Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting Information

The effect of Hydrogen Bonding on the Excited-State Proton Transfer in 2,(2'-hydroxyphenyl)benzothiazole: a TDDFT molecular dynamics study

Nawee Kungwan,[*,a,b] Felix Plasser,[b] Adélia J. A. Aquino,[b,c,e] Mario Barbatti,[d]

Peter Wolschann,[b] and Hans Lischka[*,b,e]

[a]Department of Chemistry, Faculty of Science,
Chiang Mai University, Thailand 50200

[b]Institute for Theoretical Chemistry, University of Vienna,
Währinger Straße 17, A-1090 Vienna, Austria

[c]Institute of Soil Research
University of Natural Resources and Life Sciences, Peter-Jordan-Straβe 82, A-1190, Vienna, Austria

[d]Max-Planck-Institut für Kohlenforschung, Kaiser-Wilhelm-Platz 1, D-45470, Mülheim an der Ruhr, Germany

[e]Department of Chemistry and Biochemistry,
Texas Tech University, Lubbock, Texas 79409-1061, USA

[*]Corresponding author. E-mail: naweekung@hotmail.com; hans.lischka@univie.ac.at

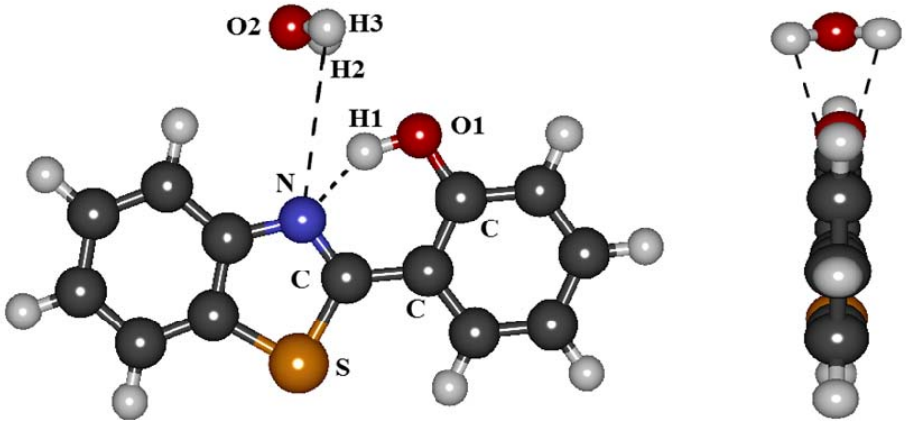

Figure 1S. Ground state optimized structures of the intramolecular hydrogen-bonded HBT-(H_2O) complex computed at the DFT/B3LYP/SVP-SV level and atom numbering scheme, left is a top view and right is a side view.

TABLE S1: Cartesian coordinates of ground-state optimized structures for HBT-$(H2O)_n$ (n=1-3) complexes at different methods with the TZVP+sp basis set

1. HBT at B3LYP/TZVP-sp

C	1.1528798	3.4900876	-0.0002222
C	0.7311322	2.1639273	-0.0000254
C	-0.6381395	1.8284912	0.0001523
C	-1.6002925	2.8424951	0.0001464
C	-1.1804124	4.1629372	-0.0000622
C	0.1834454	4.4850817	-0.0002516
N	-0.9010788	0.4731893	0.0002863
C	0.1802416	-0.2551433	0.0002026
S	1.6959403	0.6938474	-0.0000145
C	0.1687218	-1.7083373	0.0001657
C	-1.0690549	-2.4041746	-0.0000803
C	-1.0714685	-3.8034137	-0.0002851
C	0.1168569	-4.5101976	-0.0002487
C	1.3438786	-3.8388635	0.0000182
C	1.3582669	-2.4575674	0.0002196
O	-2.2577919	-1.7786973	-0.0001384
H	-2.0296615	-4.3069223	-0.0004784
H	2.2733278	-4.3933823	0.0000573
H	0.0927346	-5.5934049	-0.0004242
H	-2.0922436	-0.8022570	0.0000468
H	-2.6510597	2.5821942	0.0002933
H	-1.9157302	4.9579504	-0.0000895
H	0.4881413	5.5242004	-0.0004286
H	2.2052472	3.7439245	-0.0003704
H	2.3090123	-1.9367877	0.0004317

2. HBT-(H_2O) intermolecular hydrogen-bonded complex

2.1 at B3LYP/TZVP+sp

C	-0.9207538	2.4188573	0.5040643
C	0.1922547	1.6582513	0.0716453

C	1.3429624	2.3435435	-0.3587317
C	1.4168162	3.7252437	-0.3536328
C	0.3268256	4.4633065	0.1043270
C	-0.8207208	3.8135436	0.5266860
C	0.2411207	0.1917888	0.1334798
S	1.7478899	-0.5760624	0.7187211
C	1.0124984	-2.1463467	0.4687754
C	-0.3006291	-1.9709532	-0.0119366
N	-0.6907874	-0.6532047	-0.1865249
C	-1.0888056	-3.0920873	-0.2917691
C	-0.5611885	-4.3545389	-0.0771299
C	0.7436449	-4.5161033	0.4084869
C	1.5430142	-3.4160068	0.6848281
O	-2.0647227	1.8831859	0.9969471
O	-3.2362439	0.2302335	-0.8303054
H	-1.6806346	4.3667489	0.8818922
H	2.3135709	4.2218225	-0.7017619
H	0.3693327	5.5458227	0.1238806
H	-2.4996380	1.2628989	0.3667874
H	-2.0937672	-2.9637868	-0.6739916
H	-1.1628105	-5.2295696	-0.2894430
H	1.1353591	-5.5127635	0.5696486
H	2.5514598	-3.5445256	1.0570840
H	2.1887853	1.7665230	-0.7126521
H	-3.9225252	-0.3404284	-0.4676258
H	-2.3865813	-0.2655381	-0.7517225

2.2 at RI-MP2/TZVP+sp

C	-0.8678789	2.3838932	0.6243345
C	0.2044375	1.6422953	0.0891919
C	1.2816844	2.3184293	-0.5038278
C	1.3399849	3.7071850	-0.5061805
C	0.2859669	4.4385508	0.0413648
C	-0.7831701	3.7772014	0.6373979
C	0.2473087	0.1788451	0.1616786

S	1.6184658	-0.5791029	0.9643181
C	0.9582449	-2.1381702	0.5628575
C	-0.2781682	-1.9636302	-0.0978137
N	-0.6363640	-0.6509676	-0.3374911
C	-0.9826213	-3.0855726	-0.5586027
C	-0.5109552	-4.3481769	-0.2397930
C	0.6995602	-4.5088372	0.4603912
C	1.4236439	-3.4123595	0.9056470
O	-1.9243822	1.7973871	1.2638039
O	-3.1800684	0.3572354	-0.6700088
H	-1.6053039	4.3254251	1.0786217
H	2.1749776	4.2119765	-0.9740876
H	0.3159374	5.5208845	0.0447453
H	-2.4339506	1.2668532	0.6118464
H	-1.9050153	-2.9507783	-1.1093511
H	-1.0543696	-5.2236652	-0.5710508
H	1.0486420	-5.5060191	0.6965915
H	2.3523401	-3.5433227	1.4454805
H	2.0897130	1.7375580	-0.9333676
H	-3.8499855	-0.3009145	-0.4532807
H	-2.3329477	-0.1423486	-0.7233891

2.3 at RI-CC2/SVP-SV

C	-0.9257106	2.3986156	0.5272565
C	0.1876750	1.6550809	0.0423203
C	1.3389814	2.3427686	-0.4063472
C	1.4100517	3.7370987	-0.3739122
C	0.3235608	4.4679500	0.1336251
C	-0.8240999	3.8031936	0.5736616
C	0.2328780	0.1912500	0.1148382
S	1.6901141	-0.5636724	0.7656566
C	0.9896903	-2.1279889	0.4854200
C	-0.3188865	-1.9675722	-0.0532961
N	-0.7046686	-0.6586200	-0.2544923
C	-1.1030793	-3.1046441	-0.3723762

C	-0.5735985	-4.3893072	-0.1157592
C	0.7409173	-4.5407293	0.4362102
C	1.5303052	-3.4074739	0.7484403
O	-2.0471380	1.8326835	1.0243186
O	-3.2160849	0.2891472	-0.8183070
H	-1.6874102	4.3512085	0.9677038
H	2.3074299	4.2502211	-0.7387340
H	0.3663258	5.5633996	0.1754884
H	-2.4766942	1.2483876	0.3456158
H	-2.1092496	-2.9726978	-0.8046952
H	-1.1691746	-5.2851012	-0.3541415
H	1.1388814	-5.5499283	0.6291204
H	2.5423511	-3.5251282	1.1704275
H	2.1835631	1.7610965	-0.7972682
H	-3.7838324	-0.3108144	-0.3164554
H	-2.3473711	-0.1785688	-0.8242924

3. HBT-(H_2O) intramolecular hydrogen-bonded complex

3.1 at B3LYP/TZVP+sp

C	-0.8001702	2.4301164	0.4232832
C	0.3667521	1.7488916	-0.0066099
C	1.4745060	2.5123402	-0.4135592
C	1.4461887	3.8933501	-0.3991550
C	0.2895060	4.5497940	0.0317864
C	-0.8178667	3.8280436	0.4392332
C	0.4092440	0.2950577	0.0023822
S	1.9340734	-0.6075832	-0.1928432
C	1.0324094	-2.1052589	-0.0076991
C	-0.3303216	-1.8128109	0.1962029
N	-0.6385522	-0.4625424	0.1899946
C	-1.2472901	-2.8538617	0.3672704
C	-0.7839386	-4.1591440	0.3391763
C	0.5744419	-4.4391573	0.1395026
C	1.4968769	-3.4165726	-0.0385448
O	-1.9115140	1.7881280	0.8335839

O	-3.3764925	-0.5420709	-1.4080691
H	-1.7204735	4.3207309	0.7771604
H	2.3103485	4.4587544	-0.7226681
H	0.2551410	5.6324999	0.0466339
H	-1.7525863	0.8184513	0.7603145
H	-2.2970927	-2.6279316	0.5032659
H	-1.4825572	-4.9762571	0.4683488
H	0.9118569	-5.4680291	0.1205704
H	2.5450201	-3.6370060	-0.1957103
H	2.3674211	2.0023013	-0.7557374
H	-3.8147797	0.3130170	-1.3339191
H	-2.5013833	-0.3994537	-1.0196462

3.2 at RI-MP2/TZVP+sp

C	0.0591559	-0.0051634	0.2037697
C	1.4497252	0.0410265	-0.0434833
C	2.0757307	1.2920131	-0.1687008
C	1.3410330	2.4674708	-0.1363235
C	-0.0353410	2.4099775	0.1023469
C	-0.6746929	1.1835488	0.2253633
C	2.2258917	-1.1875850	-0.0103208
S	3.9469096	-1.1984464	0.3590271
C	3.9514518	-2.9294329	0.1446099
C	2.6407994	-3.3787560	-0.1239749
N	1.6993603	-2.3739923	-0.2370279
C	2.3991456	-4.7389326	-0.3621563
C	3.4468351	-5.6316720	-0.2043122
C	4.7424282	-5.1782033	0.1059010
C	5.0025838	-3.8325144	0.3273036
O	-0.6206120	-1.1677568	0.3592877
O	0.0194753	-3.4510584	-2.3984305
H	-1.7412357	1.1187639	0.3973353
H	1.8394158	3.4206934	-0.2516708
H	-0.6201715	3.3205172	0.1339295
H	0.0278555	-1.8921474	0.2187988

H	1.4017414	-5.0674449	-0.6242601
H	3.2787289	-6.6878327	-0.3699390
H	5.5434327	-5.8973610	0.2207794
H	6.0010568	-3.4918281	0.5677053
H	3.1422185	1.3250914	-0.3603192
H	-0.8045301	-2.9611573	-2.4948036
H	0.5006872	-2.9472548	-1.7225125

3.3 at RI-CC2/SVP-SV

C	-0.8177689	2.3824881	0.0045853
C	0.4646058	1.7521342	-0.0011274
C	1.6281804	2.5532406	-0.0061029
C	1.5455591	3.9450698	-0.0053923
C	0.2791727	4.5604876	0.0003413
C	-0.8846972	3.7904078	0.0055409
C	0.5292813	0.2993333	-0.0004314
S	2.0334838	-0.6238654	0.0000674
C	1.1006707	-2.0986248	0.0004778
C	-0.2883249	-1.7907716	0.0006291
N	-0.5637235	-0.4436857	-0.0001935
C	-1.2644314	-2.8170285	0.0005784
C	-0.8189348	-4.1587790	0.0013912
C	0.5815545	-4.4664445	0.0012924
C	1.5553238	-3.4360358	0.0009569
O	-1.9663167	1.6856678	0.0089329
O	-3.9348651	-0.4812874	-0.0096766
H	-1.8782950	4.2527765	0.0107044
H	2.4586800	4.5510306	-0.0093369
H	0.2011093	5.6547964	0.0005948
H	-1.7015201	0.7111915	0.0067914
H	-2.3309395	-2.5353489	0.0002837
H	-1.5541728	-4.9794669	0.0014180
H	0.9086349	-5.5188234	0.0017502
H	2.6312790	-3.6779362	0.0008265
H	2.6127675	2.0669465	-0.0104938

H	-3.7865852	0.1182669	0.7330862
H	-3.7644137	0.1079341	-0.7559200

4. HBT-$(H_2O)_2$ intermolecular hydrogen-bonded complex

4.1 at B3LYP/TZVP+sp

C	0.0682696	-0.1546544	0.0806558
C	1.4806801	-0.1526722	0.0926054
C	2.1468098	1.0813122	0.1988302
C	1.4609119	2.2761110	0.3188599
C	0.0657653	2.2582213	0.3273445
C	-0.6158401	1.0608518	0.2079318
C	2.2755555	-1.3812156	0.0056842
S	3.7630313	-1.3931072	-0.9834089
C	4.0357305	-3.0542075	-0.4934140
C	2.9840734	-3.4701639	0.3475486
N	2.0215311	-2.5041652	0.6043734
C	2.9868106	-4.7689874	0.8678419
C	4.0271481	-5.6195432	0.5325140
C	5.0653987	-5.1959914	-0.3086417
C	5.0815770	-3.9100881	-0.8298056
O	-0.7135743	-1.2449284	-0.0561495
H	-1.6978445	1.0298338	0.1932395
H	2.0029984	3.2081901	0.4128166
H	-0.4911158	3.1827776	0.4228470
H	-0.2602394	-2.0818438	-0.2860941
H	2.1819569	-5.0900346	1.5161226
H	4.0392577	-6.6283238	0.9261578
H	5.8669457	-5.8807549	-0.5568628
H	5.8852272	-3.5847573	-1.4780395
H	3.2299543	1.0828801	0.2166619
O	-0.0140367	-3.8295670	2.1175022
H	0.6520864	-3.1924062	1.7773188
O	-0.5053208	-3.9551695	-0.6361256
H	-0.5260707	-4.1560296	0.3206157
H	-0.6138900	-3.3148424	2.6683406

H	-1.3886872	-4.1497242	-0.9672708

4.2 at RI-MP2/TZVP+sp

C	0.0249477	-0.1553920	0.1768000
C	1.4318070	-0.1518782	0.1869215
C	2.1134825	1.0731116	0.2373250
C	1.4245406	2.2703097	0.3880349
C	0.0289362	2.2563190	0.4111433
C	-0.6603635	1.0513096	0.3394055
C	2.1978261	-1.3968166	0.0835875
S	3.3264128	-1.6176550	-1.2449810
C	3.7686212	-3.1614566	-0.5754779
C	2.9828089	-3.4127060	0.5712046
N	2.1323832	-2.3884602	0.9402115
C	3.1737923	-4.5959556	1.3002245
C	4.0494922	-5.5479762	0.8048396
C	4.7997334	-5.3022581	-0.3608625
C	4.6376291	-4.1308612	-1.0868349
O	-0.7272767	-1.2827059	0.0763375
H	-1.7424044	1.0228441	0.3409749
H	1.9668144	3.2047813	0.4468517
H	-0.5245491	3.1803287	0.5219056
H	-0.2317889	-2.0167966	-0.3473287
H	2.5872273	-4.7759360	2.1919927
H	4.1918199	-6.4763740	1.3429736
H	5.4787465	-6.0623719	-0.7262525
H	5.2106106	-3.9515312	-1.9872726
H	3.1972773	1.0631768	0.2348150
O	-0.0514699	-3.8560166	1.8577828
H	0.6514528	-3.1768024	1.7680902
O	0.2093351	-3.6649006	-0.9123543
H	0.0590215	-4.0264741	-0.0152984
H	-0.8327430	-3.3360049	2.0825051
H	-0.3790233	-4.1678509	-1.4872642

4.3 at RI-CC2/SVP-SV

C	0.0353378	-0.2087004	0.2564066
C	1.4500145	-0.1725710	0.1325778
C	2.1107516	1.0750973	0.1083691
C	1.4068668	2.2711838	0.2584710
C	0.0137151	2.2277994	0.4287211
C	-0.6581705	1.0039925	0.4332195
C	2.2381173	-1.4047650	0.0455199
S	3.5281186	-1.5409148	-1.1478258
C	3.8906402	-3.1287352	-0.5436674
C	2.9814622	-3.4543695	0.5015494
N	2.0836605	-2.4586598	0.8201598
C	3.0599171	-4.7102291	1.1382455
C	4.0339094	-5.6121751	0.7145247
C	4.9351593	-5.2796021	-0.3232095
C	4.8722067	-4.0419610	-0.9666795
O	-0.7032595	-1.3379490	0.2425345
H	-1.7445769	0.9518386	0.5374014
H	1.9381246	3.2255392	0.2516321
H	-0.5537436	3.1535109	0.5564289
H	-0.2496174	-2.0916236	-0.2188143
H	2.3506148	-4.9547399	1.9328187
H	4.1063193	-6.5919740	1.1933875
H	5.6902968	-6.0061408	-0.6342274
H	5.5679328	-3.7920655	-1.7716050
H	3.2003458	1.0865617	0.0112847
O	-0.1449296	-3.7678147	1.8941310
H	0.6311258	-3.1769016	1.7686914
O	0.0528273	-3.6660483	-0.8340778
H	-0.0408806	-3.9869951	0.0917307
H	-0.8619899	-3.1212875	1.9650596
H	-0.7251962	-4.0223003	-1.2827582

5. HBT-$(H_2O)_2$ intramolecular hydrogen-bonded complex

   5.1 at B3LYP/TZVP+sp

C	-0.8308338	2.4528177	0.4922522

C	0.3951471	1.9459004	-0.0050947
C	1.3568969	2.8601162	-0.4676259
C	1.1306330	4.2230356	-0.4416244
C	-0.0816856	4.7063113	0.0579704
C	-1.0489188	3.8323827	0.5222812
C	0.6498506	0.5125815	-0.0038837
S	2.2907952	-0.1514726	-0.1882416
C	1.6216847	-1.7671667	-0.0078859
C	0.2289838	-1.6836596	0.1870453
N	-0.2762014	-0.3916327	0.1771672
C	-0.5240256	-2.8500860	0.3566497
C	0.1350832	-4.0689485	0.3332333
C	1.5213177	-4.1419932	0.1427570
C	2.2800031	-2.9925077	-0.0342037
O	-1.8165184	1.6552018	0.9571855
O	-3.0171813	-0.3471799	-1.3045348
H	-1.9915688	4.1906046	0.9156849
H	1.8842996	4.9067179	-0.8098675
H	-0.2705574	5.7727562	0.0833337
H	-1.5173027	0.7204172	0.8835043
H	-1.5990943	-2.7993023	0.4836421
H	-0.4341707	-4.9809465	0.4620448
H	2.0107831	-5.1081625	0.1307449
H	3.3503567	-3.0516733	-0.1844878
H	2.2920230	2.4824975	-0.8640187
H	-3.3864749	0.4732434	-0.9551847
H	-2.1054082	-0.3582610	-0.9691998
H	-3.7688635	-1.9163144	-0.5859853
O	-3.9635349	-2.7388471	-0.0978785
H	-4.5133237	-3.2622259	-0.6897640

5.2 at RI-MP2/TZVP+sp

C	-0.7350304	2.4318781	0.6307375
C	0.4024287	1.8986344	-0.0142637
C	1.3499277	2.7807536	-0.5579237

C	1.1428665	4.1521626	-0.5427313
C	0.0098192	4.6684771	0.0922676
C	-0.9407373	3.8130702	0.6346612
C	0.6437377	0.4646924	0.0226043
S	2.2636174	-0.2125790	-0.0381020
C	1.5661867	-1.8102272	0.0295112
C	0.1632349	-1.7138551	0.1582280
N	-0.3280313	-0.4213769	0.1181411
C	-0.6229790	-2.8743601	0.2055950
C	0.0249836	-4.0990318	0.2460436
C	1.4269197	-4.1852386	0.1596836
C	2.2169235	-3.0454563	0.0948890
O	-1.6890333	1.6516823	1.2027000
O	-2.8821592	-0.1070440	-1.2576192
H	-1.8285514	4.1941882	1.1224646
H	1.8759310	4.8150396	-0.9826555
H	-0.1611878	5.7372053	0.1159615
H	-1.4291129	0.7206738	1.0360348
H	-1.7041250	-2.8061584	0.2392825
H	-0.5611020	-5.0074091	0.2984422
H	1.9031972	-5.1570147	0.1931167
H	3.2947472	-3.1175522	0.0316678
H	2.2206295	2.3685407	-1.0549124
H	-3.2099911	0.7341878	-0.9161939
H	-1.9974745	-0.1787924	-0.8533005
H	-3.6756053	-1.6725990	-0.6611141
O	-3.8928857	-2.5265028	-0.2427169
H	-4.5297497	-2.9247086	-0.8447474

5.3 at RI-CC2/SVP-SV

C	-0.7679472	2.4282748	0.4338563
C	0.4683126	1.9012028	-0.0248726
C	1.4812262	2.7904131	-0.4410416
C	1.2854077	4.1696276	-0.4057434
C	0.0631287	4.6833637	0.0563646

C	-0.9515660	3.8198938	0.4687449
C	0.6836421	0.4569747	-0.0200949
S	2.2855281	-0.2504302	-0.0500828
C	1.5713801	-1.8325154	0.0007542
C	0.1581713	-1.7175801	0.0763583
N	-0.3015514	-0.4173687	0.0517875
C	-0.6646218	-2.8703637	0.1322903
C	-0.0329589	-4.1325793	0.1503327
C	1.3946168	-4.2437055	0.0797287
C	2.2119625	-3.0916794	0.0165837
O	-1.7934120	1.6475351	0.8392091
O	-3.0834967	-0.0597135	-1.1893856
H	-1.9132127	4.1981345	0.8322735
H	2.0807965	4.8445938	-0.7402664
H	-0.1027537	5.7666913	0.0884024
H	-1.4991672	0.7114721	0.7486701
H	-1.7635699	-2.7673876	0.1833440
H	-0.6457406	-5.0463829	0.2025502
H	1.8644360	-5.2401713	0.0929141
H	3.3095267	-3.1779494	-0.0381297
H	2.4282439	2.3843122	-0.8177180
H	-3.1874170	0.7921667	-0.7440907
H	-2.1370673	-0.2270911	-1.0605788
H	-3.8023373	-1.4992345	-0.2638424
O	-4.0131276	-2.3580123	0.1468872
H	-4.2651425	-2.8859588	-0.6184914

6. HBT-$(H_2O)_3$ intermolecular hydrogen-bonded complex

6.1 at B3LYP/TZVP+sp

C	0.0752631	2.4128000	0.3081378
C	1.0479707	1.4733677	-0.0930867
C	2.2893930	1.9544855	-0.5448449
C	2.5624091	3.3078754	-0.6333527
C	1.5819792	4.2241019	-0.2563880
C	0.3582565	3.7781846	0.2120193

C	0.8184067	0.0231395	-0.0761757
S	2.1361614	-1.0594019	0.4699769
C	1.1000124	-2.4315562	0.1274352
C	-0.1454644	-1.9676684	-0.3453398
N	-0.2605510	-0.5893599	-0.4478725
C	-1.1439207	-2.8890743	-0.6837164
C	-0.8816435	-4.2414092	-0.5366742
C	0.3591860	-4.6900062	-0.0632613
C	1.3620855	-3.7915986	0.2732753
O	-1.1538713	2.1070366	0.7982925
O	-3.1780379	-0.1763189	-0.7987652
H	-0.4053877	4.4762143	0.5307868
H	3.5230306	3.6456707	-1.0000627
H	1.7744440	5.2882580	-0.3204243
H	-1.2919124	1.1866688	1.1241799
H	-2.1000815	-2.5363300	-1.0489504
H	-1.6460684	-4.9640130	-0.7941444
H	0.5401182	-5.7526925	0.0419128
H	2.3198641	-4.1415006	0.6367392
H	3.0362966	1.2371741	-0.8619233
H	-3.4991395	0.7378451	-0.9179751
H	-2.2213380	-0.1297883	-0.9782706
H	-2.8651758	-0.2380973	0.9849054
O	-2.4329341	-0.0285375	1.8458394
H	-2.1694099	-0.8742310	2.2233218
H	-2.7733872	2.6443423	-0.0695118
O	-3.5734797	2.6412268	-0.6264622
H	-4.2750768	3.0037192	-0.0748256

6.2 at RI-MP2/TZVP+sp

C	0.0354752	2.4252320	0.3878733
C	0.9574734	1.5473235	-0.2040956
C	2.1213988	2.0663942	-0.7870813
C	2.3201498	3.4385839	-0.8832150
C	1.3838882	4.3057980	-0.3176677

C	0.2360031	3.8031160	0.2843298
C	0.7561538	0.0951456	-0.1531577
S	1.7600904	-0.8835518	0.9118064
C	0.8982499	-2.2964646	0.3681127
C	-0.1054681	-1.9060046	-0.5489155
N	-0.1426453	-0.5568983	-0.8481652
C	-0.9223679	-2.8803651	-1.1431753
C	-0.8012277	-4.1949372	-0.7236508
C	0.1770361	-4.5667236	0.2183987
C	1.0060141	-3.6216267	0.8062396
O	-1.0952651	2.0161054	1.0341829
O	-2.9778947	-0.3114025	-0.7414058
H	-0.4949460	4.4611646	0.7366570
H	3.2136386	3.8258248	-1.3547360
H	1.5268243	5.3772652	-0.3771171
H	-1.1046889	1.0521904	1.2586619
H	-1.6781524	-2.5802798	-1.8570802
H	-1.4419615	-4.9545050	-1.1525519
H	0.2513245	-5.6017670	0.5272373
H	1.7514798	-3.9130262	1.5346609
H	2.8321390	1.3762474	-1.2267518
H	-3.3544036	0.5883337	-0.7184942
H	-2.0761074	-0.1759271	-1.0841276
H	-2.3548994	-0.5779102	0.9259848
O	-1.8158588	-0.4604045	1.7425226
H	-1.3444717	-1.2964631	1.8430823
H	-2.7130612	2.4044889	0.2824273
O	-3.5333497	2.4129874	-0.2462447
H	-4.2011143	2.7702370	0.3488699

6.3 at RI-CC2/SVP-SV

C	-0.0609089	2.4225889	0.2848023
C	0.9731449	1.5656879	-0.1621710
C	2.1823261	2.1233496	-0.6245485
C	2.3549347	3.5046578	-0.7057031

C	1.3126692	4.3499435	-0.3025781
C	0.1193824	3.8115075	0.1785467
C	0.8175440	0.1068115	-0.1450858
S	2.0582156	-0.8878268	0.6014204
C	1.1469489	-2.3008953	0.1802077
C	-0.0522719	-1.9081584	-0.4756009
N	-0.1941162	-0.5500398	-0.6594533
C	-0.9793089	-2.8857291	-0.8950517
C	-0.6897043	-4.2233889	-0.6487976
C	0.5091863	-4.6048671	-0.0039625
C	1.4356953	-3.6553485	0.4216351
O	-1.2399094	2.0005036	0.7935328
O	-3.0659767	-0.4543281	-0.6830120
H	-0.6933826	4.4560114	0.5204747
H	3.2923846	3.9182993	-1.0826506
H	1.4266683	5.4346939	-0.3662865
H	-1.2560237	1.0613611	1.1294607
H	-1.9076128	-2.5710854	-1.3750377
H	-1.3977651	-4.9940118	-0.9617382
H	0.7108511	-5.6641768	0.1720702
H	2.3580466	-3.9555340	0.9237890
H	2.9732507	1.4484246	-0.9623607
H	-3.5087109	0.4182991	-0.7056742
H	-2.1641216	-0.2489062	-0.9885393
H	-2.4658484	-0.5272008	0.9544443
O	-1.9160936	-0.3398607	1.7543042
H	-1.3733103	-1.1323295	1.8427159
H	-2.9347681	2.3212284	0.0697906
O	-3.8278336	2.1865302	-0.2952442
H	-4.3908415	2.2502810	0.4847649

7. HBT-$(H_2O)_3$ intramolecular hydrogen-bonded complex

7.1 at B3LYP /TZVP+sp

C	-0.0564935	2.4453440	0.3746554
C	1.1852405	1.7929406	0.1630713

C	2.3261869	2.5826580	-0.0517150
C	2.2577771	3.9633087	-0.0596999
C	1.0266461	4.5899124	0.1500426
C	-0.1171996	3.8404482	0.3658792
C	1.2442788	0.3391778	0.1695730
S	2.7582287	-0.5765680	-0.0597346
C	1.8350670	-2.0671171	0.0954668
C	0.4753087	-1.7617416	0.3054932
N	0.1924327	-0.4107442	0.3423154
C	-0.4611089	-2.7897866	0.4503117
C	-0.0156722	-4.1006140	0.3874796
C	1.3392441	-4.3961231	0.1828133
C	2.2790562	-3.3844321	0.0331255
O	-1.1973410	1.7570622	0.5934326
O	-4.4196035	-0.4603959	-2.1476836
H	-1.0767216	4.3128021	0.5336787
H	3.1507926	4.5509216	-0.2280584
H	0.9617812	5.6712815	0.1457428
H	-0.9713371	0.7831985	0.5653625
H	-1.5072984	-2.5467299	0.5957959
H	-0.7257649	-4.9110055	0.4963036
H	1.6611454	-5.4293477	0.1382526
H	3.3237004	-3.6184340	-0.1275446
H	3.2804852	2.0958788	-0.2158626
H	-4.2659688	0.3537307	-1.6204914
H	-3.8220168	-0.4107598	-2.9009463
H	-4.1251042	-1.4850425	-0.6151999
O	-3.9649296	-1.6416650	0.3388113
H	-4.7235131	-2.1489101	0.6471593
H	-3.1448258	1.6650373	0.1572321
O	-4.0107416	1.2682110	-0.0273830
H	-4.0109249	0.4319831	0.4693481

7.2 at RI-MP2/TZVP+sp

C	0.0350460	0.0286034	0.1019366

C	1.4401144	0.0531151	-0.0374506
C	2.0785885	1.2847260	-0.2502214
C	1.3643565	2.4735397	-0.2169049
C	-0.0220992	2.4386858	-0.0440373
C	-0.6753154	1.2281111	0.1525515
C	2.1884804	-1.1929485	-0.0256794
S	3.8846837	-1.2700768	0.4274865
C	3.8196686	-3.0058346	0.2565285
C	2.5244532	-3.3979401	-0.1442713
N	1.6263505	-2.3582867	-0.2803909
C	2.2127330	-4.7550238	-0.3080790
C	3.2360863	-5.6801554	-0.1778240
C	4.5364450	-5.2778848	0.1813555
C	4.8563982	-3.9382806	0.3570678
O	-0.6589655	-1.1322790	0.2698679
O	0.3433236	-2.7454284	-2.9367523
H	-1.7478334	1.1827647	0.2920180
H	1.8723296	3.4148907	-0.3785859
H	-0.5920509	3.3588971	-0.0277180
H	-0.0052011	-1.8627290	0.1482952
H	1.2074125	-5.0425027	-0.5922553
H	3.0254602	-6.7326991	-0.3164432
H	5.3149824	-6.0239386	0.2786716
H	5.8602279	-3.6375681	0.6267381
H	3.1506854	1.2994411	-0.4101867
H	-0.5186956	-2.3086563	-2.7999027
H	0.8172823	-2.5254592	-2.1182226
H	-0.4482088	-4.2971884	-2.3382147
O	-1.0064943	-4.8759591	-1.7779612
H	-1.2699505	-5.5952053	-2.3621949
H	-1.9261074	-1.7586954	-1.0710203
O	-2.2612215	-2.1781150	-1.8794806
H	-2.1887693	-3.1261675	-1.6848637

7.3 at RI-CC2 /SVP-SV

C	-0.1572166	2.3898066	0.5228273
C	0.9688611	1.7004418	-0.0008748
C	2.0751730	2.4434873	-0.4625719
C	2.0760479	3.8358585	-0.4107132
C	0.9623398	4.5097488	0.1157673
C	-0.1415722	3.7925515	0.5765511
C	0.9775216	0.2410540	-0.0019029
S	2.4457433	-0.6985974	-0.1677250
C	1.5121090	-2.1554231	-0.0153508
C	0.1436564	-1.8295068	0.1760025
N	-0.1166940	-0.4760454	0.1688101
C	-0.8295216	-2.8450609	0.3474626
C	-0.3981136	-4.1880905	0.3220428
C	0.9845916	-4.5123767	0.1247947
C	1.9542642	-3.4970349	-0.0423014
O	-1.2566347	1.7480588	0.9760974
O	-2.5364462	-0.2522231	-1.7960879
H	-1.0221947	4.3005337	0.9847196
H	2.9399804	4.3976110	-0.7822962
H	0.9515510	5.6051389	0.1604543
H	-1.1207475	0.7807548	0.8062270
H	-1.8856089	-2.5655472	0.4977854
H	-1.1306418	-5.0000299	0.4532128
H	1.2984880	-5.5682507	0.1087661
H	3.0168340	-3.7488421	-0.1921354
H	2.9374215	1.9137163	-0.8863681
H	-2.9733571	0.5701211	-1.4920705
H	-1.6675259	-0.1964244	-1.3734976
H	-3.4236893	-1.0699153	-0.4810071
O	-3.8622273	-1.2187982	0.3859688
H	-4.6200305	-1.7712400	0.1635060
H	-3.1202514	1.9272453	0.2981497
O	-3.8696112	1.6028975	-0.2235689
H	-4.1138144	0.7878667	0.2461760

Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics