Supporting info for

Emergence of charge-transfer-to-solvent band in the absorption spectra of hydrogen halides on ice nanoparticles: Spectroscopic evidence for acidic dissociation

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I. GEOMETRIES AND ABSOLUTE ENERGIES OF CLUSTERS ENLISTED IN TABLE II

The optimized geometries are enlisted at DFT/BHandHLYP and MP2 levels, respectively. The geometries are given in Ångstrom, energies in Hartrees.

$HF(H_2O)_4$ intact

14

E(RB+HF-LYP) = -406.050585832

O -2.197197 0.263979 0.042499

O -0.386181 2.198975 -0.145537

O 2.028915 1.043314 0.156170

O 1.605803 -1.627043 -0.084831

F -1.088182 -1.924856 0.024931

H -1.555424 -1.077142 0.031578

H -2.793882 0.457657 0.760274

H -1.569025 1.012076 -0.039970

H 0.512710 1.840955 -0.020789

H 1.948851 0.079093 0.053521

H -0.358571 2.771880 -0.906596

H 2.568989 1.199526 0.925518

H 0.660800 -1.821510 -0.026726

H 1.959297 -2.164617 -0.787609

14

MP2=-405.2234962

O 2.234022 0.249061 -0.027010

O 0.411369 2.211993 0.144165

O -2.041777 1.070705 -0.157827

O -1.642797 -1.633591 0.081909

F 1.090877 -1.948806 -0.036228

H 1.569598 -1.093067 -0.033983

H 2.808048 0.443271 -0.776679

H 1.598764 1.004195 0.049915

H -0.499696 1.858791 0.019490

H -1.971389 0.096157 -0.055603

H 0.373145 2.784714 0.918212

H -2.581601 1.218027 -0.942214

H -0.689781 -1.835302 0.022025

H -1.980189 -2.164735 0.811396

$HF(H_2O)_4$ contact ion

14

E(RB+HF-LYP) = -406.043838855

O -0.567323 -1.173218 0.751879

O -2.609537 -0.103084 -0.799826

O 1.892631 -1.391519 -0.346068

O 1.922604 1.355579 -0.306514

F -0.612163 1.232310 0.766168

H -0.575205 0.244171 0.855213

H -1.280285 -1.338453 0.127945

H 0.275729 -1.452218 0.352307

H -2.279236 0.716766 -0.428765

H -3.553454 -0.014928 -0.894079

H 2.070604 -0.440474 -0.411130

H 1.055975 1.537398 0.075515

H 2.646787 -1.797626 0.071221

H 2.041544 1.952514 -1.039502

14

MP2=-405.2174216

O -0.570979 -1.179072 0.770349

O -2.610751 -0.102100 -0.820320

O 1.899552 -1.410846 -0.356775

O 1.936111 1.364706 -0.314360

F -0.616941 1.246850 0.811350

H -0.579806 0.241992 0.877294

H -1.282776 -1.346134 0.129894

H 0.279113 -1.456408 0.359256

H -2.303178 0.725742 -0.422452

H -3.563715 -0.012827 -0.929246

H 2.085096 -0.451111 -0.419366

H 1.066820 1.555938 0.082071

H 2.664134 -1.809904 0.072854

H 2.025991 1.960392 -1.066185

$HF(H_2O)_4$ separated ion

14

E(RB+HF-LYP) = -406.030646947

O -0.744001 -0.563102 1.263454

O 1.606651 0.325067 1.151360

O -0.172122 -1.725569 -0.878294

O -1.474101 1.299153 -0.256113

F 0.744318 0.591072 -1.165801

H -1.211871 0.216570 0.820165

H -0.589618 -1.219886 0.499014

H 0.183228 -0.212458 1.461060

H 0.266012 -0.894707 -1.203939

H 0.402791 -2.468033 -1.038157

H 1.457074 0.540203 0.188341

H 2.098127 1.024210 1.570457

H -1.712195 2.217246 -0.178841

H -0.626835 1.204139 -0.767980

14

MP2=-405.2050169

O 0.043089 -0.772018 1.378973

O -1.155452 1.405377 0.880526

O 1.945328 0.225496 0.062407

O -0.669588 -1.668130 -0.879983

F -0.114737 0.753858 -1.302992

H -0.317742 -1.317743 0.592469

H 0.939012 -0.409739 1.016218

H -0.549384 0.061024 1.381050

H 1.287203 0.555841 -0.622742

H 2.521129 0.959336 0.304635

H -0.858220 1.319795 -0.081325

H -2.078691 1.678825 0.898376

H -1.484964 -2.039338 -1.232810

H -0.531320 -0.752054 -1.272580

$HF(H_2O)_5$ intact

17

E(RB+HF-LYP) = -482.456985528

O -0.704237 0.422870 1.645538

O 0.633867 1.747722 -0.247791

O 2.782556 0.021938 -0.095510

O 0.779454 -1.732177 0.377599

O -0.828383 -0.384072 -1.535633

F -2.840226 -0.077532 -0.099950

H -0.280567 -0.432535 1.527588

H -1.606762 0.308440 1.331992

H -0.338240 0.439691 -1.444714

H -0.304366 -1.040286 -1.059597

H -2.141032 -0.215648 -0.742844

H 1.633055 -1.286558 0.241688

H 0.951604 -2.642180 0.602956

H 3.428929 0.050574 -0.794826

H 2.200227 0.788641 -0.197373

H 0.131347 1.417735 0.528254

H 0.581778 2.699662 -0.247203

17

MP2=-481.473903

O -0.710629 0.433628 1.661062

O 0.641749 1.766034 -0.249557

O 2.805313 0.017750 -0.098356

O 0.778186 -1.743156 0.393718

O -0.831149 -0.384460 -1.551704

F -2.881940 -0.097823 -0.118504

H -0.288690 -0.434385 1.545897

H -1.620940 0.307452 1.344187

H -0.337867 0.448849 -1.456233

H -0.294758 -1.037417 -1.064706

H -2.158665 -0.225283 -0.755192

H 1.644366 -1.301228 0.253502

H 0.961765 -2.663543 0.615323

H 3.427961 0.040911 -0.833558

H 2.220382 0.794894 -0.202028

H 0.129964 1.434884 0.532943

H 0.593955 2.729179 -0.226621

$HF(H_2O)_5$ contact ion

17

E(RB+HF-LYP) = -482.457239223

F 0.046011 -1.258018 0.777360

O -0.038343 1.096885 0.915667

O -2.418240 1.364733 -0.333517

O -2.395672 -1.375239 -0.465611

O 2.284672 1.498675 -0.421248

O 2.521752 -1.240702 -0.381622

H 0.010064 -0.234799 0.888981

H -0.861097 1.391132 0.485638

H -3.203338 1.727742 0.066275

H -2.574145 0.417709 -0.474256

H -2.444287 -1.934730 -1.235249

H -1.551730 -1.552990 -0.032701

H 0.729366 1.451621 0.434201

H 2.530590 0.563948 -0.498601

H 2.441106 1.910254 -1.265957

H 1.678190 -1.452960 0.036718

H 3.197837 -1.719582 0.089365

17

MP2=-481.4732676

F 0.042862 -1.259066 0.860670

O -0.037579 1.112087 0.977536

O -2.391446 1.377623 -0.363119

O -2.376487 -1.386792 -0.481905

O 2.272984 1.511223 -0.424541

O 2.484464 -1.255607 -0.422255

H 0.008465 -0.212101 0.961279

H -0.862519 1.392803 0.518923

H -3.200710 1.743250 0.011063

H -2.556173 0.421748 -0.503467

H -2.375078 -1.953667 -1.260892

H -1.539351 -1.563240 -0.013331

H 0.731973 1.455048 0.469430

H 2.512937 0.567135 -0.528147

H 2.404244 1.926520 -1.283849

H 1.656771 -1.461760 0.051514

H 3.177381 -1.761525 0.016534

$HF(H_2O)_5$ separated ion

17

E(RB+HF-LYP) = -482.447391887

F -0.773240 1.564004 -0.205604

H -1.119417 0.540705 -1.250747

H -2.063554 -0.324564 -2.205589

H -0.840739 -1.295925 -0.637376

H -1.112718 0.838143 1.065832

H -2.040364 0.240577 2.222050

H -0.814381 -1.093633 0.958580

H 0.802894 1.590188 -0.197531

H 2.146144 2.069977 0.443827

H 0.540051 -1.597742 0.182153

H 2.033837 -0.192932 0.040228

H 2.590181 -1.542029 -0.538895

O -1.241061 -0.332132 -1.726200

O -0.466873 -1.700749 0.218588

O -1.217595 0.122151 1.757892

O 1.774533 1.423581 -0.148740

O 2.005649 -1.176451 0.119450

17

MP2=-481.4643128

F -0.797437 1.572830 -0.206544

H -1.122864 0.548475 -1.263776

H -2.060543 -0.340912 -2.217770

H -0.839934 -1.284720 -0.643790

H -1.118128 0.850447 1.074788

H -2.042261 0.231908 2.235601

H -0.816502 -1.078775 0.965696

H 0.794728 1.596637 -0.200925

H 2.138237 2.071569 0.458666

H 0.543342 -1.600973 0.187164

H 2.039925 -0.200373 0.043021

H 2.580440 -1.551339 -0.564307

O -1.216749 -0.334638 -1.753132

O -0.474603 -1.706598 0.222536

O -1.197503 0.129760 1.784004

O 1.775899 1.423765 -0.155511

O 2.017297 -1.193894 0.132197

$HCl(H_2O)_4$ intact

14

E(RB+HF-LYP) = -766.411922282

O 0.178925 -0.216988 2.883093

O -1.881612 1.386311 2.311130

O -2.121408 1.766603 -0.355214

O -0.705310 -0.203828 -1.618692

Cl 1.394263 -1.493224 0.566450

H 0.838478 -0.911211 1.640146

H 0.770043 0.261252 3.458958

H -0.587626 0.362143 2.697033

H -1.989167 1.573412 1.361353

H -1.649732 1.080242 -0.853394

H -2.748211 1.198945 2.660492

H -1.926266 2.601217 -0.771576

H -0.025260 -0.585858 -1.055538

H -1.130881 -0.931049 -2.065103

14

MP2=-765.2039975

O 0.185724 -0.227624 2.902431

O -1.907602 1.403248 2.335686

O -2.128729 1.791960 -0.365260

O -0.704713 -0.219182 -1.625019

Cl 1.426545 -1.489699 0.531067

H 0.882223 -0.936612 1.599255

H 0.767979 0.269424 3.489005

H -0.587913 0.357289 2.721915

H -2.010309 1.594467 1.376998

H -1.650951 1.095114 -0.861217

H -2.790448 1.196116 2.661611

H -1.902815 2.626392 -0.790757

H -0.020795 -0.611881 -1.058075

H -1.141960 -0.961045 -2.058502

$HCl(H_2O)_4$ contact ion

14

E(RB+HF-LYP) = -766.412230102

O 0.420447 -1.263002 -0.891224

O 2.317383 -0.978606 0.847298

O -1.924802 -1.517810 -0.008896

O -2.139378 1.041587 0.606388

Cl 0.778467 1.513273 -0.396529

H 0.511214 -0.234384 -0.918362

H 1.092871 -1.505143 -0.212131

H -0.519228 -1.465355 -0.564268

H 2.178906 -0.024823 0.770992

H 2.549364 -1.177494 1.749898

H -2.147505 -0.610192 0.292962

H -1.277535 1.392822 0.323630

H -2.641274 -1.836739 -0.551734

H -2.369950 1.478314 1.421470

14

MP2=-765.2004712

O 0.422784 -1.281524 -0.820706

O 2.157515 -0.983154 1.140354

O -1.994470 -1.522543 -0.049689

O -2.182659 1.081899 0.540249

Cl 0.787066 1.457300 -0.378501

H 0.539002 -0.215437 -0.808185

H 1.051121 -1.551034 -0.102829

H -0.538574 -1.476379 -0.535170

H 2.062292 -0.028469 0.960428

H 3.097184 -1.152465 1.272530

H -2.214254 -0.597712 0.229842

H -1.297743 1.414340 0.278366

H -2.687525 -1.809242 -0.656104

H -2.372759 1.476866 1.398910

$HCl(H_2O)_4$ separated ion

14

E(RB+HF-LYP) = -766.416324005

O 1.804311 0.008845 -0.002366

O 0.451499 -1.429404 -1.575083

O 0.453027 -0.656492 2.019692

O 0.436514 2.088811 -0.443845

Cl -1.728546 -0.006199 0.002026

H 1.407974 0.925962 -0.153979

H 1.409978 -0.320003 0.870703

H 1.410876 -0.584370 -0.721388

H -0.419721 -0.524981 1.594236

H 0.434473 -1.484054 2.493495

H -0.419576 -1.124112 -1.247657

H 0.423314 -1.452980 -2.528044

H 0.407157 2.926355 0.011175

H -0.432150 1.649146 -0.339709

14

MP2=-765.2031752

O 1.810536 0.007500 -0.003128

O 0.451782 -1.450546 -1.578450

O 0.454046 -0.639352 2.044482

O 0.437560 2.093791 -0.470489

Cl -1.705707 -0.008440 0.002567

H 1.401607 0.931449 -0.161165

H 1.407412 -0.319854 0.878416

H 1.406935 -0.594157 -0.725203

H -0.418829 -0.518454 1.591605

H 0.426526 -1.490170 2.498628

H -0.420630 -1.122759 -1.242326

H 0.417589 -1.421433 -2.542222

H 0.401995 2.914528 0.035457

H -0.431694 1.634420 -0.348916

$HCl(H_2O)_5$ intact

17

E(RB+HF-LYP) = -842.821548766

O -0.091560 0.412864 1.744072

O 1.126466 1.759443 -0.227990

O 3.230526 -0.034539 -0.208331

O 1.214432 -1.730931 0.387639

O -0.385619 -0.339211 -1.535351

Cl -2.942278 -0.037576 -0.064776

H 0.265899 -0.454385 1.522781

H -1.040371 0.349746 1.625464

H 0.098337 0.481479 -1.399001

H 0.109548 -1.007047 -1.047549

H -1.854936 -0.187273 -0.812750

H 2.070203 -1.305974 0.203673

H 1.376480 -2.641511 0.618166

H 3.816850 -0.038791 -0.959415

H 2.668975 0.750735 -0.276218

H 0.661163 1.438596 0.571420

H 1.092619 2.712201 -0.225704

17

MP2=-841.4576492

O -0.115925 0.420528 1.749144

O 1.130716 1.777599 -0.223906

O 3.245962 -0.037413 -0.217013

O 1.215379 -1.745379 0.410247

O -0.377442 -0.345651 -1.567508

Cl -2.937962 -0.032317 -0.036341

H 0.249822 -0.455675 1.531692

H -1.069818 0.339575 1.601767

H 0.117998 0.479964 -1.432088

H 0.130074 -1.012749 -1.072110

H -1.881824 -0.183489 -0.802616

H 2.080798 -1.319937 0.219497

H 1.397243 -2.661188 0.651466

H 3.791766 -0.042336 -1.011341

H 2.676404 0.755631 -0.275713

H 0.647301 1.449517 0.574950

H 1.116242 2.741147 -0.183997

$HCl(H_2O)_5$ contact ion

17

E(RB+HF-LYP) = -842.829411756

Cl -0.066310 -1.649889 -0.673342

O 0.050918 1.211616 -1.053490

O 2.235009 1.615952 0.172207

O 2.535555 -0.914217 0.899467

O -2.049752 1.797463 0.251811

O -2.656051 -0.726641 0.814855

H -0.000333 0.194941 -1.055994

H 0.917739 1.460548 -0.601724

H 3.007749 1.958899 -0.269192

H 2.460177 0.732191 0.533994

H 2.584527 -1.291415 1.773435

H 1.788959 -1.340025 0.445838

H -0.747697 1.548302 -0.538659

H -2.405443 0.922118 0.513953

H -2.080807 2.372233 1.011710

H -1.890028 -1.189416 0.435619

H -3.432996 -1.193649 0.519033

17

MP2=-841.4598022

Cl -0.072011 -1.655776 -0.531408

O 0.041511 1.151955 -1.038956

O 2.240919 1.649233 0.180510

O 2.620674 -0.911351 0.855729

O -2.065274 1.836355 0.258094

O -2.751745 -0.708020 0.752669

H -0.007290 0.116124 -0.966627

H 0.910551 1.430322 -0.590735

H 3.001984 2.004125 -0.294105

H 2.505415 0.758117 0.523220

H 2.733969 -1.309519 1.726263

H 1.829786 -1.338233 0.461258

H -0.753678 1.518694 -0.522585

H -2.456534 0.958423 0.496130

H -2.046713 2.364922 1.064420

H -1.963848 -1.186051 0.415248

H -3.516499 -1.170308 0.390397

$HCl(H_2O)_5$ separated ion

17

E(RB+HF-LYP) = -842.829663417

Cl 1.714300 1.005045 -0.090113

H 1.162835 -0.261638 1.469838

H 1.332335 -1.448527 2.483032

H -0.249886 -1.574331 0.923829

H 1.156741 -0.470380 -1.455242

H 1.337820 -1.801728 -2.263945

H -0.236569 -1.692950 -0.697454

H -0.210835 1.951151 -0.138635

H -1.202608 2.919121 0.547149

H -1.580930 -1.118223 0.059902

H -2.120815 0.874214 -0.016188

H -3.252756 0.009318 -0.676425

O 0.694183 -0.971386 1.959639

O -0.822729 -1.794939 0.119911

O 0.693693 -1.252707 -1.824941

O -1.149244 2.209602 -0.087499

O -2.575707 0.000457 -0.005104

17

MP2=-841.4592466

Cl 1.632808 0.977246 -0.105162

H 1.153515 -0.260791 1.471421

H 1.369164 -1.467951 2.463613

H -0.235060 -1.578013 0.934833

H 1.139511 -0.488249 -1.471389

H 1.364793 -1.842911 -2.243990

H -0.225592 -1.708710 -0.699764

H -0.230079 1.990440 -0.134792

H -1.215219 2.943119 0.598901

H -1.564297 -1.101366 0.061823

H -2.114153 0.898483 -0.013860

H -3.205575 0.010918 -0.725086

O 0.692219 -0.970631 1.989704

O -0.817467 -1.809143 0.126824

O 0.683266 -1.280919 -1.856721

O -1.175392 2.261904 -0.082380

O -2.562613 0.008673 -0.006222

$HBr(H_2O)_4$ intact

14

E(RB+HF-LYP) = -319.553977267

O -0.082454 2.250006 0.058497

O -2.660158 1.572892 0.140056

O -3.071208 -1.068001 -0.252234

O -0.723244 -2.400911 0.191745

Br 1.849005 -0.100351 -0.038561

H 0.906034 1.049301 0.010674

H 0.025333 2.885266 -0.645162

H -1.032055 2.014094 0.104415

H -2.850506 0.632033 -0.025322

H -2.269152 -1.589005 -0.089190

H -3.200721 1.844084 0.876410

H -3.473936 -1.410397 -1.044932

H 0.046803 -1.836869 0.073586

H -0.570481 -2.908113 0.984641

14

MP2=-318.8187096

O -0.072549 2.266062 0.065362

O -2.707431 1.601136 0.151587

O -3.094376 -1.078085 -0.280062

O -0.708140 -2.400480 0.212286

Br 1.885269 -0.155679 -0.085253

H 0.983149 0.979097 -0.012432

H 0.014352 2.934522 -0.625025

H -1.032515 2.044323 0.114215

H -2.894719 0.653140 -0.027769

H -2.279993 -1.594059 -0.106467

H -3.249880 1.841271 0.911148

H -3.469893 -1.432837 -1.093586

H 0.074562 -1.838738 0.089059

H -0.554576 -2.885647 1.031558

$HBr(H_2O)_4$ contact ion

14

E(RB+HF-LYP) = -319.561467028

O 0.600033 1.678855 -0.876457

O -0.539058 2.305302 1.337810

O 2.849849 0.644415 -0.554766

O 1.978282 -1.666219 0.367049

Br -1.141383 -0.663277 -0.035173

H -0.006175 0.868134 -0.866178

H 0.302476 2.164070 -0.061255

H 1.558451 1.331738 -0.775945

H -0.976886 1.441577 1.341225

H -1.196288 2.966668 1.539211

H 2.665683 -0.244294 -0.176112

H 1.014149 -1.586124 0.284259

H 3.471002 0.544457 -1.271564

H 2.152089 -2.070242 1.213003

14

MP2=-318.8202705

O 0.284145 0.283385 1.928320

O 2.435314 1.074882 0.686793

O -1.645325 1.886129 1.669053

O -2.164817 1.199497 -0.848949

Br 0.279481 -0.977687 -0.788253

H 0.183701 -0.313684 1.084829

H 1.149972 0.743669 1.737375

H -0.495260 0.960042 1.905504

H 2.157372 0.508846 -0.060520

H 3.375590 0.912353 0.828679

H -1.939534 1.748951 0.730051

H -1.518804 0.481231 -1.021565

H -2.427676 1.820320 2.230017

H -2.150350 1.764659 -1.630541

$HBr(H_2O)_4$ separated ion

14

E(RB+HF-LYP) = -319.564700494

O 0.028297 -0.351559 2.808586

O -1.278862 1.803948 2.571046

O 2.127487 0.571977 1.753885

O -0.690157 -1.510147 0.681480

Br -0.118054 1.465527 -0.401076

H -0.311287 -0.930750 2.054140

H 0.940884 -0.017998 2.521779

H -0.567576 0.460927 2.844252

H 1.712312 0.950003 0.956046

H 2.742752 1.213307 2.100379

H -1.085562 1.962278 1.626237

H -2.189731 2.032274 2.736394

H -1.466190 -2.005520 0.434057

H -0.601909 -0.746145 0.080146

14

MP2=-318.8233365

O 0.021025 -0.351984 2.816624

O -1.269028 1.833657 2.590319

O 2.132669 0.550971 1.740153

O -0.659665 -1.533332 0.669365

Br -0.129594 1.450375 -0.359200

H -0.317586 -0.933912 2.049310

H 0.942086 -0.013383 2.520601

H -0.578008 0.472265 2.847725

H 1.685993 0.939122 0.950000

H 2.733650 1.222567 2.085922

H -1.069713 1.965692 1.630490

H -2.203973 2.033006 2.721767

H -1.470616 -1.993527 0.421582

H -0.574834 -0.743393 0.082694

$HBr(H_2O)_5$ intact

17

E(RB+HF-LYP) = -395.963551910

O 0.637346 0.445354 1.770349

O 1.818357 1.755859 -0.248778

O 3.904287 -0.061085 -0.243147

O 1.880887 -1.724354 0.414764

O 0.288776 -0.346073 -1.533000

Br -2.427728 -0.017892 -0.031995

H 0.970429 -0.429712 1.540865

H -0.317009 0.396267 1.708588

H 0.771526 0.474678 -1.392947

H 0.771820 -1.011412 -1.030293

H -1.208121 -0.185511 -0.826017

H 2.737373 -1.310492 0.209751

H 2.037608 -2.633531 0.653954

H 4.471808 -0.085742 -1.008025

H 3.351291 0.730011 -0.311109

H 1.365047 1.450705 0.562981

H 1.793326 2.708701 -0.259918

17

MP2=-395.0703989

O 0.613473 0.448029 1.774062

O 1.821587 1.777241 -0.245287

O 3.916875 -0.062737 -0.251833

O 1.883993 -1.743041 0.438488

O 0.300096 -0.356864 -1.573733

Br -2.420071 0.002668 0.004948

H 0.948757 -0.437760 1.543918

H -0.349682 0.385660 1.699408

H 0.797520 0.467442 -1.436916

H 0.795948 -1.022590 -1.065214

H -1.242324 -0.175081 -0.811328

H 2.749774 -1.327480 0.227138

H 2.062689 -2.655664 0.694360

H 4.450781 -0.086923 -1.054007

H 3.358229 0.737991 -0.312316

H 1.349395 1.463414 0.565363

H 1.809983 2.741466 -0.221028

$HBr(H_2O)_5$ contact ion

17

E(RB+HF-LYP) = -395.976685466

Br -0.115454 -1.480227 -0.358171

O 0.120028 1.486404 -1.127554

H 0.027779 0.488327 -1.031828

H 1.005352 1.743277 -0.707739

O 2.319426 1.957177 0.020271

H 3.092664 2.214827 -0.475123

H 2.535160 1.135091 0.511682

O 2.634187 -0.423225 1.132422

H 2.691613 -0.653157 2.055755

H 1.897767 -0.932796 0.758648

H -0.663899 1.907518 -0.645141

O -1.927135 2.318982 0.102679

H -2.340128 1.517472 0.489333

H -1.923314 3.004008 0.765555

H -2.015775 -0.618574 0.752498

O -2.736023 -0.030943 1.031207

H -3.550197 -0.465209 0.790146

17

MP2=-395.0767548

Br -0.122516 -1.464488 -0.194830

O 0.108712 1.425446 -1.095492

H 0.019241 0.420632 -0.917060

H 1.000158 1.715704 -0.689252

O 2.330063 1.992361 0.018841

H 3.090185 2.260207 -0.511792

H 2.585856 1.159106 0.492106

O 2.705582 -0.427774 1.081859

H 2.831621 -0.683728 2.003166

H 1.920482 -0.924409 0.766917

H -0.670960 1.881900 -0.618304

O -1.938451 2.360468 0.107422

H -2.391835 1.552985 0.461161

H -1.883660 2.995858 0.831114

H -2.081981 -0.612837 0.719474

O -2.825043 -0.017664 0.954847

H -3.625395 -0.464817 0.654462

$HBr(H_2O)_5$ separated ion

17

E(RB+HF-LYP) = -395.977884030

Br -1.669143 0.211428 -0.038808

H -0.436620 -1.013933 -1.503316

H -0.036850 -2.313066 -2.275176

H 1.346913 -1.530007 -0.711499

H -0.459778 -0.817651 1.586497

H -0.054860 -1.987865 2.543619

H 1.348561 -1.412878 0.913015

H -0.092729 1.922509 -0.125595

H 0.485433 3.157864 0.594993

H 2.353125 -0.446930 0.020802

H 2.077660 1.605521 -0.039163

H 3.433260 1.236168 -0.739398

O 0.315030 -1.538215 -1.844826

O 1.936433 -1.374724 0.092419

O 0.292177 -1.277792 2.010083

O 0.687314 2.499920 -0.065098

O 2.826031 0.965848 -0.055891

17

MP2=-395.0772054

Br -1.575811 0.207944 -0.052561

H -0.418575 -1.020383 -1.520151

H -0.046664 -2.356233 -2.260086

H 1.338928 -1.545934 -0.718134

H -0.450174 -0.809446 1.586625

H -0.081211 -2.010333 2.534211

H 1.336713 -1.424937 0.922761

H -0.097916 1.958603 -0.116241

H 0.485451 3.183642 0.636865

H 2.332767 -0.441375 0.022291

H 2.064457 1.622791 -0.037223

H 3.399142 1.223630 -0.777291

O 0.332662 -1.554326 -1.880018

O 1.934339 -1.390418 0.095513

O 0.297183 -1.272140 2.041149

O 0.686691 2.548010 -0.060445

O 2.813977 0.967096 -0.054609

II. FULL CITATIONS FOR ITEMS [51] AND [52]

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