Supplementary materials

Table 1. Absolute energies (in -au) and zero-point vibrational energies (ZPVE in kcal mol^{-1}) of al computed structures in the present study.

structure	HF/6-31+G* (C,H,Li) 3-21G (Br, Zn,Mg) optimization	ZPVE (x 0.89)	B3LYP/6-311+G* energy
1	78.03548	30.5	78.60801
2	4445.61235	41.9	4470.88157
3	4523.67374	74.2	4549.48741
4	4523.70167	76.6	4549.51759
5	84.86688	24.4	85.50337
6	4530.59989	67.8	4556.45889
7	4530.54015	70.1	4556.43039
8	123.92103	40.7	124.85510
9	4406.57538	25.4	4431.55482
10	1962.95236	66.3	1974.66839
11	2836.05415	25.1	2852.32726
12	7281.73996	68.1	7323.24727
13	7291.70300	70.1	7323.23919
LiBr	2567.59190	0.8	2581.75531
TS1	4523.63872	76.2	4549.47241
TS2	4530.53030	68.8	4556.42085
TS3	7281.69645	69.1	7323.22356
TS4	4608.60317	102.5	4635.06453
TS5	4608.59895	102.4	4635.06280
TS6	4608.60295	102.5	4635.06361
TS7	4608.59761	102.2	4635.05910

Structures (xmol (xyz) coordinates in Å)

6 (number of atoms)
1 (number of structure in text)
C 0.000000000 0.000000000 0.000000000
C 1.321081000 0.000000000 0.000000000
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H-0.565915576-0.915162290 0.000000000
H 1.886996576 0.915162290 0.000000000
H 1.886996576-0.915162290-0.000000000

10
2
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C-3.511966339 1.135897190-0.242672488
C-2.828546403 0.249747769 0.468237259
H-3.566348059 1.081462617-1.317596962
H-2.824522112 0.364209387 1.542305408
C-2.029366441-0.893452004-0.058521349
H-2.199092972-1.775494889 0.552149481
H-2.341306499-1.133866718-1.070582712
Zn-0.211505915-0.450541715-0.049275209
Br 2.043987230 0.288149112 0.015418911

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H 4.797181197 0.151660927 0.177367639
C 3.914163406-0.247098181-0.289744047
C 2.927212252-0.774706595 0.427361335
H 3.884293101-0.224947555-1.367527067
H 3.045503850-0.777414434 1.502199424
C 1.647444902-1.336254233-0.074668883
H 1.757505598-1.652083657-1.110483478
H 1.391408800-2.224668757 0.497752542
Zn 0.124077082-0.167549483 0.005946859
Br-2.281113388-0.264822531-0.017242477
C 0.680977599 2.053508431-0.641451490
C 0.604732920 2.084597963 0.684898169
H 1.615023110 1.849495822-1.135491385
H-0.179519517 2.266137601-1.251545042
H 1.476677282 1.907019476 1.290374361
H-0.318603770 2.319789362 1.184063407

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Zn-0.076988643-0.306053485-0.225657579
C-0.897401540 1.924123873-0.478399124
C-1.677699204 1.356885162 0.440056268
H-0.021217111 2.482928798-0.204391339
H-1.156369695 1.889862461-1.524443776
H-1.388153331 1.446182649 1.478240648
H-3.740482800 0.978126033 0.750978392
H-3.196932775 0.686319306-0.887573671
H-1.304299940-2.496824443 0.058750268
H-2.535081485-1.034281935 1.541206545
H-3.663342569-1.443321256 0.282357865
H-1.869726703-1.669016289-1.361244108
Br 2.282915241-0.002880810 0.144115498

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H 0.019678906-1.617745259 0.000000000
H-1.638150784-0.885039285 0.000000000

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H-1.897009810-1.679382725 1.746654017
H-2.053799874-2.209890124 0.064935683
Zn-0.754124186 0.062934512 0.359533949
C 0.789533176 1.889368395 2.195485212
C-0.273207902 1.655027503 1.419956910
Li 1.270833016 1.751129526-0.156542407
Br 0.581278841 0.450720866-1.906794003
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H 0.876653716 2.742788413 2.851400775
H 1.611802081 1.187480109 2.261587025
H 0.419712207-2.006262884 2.893303474
H 1.695657710-2.868793166 1.894878173
H 0.296722309-2.806208894-0.039876157

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C-1.167051926-1.186136690 0.729660123
Li-0.245075633 0.734452169 1.021206123
C-1.664899376 2.426981386-0.139778877
C-2.510425524 1.451545514 0.180932123
Zn 0.410661065-1.242459930-0.211041877
Br 2.051297347 0.606278820 0.029929123
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H-2.186455714 0.204217465-1.523537877
H-1.117196043-1.951345698 1.501439123
H-3.277169903-1.038746369 1.036299123
H-2.903743037-1.912997426-0.410184877

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C-0.101668029-0.070950103-0.542750357
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C 0.837209413 0.910562847-0.231475656

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H 0.622027332 1.617012723 0.562583211
Li 0.918591325-0.702202768 1.163982011

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H 1.681759438 4.107510575 0.000000000
C 1.610505746 3.031043717 0.000000000
C 0.448781698 2.390670643 0.000000000
H 2.556047833 2.513919748 0.000000000
H-0.419878324 3.034413000 0.000000000
Zn 0.107283843 0.578064549 0.000000000
Br-0.554061969-1.700801884 0.000000000

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C-0.511271063 1.979973653-0.503504809
Zn 0.521555559 0.395567516-0.366327484
C 0.886308047-1.492731495-0.317427991
C-0.393005975-2.012735336 0.246582542
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H 1.731077860-1.792205817 0.292929575
H-1.226417303-2.042917127-0.441385718
H-1.596957336-2.727099443 1.811379245
H 0.156414631-2.405481600 2.241646291
H-0.484094829 2.576089221-1.405525698
H-1.940730074 3.327476259 0.297326700
H-1.460215910 1.953305417 1.385537090

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H-2.770933116-2.392180980 0.000000000
H-4.407181022-1.607363917 0.000000000
Br 1.591337096 0.385035209 0.000000000

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C-2.383797875 0.222395590-3.244216562
C-1.468828492-0.944301555-3.099633475
Zn-0.827742388-0.816511039-1.292552359
C-1.878621719-1.138122673 1.452923978
C-1.677832146-0.292874975 0.431272552
Br 1.658781093-1.126121093-0.402771954
Mg 0.367321845 0.230743179 1.301926224
Br 1.023032623 1.917367390 2.877312335
H-0.657606954-0.887311779-3.818242170
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H-2.367233987 0.542306855 0.425219432
H-2.658193816-1.009861594 2.187874196
H-1.291748716-2.039445331 1.576490851
H-3.362445229 0.107141018-2.799078320

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C 3.242466946 4.121355922-0.877103570
C 2.273698034 3.843084082-0.021213696
H 3.860261647 3.351489680-1.308527000
H 1.687807051 4.654262645 0.383730546
C 1.897133090 2.468287639 0.455369715
H 2.584569609 1.744330230 0.008196066
H 2.040988533 2.411044773 1.533609878
C 0.445635610 2.083277650 0.140595841
H 0.326230305 2.096867605-0.941882280
H-0.185118094 2.891592220 0.511021573
H 0.062631460 0.802874069 1.821988875
Zn-1.719312023 0.285193252 0.309044819
Br-3.867636580-0.506797008-0.355412072
Br 3.085396606-2.428368590-0.121866551

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TS1
H-0.708340122-2.398733263 0.335542917
C-1.211615016-1.628444647-0.230784010
C-2.447109937-1.210040121 0.309703786
H-1.215998695-1.820357426-1.296409496
H-2.597493909-1.381207041 1.365717566
C-3.377841124-0.436706648-0.333336746
H-3.358079655-0.378489066-1.408768279
H-4.328167325-0.245390063 0.132781650
Zn-0.011891558-0.030659308-0.090983911
Br 2.394145563-0.014668723 0.163501984
C-2.491556473 1.579690872 0.013581351
C-1.100896640 1.682164942-0.105386558
H-3.130657097 1.865499145-0.797983579
H-2.945843897 1.645177575 0.982826101
H-0.757540544 2.154429242-1.015498881
H-0.622111595 2.072269029 0.786072939

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TS2
H-1.576952133-1.551146568-1.901426494
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C-2.147496072 0.435894621-1.443216267
H-2.396140254-1.315398418-0.288828210
C-1.574124021 1.160973639-2.510761784
H-1.210933694 0.576306918-3.341186385
H-2.109732645 2.048488142-2.810229378
Zn 0.064478001-0.437816817-0.363165337
Br 0.818820279-0.522573027 2.085021191
C 0.029149758 1.899066112-1.823799352
C 0.974245194 0.955689630-1.287452922
Li 1.740482182 1.181439384 0.628041166
H 1.709369591 0.651732612-2.026625527
H 0.307811316 2.430348992-2.724414067
H-0.443506832 2.578201042-1.128384175

H-2.715111969 1.006441775-0.722576407

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TS3
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C 1.619523776-3.214189422-0.549589232
C 0.868536821-3.559476764 0.578590524
H 2.683968773-3.120304864-0.403733437
C-0.500546805-3.842183782 0.596416015
H-0.941229561-4.207635143-0.316730782
H-0.891838498-4.290599862 1.494360957
Zn 0.845303455-1.348948677-0.687824480
Br 1.801282633 0.954024261-0.129795009
C-1.385102306-2.062268471 0.671842218
C-1.062648304-1.186033862-0.412462416
Mg-0.921901105 0.899392310 0.034877036
H-1.691560208-1.383344344-1.275233595
H-2.363592435-2.514487778 0.705652776
H-1.040041742-1.809649933 1.662453426
H 1.347138447-3.424451385 1.537658569
Br-2.085884360 2.967742511 0.501046560

22
TS4
H 0.265782073-2.777090504 0.283701363
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C-0.985989395-1.547539068 1.480616028
H 1.084393924-1.909643515 1.663905870
C-2.213984238-1.561423709 0.769454059
Zn 0.414580075-0.348249731-0.340841233
Br 2.200501388 1.499480694-0.256788871
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C-1.211558098 0.338937092-1.058128499
Li-0.028362669 2.040175209-1.050567864
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H-3.253017253-0.042764780-0.530749235
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H-2.753267751 2.066646569 0.683801007
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H-3.407209238-2.534291153-0.730860791
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H-2.270925620-3.611462912 0.061416745

22
TS5
H 0.553730357-2.727867249 0.451049361
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C-0.900150918-1.588231017 1.480081620
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C-2.050410368-1.751754007 0.666457227
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H-3.063264027 0.710299261 1.423774318
H-1.417664098 1.244660426 1.122390786
H-1.904251544-2.452019432-0.143208254
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H-3.513589090-2.995321899 1.664064704
H-3.458446599-1.359164386 2.277987210

22
TS6
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H 0.771273083-1.284240870 2.334761147
C-2.262546265-1.328654295 0.722269881
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Br 2.284585126 1.573323172 0.059275893
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C-0.886013002 0.196069847-1.224271688
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H-3.150865251-2.811694539-0.564591025
H-1.423612289-2.620631530-0.789259201
H-2.041524042-3.484006508 0.610859573
H-2.303015225 0.889769589 0.222149409
H-3.582533630 0.863082188-1.930304609
H-3.315898511-0.860839149-2.062067346
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22
TS7
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H 1.302971591-2.107960987 1.275754574
C-2.047604904-1.505273259 0.794818182
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Br 2.340733340 1.502392914-0.052542960
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C-1.026180269 0.420028345-1.088266312
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H-1.195032439 0.268949679-2.152061213
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H-2.387173395 0.710907076 0.549909480
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H-3.286151726-0.909960211-1.880572604
H-4.304978858-0.506508662-0.504713695