	-2.869818	-0.205635	0.160159

Table S3: *Ab initio* coordinates of the equilibrium structure of $^{13}CC_5H_6 - H_2O$ complex at MP2/6-311++g(d,p) level, including BSSE CP corrections

Atom	X / Å	Y / Å	Z / Å
^{13}C	-0.371473	0.950480	1.084740
C	-0.577476	-0.407225	1.363890
C	-0.829698	-1.305537	0.319368
C	-0.941632	-0.836183	-0.995915
C	-0.734773	0.520684	-1.275504
C	-0.482993	1.419679	-0.231149
H	-0.495552	-0.770030	2.384734
H	-0.985673	-2.358969	0.535599
H	-1.147162	-1.531905	-1.805139
H	-0.815291	0.883828	-2.296389
H	-0.329060	2.473426	-0.446888
H	-0.173658	1.647319	1.894802
H	2.575221	-0.932310	-0.713372
H	2.040903	0.182337	0.135352
O	2.869818	-0.205635	-0.160159

Table S4: *Ab initio* coordinates of the equilibrium structure of $C_6H_6 - H_2^{18}O$ complex at MP2/6-311++g(d,p) level, including BSSE CP corrections

Atom	X / Å	Y / Å	Z / Å
C	-0.371473	0.950480	1.084740
C	-0.577476	-0.407225	1.363890
C	-0.829698	-1.305537	0.319368
C	-0.941632	-0.836183	-0.995915
C	-0.734773	0.520684	-1.275504
C	-0.482993	1.419679	-0.231149
H	-0.495552	-0.770030	2.384734
H	-0.985673	-2.358969	0.535599
H	-1.147162	-1.531905	-1.805139
H	-0.815291	0.883828	-2.296389
H	-0.329060	2.473426	-0.446888
H	-0.173658	1.647319	1.894802
H	2.575221	-0.932310	-0.713372
H	2.040903	0.182337	0.135352
^{18}O	2.869818	-0.205635	-0.160159

Table S5: *Ab initio* coordinates of the equilibrium structure of $Ne - C_6H_6 - H_2O$ complex at MP2/6-311++g(d,p) level, including BSSE CP corrections

Atom	X / Å	Y / Å	Z / Å
C	-0.128491	-1.324785	0.218031
C	-0.076518	-0.446912	1.309030
C	-0.043449	0.936446	1.092771
C	0.004820	1.439487	-0.213844
C	-0.048361	0.562416	-1.304710
C	-0.081336	-0.821164	-1.088900
H	-0.109035	-0.837767	2.322318
H	-0.008132	1.617198	1.939000
H	0.040188	2.512728	-0.381555
H	-0.017882	0.952860	-2.318246
H	-0.116239	-1.502104	-1.934930
H	-0.156216	-2.398140	0.385733
H	-3.420935	0.786149	-0.028603
H	-2.697727	-0.526429	0.006705
O	-3.586382	-0.158881	-0.006664
Ne	3.741705	-0.140637	-0.001138

Table S6: *Ab initio* coordinates of the equilibrium structure of $Ar - C_6H_6 - H_2O$ complex at MP2/6-311++g(d,p) level, including BSSE CP corrections

Atom	X / Å	Y / Å	Z / Å
C	-0.540151	-1.315270	0.218834
C	-0.498984	-0.436226	1.309352
C	-0.482749	0.947312	1.092331
C	-0.440484	1.450182	-0.214558
C	-0.482869	0.571926	-1.304943
C	-0.499006	-0.811833	-1.088371
H	-0.526836	-0.826889	2.322853
H	-0.455812	1.628911	1.938186
H	-0.418177	2.523682	-0.382859
H	-0.457049	0.962153	-2.318692
H	-0.525528	-1.493615	-1.934027
H	-0.554813	-2.388790	0.387128
H	-3.858043	0.755259	-0.029269
H	-3.118901	-0.548391	0.006831
O	-4.011967	-0.191704	-0.006822
Ar	3.315353	-0.084180	-0.000636

Table S7: *Ab initio* coordinates of the equilibrium structure of $Kr - C_6H_6 - H_2O$ complex at MP2/6-311++g(d,p) level, including BSSE CP corrections

Atom	X / Å	Y / Å	Z / Å
C	-1.186679	-1.312101	0.204664
C	-1.150380	-0.443305	1.303516
C	-1.143789	0.942332	1.099761
C	-1.105977	1.457974	-0.202279
C	-1.143451	0.589966	-1.301014
C	-1.149839	-0.795886	-1.097675
H	-1.174551	-0.843818	2.313271
H	-1.120490	1.615963	1.952119
H	-1.091149	2.533189	-0.360258
H	-1.120608	0.990012	-2.311023
H	-1.172413	-1.469730	-1.949813
H	-1.193617	-2.387292	0.362640
H	-4.517851	0.739660	-0.018209
H	-3.772379	-0.560670	0.004220
O	-4.667173	-0.208208	-0.004355
Kr	2.605031	-0.044043	0.000002