Electronic Supplementary Material (ESI) for RSC Advances.

Theoretical insights into structure, bonding, reactivity and importance of ion-pair interactions in Kirby's tetrafluoroboric acid salts of twisted amides

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Supporting Information

Table S1. Energies (in Hartree) of the amides (**1**-**3**), products of hydrolyses (**4**-**7**), transition states (**8**,**9**), cations ($\mathbf{1}^+$-$\mathbf{3}^+$), $[BF_4]^-$ and water.

	Energy			
	Gas-phase	Disp	Methanol	Acetonitrile
(**1**)				
PBE-D3(BJ)	-905.203138	-0.037741		
PBE0-D3(BJ)	-905.259820	-0.033263	-905.294931	-905.295176
TPSS-D3(BJ)	-906.339605	-0.047373		
TPSSH-D3(BJ)	-906.250163	-0.044092		
(**2**)				
PBE-D3(BJ)	-944.481850	-0.042235		
PBE0-D3(BJ)	-944.546366	-0.037320	-944.580977	-944.581219
TPSS-D3(BJ)	-945.681865	-0.053022		
TPSSH-D3(BJ)	-945.589181	-0.049402		
(**3**)				
PBE-D3(BJ)	-1023.038753	-0.051421		
PBE0-D3(BJ)	-1023.118924	-0.045660	-1023.152744	-1023.152979
TPSS-D3(BJ)	-1024.366619	-0.064606		
TPSSH-D3(BJ)	-1024.266632	-0.060279		
(**4**)				
PBE0-D3(BJ)	-981.673895	-0.036525		-981.706280
(**5**)				
PBE0-D3(BJ)	-1020.957669	-0.041024		-1020.988798
(**6**)				
PBE0-D3(BJ)	-1020.953706	-0.041804		-1020.988631
(**7**)				
PBE0-D3(BJ)	-1099.526562	-0.050246		-1099.561500
($\mathbf{1}^+$)				
PBE0-D3(BJ)	-480.791764	-0.027560	-480.878626	-480.879174
($\mathbf{2}^+$)				
PBE0-D3(BJ)	-520.079653	-0.031569	-520.164562	-520.165100
($\mathbf{3}^+$)				
PBE0-D3(BJ)	-598.653675	-0.039744	-598.735962	-598.736486
$[BF_4]^-$				
PBE0-D3(BJ)	-424.313600	-0.001483	-424.407606	-424.408182
H_2O				
PBE0-D3(BJ)	-76.381111	-0.000277		-76.392227

Table S2. Numerical Frequencies (cm^{-1}) and enthalpies of amides (**1-3**), hydrolysis products (**4-7**) and transition states (**8**, **9**) at DFT/PBE-D3(BJ) in acetonitrile.

1-Azatricyclo[3.3.1.1^{3,7}]decan-2-one, tetrafluoroboric acid salt (1)

The IR spectrum

wavenumber	T**2
22.59	0.4861
53.99	1.4722
61.50	5.1176
71.00	0.2984
88.15	10.1280
107.60	7.3856
176.15	38.0423
270.98	2.1570
274.07	4.2863
331.11	0.1734
353.62	7.1343
359.29	2.0915
364.49	0.3173
385.08	0.2911
423.13	5.6874
433.56	16.9584
465.40	43.5342
482.61	15.4873
483.95	9.1238
503.34	46.8857
574.46	78.3162
611.66	37.4127
624.47	0.0509
687.75	54.3342
700.02	98.9735
761.99	0.3659
768.95	17.8418
805.02	2.4767
816.01	94.7897
844.11	247.6080
848.08	64.5144
872.62	4.7345
881.23	0.8191
896.91	5.6420
942.09	12.1384
948.36	13.3099
978.27	2.6811
999.97	117.3191
1004.17	55.7239
1009.93	349.9247
1025.02	170.2227
1032.47	0.3054
1060.40	2.6699
1081.84	3.0648
1087.12	0.0913
1098.81	50.6453
1138.48	23.6969

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   1155.56      99.0420
   1158.64     500.8882
   1189.36      13.1908
   1224.43       6.3351
   1240.35       9.6688
   1267.90       8.1087
   1279.95      13.8495
   1297.31       5.9513
   1299.27       2.9939
   1301.23       8.0276
   1320.91       0.7743
   1328.28       4.7505
   1333.34       0.1754
   1336.68       1.3210
   1359.75       2.9687
   1423.91      17.4806
   1425.29      18.3832
   1437.44      27.7073
   1442.42      11.0795
   1448.44      20.5054
   1463.95       8.9916
   1485.60      28.6795
   1814.94     534.8474
   2554.27    2470.7766
   2974.14      48.1671
   2976.49      29.1568
   2977.80      28.9441
   3001.16       9.7804
   3003.36      29.8995
   3008.04      32.9557
   3013.95      12.0949
   3019.14      36.8226
   3022.15      22.8700
   3022.55      40.2025
   3035.52      15.1417
   3062.68       3.7718
   3064.12       6.3292

ENTHALPY
Total free energy                        ...   -904.98976722
Thermal Enthalpy correction              ...         0.00094421
------------------------------------------------------------------
Total Enthalpy                                 -904.98882301 Hartree
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3-Methyl-1-azatricyclo[3.3.1.1^{3,7}]decan-2-one, tetrafluoroboric acid salt (2)

```
The IR spectrum
     wavenumber  T**2

     24.00       0.5319
     50.00       2.7561
     59.03       3.1532
     62.96       1.4060
     90.19       9.9609
    106.13       7.3633
```

173.85	41.6314
217.47	0.0847
241.86	0.3669
243.33	0.0645
302.24	14.3130
323.15	0.6826
331.30	0.3246
353.69	10.8605
363.10	0.3444
366.17	0.1846
388.99	0.1864
407.84	10.9952
431.59	6.1394
474.33	13.9515
483.30	9.3586
484.51	15.8671
503.01	43.2068
546.25	4.5460
596.81	70.1857
631.51	0.4816
652.50	78.7501
697.92	109.3251
764.71	0.0518
770.95	56.9508
795.40	13.9989
811.60	1.4890
818.18	174.4130
846.66	198.9887
872.59	0.7963
875.22	3.8677
894.99	0.2869
909.08	18.9782
944.53	29.7970
953.84	41.3665
967.13	30.0031
979.60	6.7007
1004.83	188.4060
1015.35	255.6368
1017.54	191.8456
1035.71	21.1821
1057.66	0.6251
1078.76	3.2813
1082.11	4.1024
1115.67	3.9696
1140.35	34.5157
1153.60	354.3791
1156.41	8.4312
1161.21	247.3631
1184.36	0.3079
1237.79	3.8358
1263.94	24.3090
1269.70	4.8259
1279.11	6.6051
1298.95	4.2705

```
   1299.96       4.7499
   1320.41       0.0407
   1326.33       2.8810
   1329.59       0.8427
   1336.47       0.4520
   1359.98      13.5841
   1362.73       1.8114
   1420.68       0.2052
   1424.31      25.1417
   1427.06      22.5111
   1429.91       2.1830
   1439.10      42.4021
   1443.50       5.9263
   1446.67      29.4522
   1461.33      15.4470
   1486.68      25.2827
   1807.14     486.3938
   2558.27    2506.7281
   2966.12      36.7675
   2968.17      34.7011
   2975.55      37.8134
   2981.02      27.4621
   2999.45      11.7015
   3002.63      36.6588
   3006.45      24.0886
   3011.50      25.9297
   3014.03      23.4014
   3016.30      17.8595
   3020.45      43.8064
   3057.89      23.9475
   3058.40      22.6025
   3060.64       3.9266
   3066.96       4.8093

ENTHALPY
Total free energy                  ...   -944.23983925 Hartree
Thermal Enthalpy correction        ...      0.00094421 Hartree
------------------------------------------------------------------
Total Enthalpy                     ...   -944.23889504 Hartree
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3,5,7-Trimethyl-methyl-1-azatricyclo[3.3.1.1^{3,7}]decan-2-one, tetrafluoroboric acid salt (3)

```
The IR spectrum
     wavenumber  T**2

     44.12       3.0516
     56.84       2.2884
     58.22       1.7705
     79.42      10.5130
    103.13       6.4323
    169.67      35.2049
    211.93       0.0231
    215.19       0.0185
```

219.09	0.0060
232.07	0.0481
232.82	0.0923
234.82	0.2629
246.10	0.8310
247.83	0.3465
295.38	0.0067
313.52	13.3234
331.02	0.5476
353.65	11.0609
367.54	0.3533
377.24	1.9006
396.27	0.4241
408.90	6.4080
425.40	20.5489
429.88	2.4600
479.27	1.3697
483.64	7.3856
490.52	27.2518
501.11	0.3389
502.95	41.6501
510.17	0.1830
556.64	3.7862
656.83	168.3334
682.35	61.0762
702.51	46.3468
758.89	0.2848
789.62	0.0243
819.01	79.9529
840.14	205.8352
845.70	9.0857
864.82	140.6876
872.60	7.7868
880.67	0.0835
890.44	1.1163
902.45	12.8871
916.23	12.1989
937.56	1.9920
956.31	1.1598
967.85	5.9333
989.58	153.3307
992.57	32.8969
1003.51	151.4540
1006.14	22.5526
1017.50	356.9940
1073.44	2.4207
1078.35	1.1616
1084.59	1.0961
1089.69	0.6897
1109.49	26.8744
1153.32	638.3387
1161.94	0.9239
1171.49	5.6027
1203.55	0.1948

1210.00	1.0453
1227.14	2.3984
1249.45	0.7625
1261.68	5.7938
1274.92	6.5926
1285.83	10.5572
1296.43	3.3464
1305.44	7.5884
1325.14	0.7798
1333.49	0.6034
1351.49	1.5933
1356.34	10.1289
1359.72	9.6630
1362.19	8.8298
1417.84	1.4076
1420.84	9.6330
1425.84	12.0704
1427.87	14.4186
1428.17	3.4193
1430.21	4.4489
1432.29	19.5768
1434.24	26.3777
1437.60	46.5177
1440.98	18.0292
1446.72	12.5709
1458.21	17.0089
1484.49	22.3953
1808.32	499.9433
2567.56	2577.278
2955.42	52.4881
2958.54	34.0129
2961.36	23.1612
2966.45	64.2689
2968.27	30.0424
2981.17	25.5622
2996.16	17.0713
3002.58	31.5193
3005.26	25.8265
3006.62	38.9290
3009.04	10.5064
3039.60	34.7740
3041.73	36.5647
3045.09	34.3021
3045.40	32.8964
3055.91	4.2644
3058.54	22.6291
3059.26	25.6405
3061.95	6.3801

ENTHALPY

Total free energy	...	-1022.73981113 Hartree
Thermal Enthalpy correction	...	0.00094421 Hartree
Total Enthalpy	...	-1022.73886692 Hartree

(4)

The IR spectrum

wavenumber	T**2
28.93	5.1471
34.40	0.8971
48.71	2.6739
60.12	6.5734
90.04	10.3652
101.86	9.0467
127.57	7.7925
152.94	15.4640
196.14	32.1641
260.78	13.9625
268.43	0.3525
317.24	31.0110
327.71	0.0960
348.66	8.3831
358.97	0.6240
364.24	4.6192
385.91	1.0942
413.13	5.2468
460.83	1.3601
483.64	2.3043
487.37	3.0179
496.18	1.6596
510.64	76.7758
533.16	27.4771
572.73	1.5900
639.41	7.0220
689.64	227.4305
714.47	36.0084
726.11	264.8600
742.84	75.8130
755.55	30.7167
780.29	26.0931
834.08	2.7403
848.89	237.1383
856.18	14.4783
876.88	89.0100
893.23	56.2294
905.04	1.7587
923.77	11.8861
940.36	20.8644
951.39	29.0726
976.78	425.9255
993.16	44.1868
1031.26	3.1352
1055.23	49.8487
1066.31	56.2668
1073.21	55.5398
1081.94	90.3565
1099.38	4.0129
1119.47	357.3056

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   1125.90      13.4684
   1151.44     227.7222
   1167.39     325.6512
   1178.92      27.6284
   1211.13       8.3634
   1232.16      17.8351
   1265.21       4.6298
   1268.93       4.2007
   1293.87      13.8111
   1298.95       9.6419
   1306.69       3.4049
   1309.15      11.6234
   1323.17      14.9889
   1331.42       0.4008
   1345.14       0.9946
   1348.43      10.8272
   1352.69       6.2535
   1372.43       0.9805
   1397.69      10.1974
   1418.28      20.2247
   1426.91      10.4520
   1433.11      16.2781
   1440.02      29.6783
   1450.39       9.9441
   1463.26      50.3658
   1690.14     154.8615
   1737.55     549.5540
   2946.66    1490.8693
   2964.96      32.9808
   2968.23      17.1185
   2976.69       1.7862
   2981.01      33.6431
   2986.28      55.2180
   2991.32      23.4267
   3000.98      33.2095
   3007.48      43.5819
   3010.65      35.8820
   3029.56      17.8648
   3036.43      25.7682
   3052.98      16.6330
   3070.32       6.8973
   3248.40     491.4892
   3350.20     601.6440

ENTHALPY
Total free energy                ...   -981.37180406 Hartree
Thermal Enthalpy correction      ...      0.00094421 Hartree
------------------------------------------------------------------
Total Enthalpy                   ...   -981.37085985 Hartree
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(5)

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The IR spectrum
     wavenumber  T**2
     10.01       8.9302
     37.64       5.6974
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56.05	0.4306
70.18	1.1907
93.59	8.9227
104.67	6.8768
111.76	11.1831
124.47	0.5717
173.95	41.8483
223.55	0.7459
227.43	11.2356
254.76	0.9882
284.52	12.6098
289.03	9.4185
313.11	18.4573
332.29	1.2414
354.07	0.5456
364.39	3.2173
367.96	0.6288
393.37	0.1804
420.48	5.1883
461.59	9.1560
483.10	0.4349
486.90	7.1234
490.02	16.4142
504.13	29.2927
530.04	31.1721
553.58	5.3589
624.28	360.4729
643.59	55.0688
698.31	27.6467
711.84	83.0573
753.57	52.6365
762.51	9.8816
772.42	1.3319
778.49	94.4288
823.57	10.9616
840.75	59.3225
850.18	2.6251
872.56	164.1615
893.26	3.3955
906.71	9.8172
926.02	11.4410
943.77	33.0638
964.76	16.6498
982.15	230.3687
987.28	175.3674
999.26	70.7466
1037.04	34.7865
1038.98	7.2122
1059.07	11.8656
1074.18	59.1747
1088.19	62.5672
1103.33	153.5734
1116.05	6.6875
1141.63	66.8956

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   1147.86     334.4443
   1166.56     428.9627
   1187.77      15.8262
   1223.50       5.7043
   1261.18       8.0377
   1268.60       5.3956
   1273.29       6.0357
   1289.67       6.6666
   1305.12       5.0139
   1317.08      10.9589
   1325.72       1.2756
   1329.52      10.1153
   1335.92       1.4838
   1344.78       0.7024
   1349.90       0.5045
   1362.58      12.2242
   1374.99       0.2897
   1384.04      12.5492
   1410.95      18.7416
   1421.00       5.5702
   1428.28      11.9827
   1431.29      35.0427
   1435.26       3.3784
   1437.38      49.0274
   1450.49       7.4777
   1464.00      51.5115
   1628.97     328.9582
   1709.69     435.1735
   2924.04    1277.8169
   2962.81      35.4819
   2965.38      14.9787
   2968.94       3.2935
   2970.91      60.3187
   2980.80      50.4062
   2983.80      32.0831
   3003.87      33.2916
   3006.18      47.9517
   3010.97      35.2169
   3031.42      21.2192
   3038.65      23.3718
   3047.96      30.8588
   3053.18      29.8578
   3059.75      10.8084
   3070.74       4.9086
   3330.76     206.6532
   3469.39     344.9334
ENTHALPY
Total free energy                  ...  -1020.61768512 Hartree
Thermal Enthalpy correction        ...      0.00094421 Hartree
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Total Enthalpy                     ...  -1020.61674092 Hartree
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(6)

The IR spectrum

wavenumber	T**2
31.63	7.1310
39.37	0.6079
51.35	5.2530
54.87	2.0203
93.02	8.0660
157.32	51.5660
167.40	24.4807
188.02	136.2307
210.31	7.2921
254.63	6.2628
270.11	4.7966
276.04	2.3557
297.19	154.5789
305.17	27.2830
331.85	0.1605
346.65	35.8190
350.25	13.0124
366.88	0.7680
384.29	3.9050
418.16	11.4132
442.43	3.3939
449.80	3.0802
476.22	1.4040
483.06	10.2278
484.23	6.2469
501.91	39.4965
506.11	3.6081
517.45	19.9644
540.64	8.8291
627.53	71.9623
665.64	19.0511
686.00	5.7840
696.28	111.7790
772.37	35.0183
799.64	24.2516
809.89	2.3696
825.02	163.5718
848.35	226.8049
873.69	0.9713
877.09	9.2159
904.92	9.3400
906.12	2.6285
936.94	47.4435
942.53	91.2711
956.05	49.9595
974.55	29.3464
978.67	6.8129
1015.42	157.8625
1019.90	393.2318
1032.55	2.9869
1048.71	71.1739
1049.98	31.2182
1079.34	29.7566

```
   1083.93       3.4068
   1091.00     230.7436
   1123.64       3.4713
   1143.36      86.4368
   1147.56      92.8103
   1156.74     456.9571
   1171.68      35.2604
   1199.79      67.7494
   1240.54      27.9500
   1251.81       4.1244
   1256.22      81.6715
   1275.60       3.5477
   1280.33      76.2020
   1300.25      14.1704
   1300.81      11.0619
   1322.78       8.2538
   1325.28       9.5390
   1327.45       1.7444
   1328.98       2.3128
   1347.65       8.3829
   1360.16      11.0958
   1379.40      23.2527
   1421.39       6.8755
   1426.28      15.2099
   1429.19      25.4198
   1434.77      16.6675
   1441.49      20.3245
   1442.99      63.3102
   1449.09      44.3593
   1462.48      18.1609
   1507.08      71.1243
   2795.25    1847.2438     -
   2930.43      77.4465
   2969.07      41.6193
   2971.82      24.9212
   2978.98      39.5321
   2996.14      28.5478
   2999.64      36.3067
   3008.47      38.6409
   3012.88      46.0690
   3019.31      25.2829
   3025.63      26.6425
   3027.98      18.4585
   3046.51      28.1542
   3062.14      27.8881
   3068.77       8.8855
   3079.15       5.2711
   3636.35     136.6395
   3699.31      91.3798
ENTHALPY
Total free energy                ...  -1020.61280582 Hartree
Thermal Enthalpy correction      ...      0.00094421 Hartree
------------------------------------------------------------------
Total Enthalpy                   ...  -1020.61186161 Hartree
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(7)

The IR spectrum

wavenumber	T**2
28.80	7.6246
38.87	1.8795
46.59	5.6594
53.90	1.2162
91.18	9.0133
137.62	13.8548
160.12	144.8175
163.34	55.6065
204.68	2.2836
217.45	0.6021
219.44	0.1402
231.22	1.2574
233.90	7.8340
246.83	1.7146
257.00	1.2893
260.93	10.3476
274.52	3.9629
298.71	160.5482
313.09	7.8209
331.18	1.5436
335.76	9.7228
347.30	37.6645
350.45	10.8018
399.33	0.5535
414.99	1.3533
422.25	6.9293
435.67	7.6684
458.98	1.7754
477.89	1.2069
481.23	7.7820
484.26	7.5693
488.07	1.6510
497.15	20.7649
502.43	31.1596
546.99	15.2069
560.05	5.2084
610.78	6.5740
657.97	105.8747
693.71	109.7595
704.81	3.1969
782.19	0.1777
819.00	71.1576
844.90	215.0655
849.23	41.2460
866.00	147.1856
874.46	0.2388
876.14	2.1843
894.48	1.1938
900.27	27.3938
914.13	11.7036

935.02	41.6337
952.54	56.8761
958.64	5.4325
967.04	9.4250
984.74	29.7507
1000.99	19.8589
1019.82	451.3846
1027.58	54.1758
1031.92	84.0411
1072.82	143.3459
1078.98	15.4688
1082.28	5.7511
1087.24	18.4705
1096.11	159.0389
1097.52	17.3823
1152.32	616.0069
1172.78	51.4404
1197.81	82.1669
1203.63	0.4753
1213.42	5.2921
1230.50	4.2336
1247.58	0.5679
1256.11	54.0435
1260.96	61.8277
1272.25	18.2499
1280.81	55.7601
1295.49	20.1239
1304.27	9.1607
1314.35	9.2959
1335.20	1.6858
1342.97	10.4824
1353.14	4.4480
1354.86	15.1502
1357.80	10.2516
1377.84	24.8593
1419.77	2.8890
1422.22	3.1604
1426.50	4.6285
1427.86	11.2724
1428.50	14.9662
1431.37	18.3884
1433.49	36.8124
1435.89	8.6424
1440.78	36.7425
1442.23	42.0648
1450.58	40.0672
1460.75	19.1085
1506.50	66.1000
2789.00	1929.9345
2923.25	74.5013
2950.53	34.8148
2962.31	24.0461
2964.66	75.5930
2966.73	45.0917

```
   2979.14      34.7241
   2988.93      24.6164
   2994.82      39.1307
   3012.15      29.8691
   3018.70      18.1135
   3020.67      14.6039
   3033.98      25.0204
   3034.17      48.9334
   3040.93      33.3666
   3042.22      48.6676
   3047.42      28.2884
   3062.08      25.5561
   3063.08       8.7439
   3072.09       5.8976
   3637.66     134.7973
   3697.84      93.8715
ENTHALPY
Total free energy                ...  -1099.11350361 Hartree
Thermal Enthalpy correction      ...      0.00094421 Hartree
------------------------------------------------------------------
Total Enthalpy                   ...  -1099.11255940 Hartree
```

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(7)

```
The IR spectrum
     wavenumber  T**2
   -212.40       0.0000
     45.80       0.1682
     50.67       4.9198
     65.65      18.4385
     80.93       2.8229
    105.46       4.0329
    111.27      16.5992
    137.95       6.3223
    157.82      13.8145
    209.22      19.4885
    224.60       6.6970
    264.00       8.8213
    307.88      22.5328
    332.17       1.4027
    333.92       2.2350
    338.10      38.2098
    351.70      10.3589
    363.42      26.6938
    375.41       3.2266
    388.07      28.9695
    444.74      12.7178
    482.62      31.0705
    488.88       8.2455
    492.74       3.8600
    498.39      21.4647
    580.87      11.8027
    616.12      90.5304
    630.93       1.9421
    658.74      90.5815
    723.94      38.0237
```

736.29	105.7208
751.60	3.8015
768.73	76.2347
806.87	202.4599
856.42	87.3094
866.80	10.1052
876.27	61.4033
878.59	93.1460
895.25	295.1592
896.70	136.5401
929.53	3.7936
953.93	7.3075
956.10	4.4208
985.56	302.7635
993.59	161.1446
1008.94	35.0573
1039.98	5.5404
1063.07	1.5981
1081.15	4.9071
1097.61	24.4077
1115.09	0.8986
1129.08	136.9640
1129.97	194.1764
1137.34	424.7952
1168.28	29.2685
1179.56	3.1119
1206.12	24.8900
1225.20	25.1802
1250.86	9.2873
1274.77	5.1734
1281.33	36.7486
1283.71	12.0655
1307.29	1.0722
1309.06	2.4186
1330.81	4.7287
1335.48	3.5338
1338.28	0.9488
1345.61	3.0484
1370.00	5.3462
1411.38	28.9767
1415.72	27.4967
1430.18	16.4472
1433.01	17.8983
1439.05	11.0823
1448.93	5.4740
1640.92	81.0709
2072.70	727.9208
2569.01	2643.0661
2887.91	50.3543
2890.88	102.8894
2942.57	27.9419
2958.03	45.8958
2976.47	33.6839
2981.09	30.2694

```
   2996.18      27.9488
   2998.31      52.9278
   3001.07      48.3185
   3004.49      47.8376
   3046.47       2.3781
   3054.74      12.9767
   3064.41       3.0034
   3271.32     965.3044
   3430.14      18.8901
ENTHALPY
--------
Total free energy                  ...   -981.30549134 Hartree
Thermal Enthalpy correction        ...      0.00094421 Hartree
-----------------------------------------------------------------------
Total Enthalpy                     ...   -981.30454713 Hartree
```

(9)

```
The IR spectrum
      wavenumber  T**2
  -1537.58       0.0000
     25.30       1.9383
     37.93       2.7994
     59.69       2.9061
     63.69       1.9913
    100.24       7.5708
    123.03      10.3090
    167.41      36.2381
    194.10       0.7879
    214.62       0.0504
    217.04       0.0509
    222.05       2.2955
    230.22       1.7723
    239.62       1.0882
    246.75       1.5634
    253.38       0.5996
    255.63       0.5723
    294.58      40.6491
    302.38      22.0123
    320.91      13.8993
    332.24       0.2330
    354.47       9.3864
    387.35     113.0692
    398.57       2.9750
    400.93      36.5135
    419.20       4.5863
    427.36      10.0961
    430.30      54.9749
    455.31      15.4345
    480.25       0.6780
    484.16       8.7801
    488.54      19.0115
    501.17      16.7719
    503.44      39.4598
    524.14     101.7139
```

552.19	16.3252
624.16	51.5695
658.64	154.6808
700.99	201.5877
703.24	141.8170
782.82	1.2394
798.92	15.3237
816.50	145.5338
841.95	278.6144
849.81	5.3440
865.37	13.1362
871.03	104.9880
878.14	5.5964
891.23	58.1677
893.80	6.1938
907.45	2.6176
916.07	3.6804
941.45	2.5803
956.64	5.1928
968.73	2.6617
990.97	3.3145
1002.41	5.8870
1015.02	640.3249
1020.77	14.1887
1046.38	109.1950
1072.73	1.5617
1081.63	5.6122
1084.51	0.9538
1089.08	0.6647
1108.20	69.0373
1152.07	626.4588
1174.57	16.8236
1191.94	7.6539
1203.65	6.6092
1214.95	5.0598
1229.67	19.0890
1248.66	0.5585
1263.22	7.1908
1278.90	6.0390
1286.40	23.6911
1296.42	3.7245
1303.10	68.8357
1310.36	46.0797
1322.63	34.9916
1334.34	1.4440
1350.69	41.9366
1352.75	1.8333
1354.14	10.4004
1365.74	3.2180
1400.81	287.9389
1415.27	2.1535
1418.39	9.9239
1426.20	8.7390
1427.26	4.2997

```
   1428.99      10.8790
   1432.03       7.3716
   1434.69      19.3236
   1437.11      73.3494
   1437.94      51.2728
   1440.12      19.3506
   1451.19      10.8936
   1456.11      23.3298
   1511.39     158.7743
   1946.46     125.8178
   2618.12    2337.9443
   2951.03      62.6769
   2953.70      27.7305
   2961.71      33.9773
   2965.00      37.3642
   2966.27      68.8813
   2968.93      32.0081
   2994.81      39.6876
   2998.20      43.9472
   3015.12      20.0031
   3015.56      15.6115
   3023.75       7.3783
   3028.37      33.0472
   3036.93      30.9107
   3038.27      40.1940
   3042.38      40.2918
   3043.48      38.0603
   3066.50      14.4352
   3071.92       2.7015
   3073.59       5.8855
   3653.75     144.2072
ENTHALPY
--------
The enthalpy is H = U + kB*T
                kB is Boltzmann's constant
Total free energy                ...  -1099.06183518 Hartree
Thermal Enthalpy correction      ...      0.00094421 Hartree
-------------------------------------------------------------------
Total Enthalpy                   ...  -1099.06089098 Hartree
```

H_2O

```
The IR spectrum
   wavenumber  T**2
   1554.48     109.7273
   3709.34      19.8719
   3796.13     110.8861
ENTHALPY
--------
Total free energy                ...    -76.36806255 Hartree
Thermal Enthalpy correction      ...      0.00094421 Hartree
-------------------------------------------------------------------
Total Enthalpy                   ...    -76.36711835 Hartree
```

Cartesian coordinates of all optimized geometries of the amides, products of hydrolyses, transition states using DFT-D3(BJ) methods with different density functional.

1-Azatricyclo[3.3.1.1^{3,7}]decan-2-one, tetrafluoroboric acid salt (1)

PBE

C	-2.508710	-0.195659	-1.495081
C	-1.615727	-1.337282	-0.988680
C	-0.179485	-0.836762	-0.877360
C	-2.446761	0.985076	-0.495203
C	-1.018879	1.442250	-0.367329
C	-2.099769	-1.815396	0.390428
C	-2.927618	0.507164	0.898973
C	-2.028460	-0.640878	1.380710
C	-0.589266	-0.141083	1.475877
H	-2.187650	0.135410	-2.493494
H	-3.554964	-0.525585	-1.578940
H	-1.629770	-2.169911	-1.706692
H	0.219821	-0.455939	-1.825891
H	-3.036679	1.840139	-0.847664
H	0.525051	-1.587761	-0.500310
H	-3.133081	-2.186483	0.321024
H	0.900686	0.644283	0.187291
H	-3.972067	0.172760	0.810548
H	-1.474385	-2.648385	0.743853
H	-2.910101	1.343405	1.613322
H	0.129161	-0.907437	1.792306
H	-2.343428	-0.967563	2.382399
H	-0.489719	0.723412	2.146364
B	3.036821	-0.244400	0.166613
N	-0.129412	0.310941	0.108675
O	-0.549378	2.524934	-0.569229
F	2.904401	-0.730570	-1.142127
F	2.326267	1.064865	0.207754
F	4.336233	-0.065996	0.566551
F	2.303408	-1.089088	1.056102

PBE0

C	-2.495359	-0.193070	-1.484523
C	-1.607646	-1.327798	-0.981937
C	-0.181120	-0.826918	-0.865334
C	-2.435204	0.975838	-0.488353
C	-1.011578	1.422230	-0.357901
C	-2.090602	-1.805720	0.386519
C	-2.916284	0.500548	0.893056
C	-2.022837	-0.640395	1.372395
C	-0.592276	-0.142151	1.468054
H	-2.173929	0.137702	-2.475195
H	-3.533465	-0.523280	-1.571713

H	-1.616488	-2.153316	-1.696646
H	0.217224	-0.448517	-1.806907
H	-3.014103	1.829598	-0.838658
H	0.516562	-1.574440	-0.490939
H	-3.116563	-2.175539	0.315018
H	0.873606	0.639407	0.187355
H	-3.953222	0.166998	0.805031
H	-1.468750	-2.633110	0.737339
H	-2.900322	1.329872	1.604790
H	0.119012	-0.904895	1.782310
H	-2.334893	-0.966183	2.366970
H	-0.495752	0.713825	2.138137
B	3.007115	-0.236011	0.158471
N	-0.137166	0.309266	0.114442
O	-0.545891	2.492035	-0.562344
F	2.875667	-0.751263	-1.124424
F	2.320412	1.053296	0.169367
F	4.297049	-0.071393	0.551955
F	2.273344	-1.048152	1.054456

PBE0 methanol

C	-2.654353	-0.176681	-1.440226
C	-1.797889	-1.356118	-0.991174
C	-0.342497	-0.931863	-0.983963
C	-2.469997	0.994372	-0.458243
C	-1.028984	1.362668	-0.439586
C	-2.205651	-1.802310	0.410991
C	-2.868598	0.548787	0.960516
C	-2.008943	-0.639020	1.380240
C	-0.552538	-0.217997	1.377084
H	-2.385896	0.132980	-2.452475
H	-3.711174	-0.450065	-1.446731
H	-1.898278	-2.179955	-1.699469
H	-0.010582	-0.573388	-1.958123
H	-3.033836	1.870765	-0.773379
H	0.330205	-1.719939	-0.648459
H	-3.252347	-2.113397	0.411914
H	0.814078	0.515233	-0.024649
H	-3.924323	0.271611	0.944303
H	-1.606263	-2.660850	0.724156
H	-2.753972	1.377040	1.662987
H	0.126540	-1.026188	1.644860
H	-2.263090	-0.941307	2.397360
H	-0.366126	0.633134	2.031493
B	3.298419	-0.084105	0.293943
N	-0.174570	0.206092	-0.015281
O	-0.496317	2.392497	-0.699657
F	4.140649	-0.438245	-0.751835
F	2.448541	0.979545	-0.135149
F	4.029686	0.339451	1.396125
F	2.474646	-1.164282	0.643219

TPSS

C	-2.508210	-0.198673	-1.495574
C	-1.616325	-1.342659	-0.987768
C	-0.176383	-0.848640	-0.881605
C	-2.441978	0.986350	-0.497336
C	-1.013768	1.442428	-0.374207
C	-2.099916	-1.818644	0.393702
C	-2.923271	0.509994	0.899644
C	-2.026454	-0.641366	1.382635
C	-0.585176	-0.146498	1.480575
H	-2.187588	0.128941	-2.489955
H	-3.550843	-0.525378	-1.573439
H	-1.635001	-2.172562	-1.701398
H	0.219621	-0.468497	-1.825085
H	-3.030126	1.836230	-0.849218
H	0.520086	-1.593411	-0.494464
H	-3.129943	-2.185399	0.325843
H	0.892145	0.639934	0.186018
H	-3.963403	0.178514	0.811138
H	-1.475099	-2.646289	0.746094
H	-2.899535	1.343650	1.609469
H	0.127705	-0.914330	1.784844
H	-2.341400	-0.964391	2.380189
H	-0.481915	0.715623	2.144492
B	3.023605	-0.225167	0.167597
N	-0.125824	0.309683	0.105693
O	-0.540522	2.520545	-0.583171
F	2.884523	-0.680466	-1.149390
F	2.344907	1.083518	0.239482
F	4.324459	-0.094337	0.574565
F	2.272171	-1.080240	1.031419

TPSSH

C	-2.533636	-0.216693	-1.486307
C	-1.602053	-1.328539	-0.990851
C	-0.176210	-0.798204	-0.920774
C	-2.475405	0.974587	-0.501822
C	-1.056927	1.458102	-0.421862
C	-2.040276	-1.804360	0.401060
C	-2.911715	0.500197	0.904347
C	-1.976997	-0.620222	1.375574
C	-0.551126	-0.088221	1.436945
H	-2.245842	0.109652	-2.488664
H	-3.566168	-0.571434	-1.537387
H	-1.612596	-2.162879	-1.695557
H	0.186967	-0.418108	-1.874744
H	-3.087767	1.806514	-0.847512
H	0.543361	-1.522147	-0.544258
H	-3.058868	-2.198879	0.359145
H	0.858587	0.731523	0.126638
H	-3.942256	0.141693	0.842765
H	-1.386484	-2.609523	0.745202
H	-2.894714	1.338118	1.605827

H	0.187359	-0.832447	1.730863
H	-2.259551	-0.941389	2.380592
H	-0.456508	0.780977	2.088931
B	2.982375	-0.320647	0.252558
N	-0.137181	0.365192	0.052315
O	-0.610707	2.534438	-0.671240
F	2.813653	-0.578470	-1.111375
F	2.336084	0.966589	0.515962
F	4.289357	-0.267374	0.641910
F	2.241786	-1.279582	0.992508

3-Methyl-1-azatricyclo[3.3.1.1^{3,7}]decan-2-one, tetrafluoroboric acid salt (2)

PBE

C	-2.501668	-0.187797	-1.490175
C	-1.616586	-1.334077	-0.985697
C	-0.178982	-0.840972	-0.875038
C	-2.457649	1.015256	-0.507301
C	-1.011779	1.443132	-0.369599
C	-2.103009	-1.810683	0.392012
C	-2.916989	0.516240	0.893145
C	-2.026979	-0.634844	1.378904
C	-0.586780	-0.141979	1.475731
H	-2.180717	0.140976	-2.490344
H	-3.550371	-0.512315	-1.574863
H	-1.637036	-2.165134	-1.705560
H	0.222112	-0.462457	-1.823751
H	0.523385	-1.592898	-0.495815
H	-3.138007	-2.177028	0.322223
H	0.899637	0.640740	0.185258
H	-3.964176	0.188043	0.803972
H	-1.481169	-2.645817	0.746503
H	-2.898289	1.353895	1.607193
H	0.129804	-0.910186	1.791780
H	-2.347507	-0.956475	2.380594
H	-0.484087	0.722795	2.145428
B	3.038578	-0.246894	0.164312
N	-0.130142	0.307317	0.108162
O	-0.525263	2.519291	-0.569545
F	2.905086	-0.736928	-1.142979
F	2.327497	1.061620	0.202914
F	4.338896	-0.066363	0.561569
F	2.307917	-1.089926	1.057336
C	-3.313165	2.176363	-0.998172
H	-2.973761	2.530805	-1.979788
H	-4.358693	1.852022	-1.086972
H	-3.268189	3.023858	-0.302473

PBE0

C	-2.491425	-0.185727	-1.480294
C	-1.610504	-1.324343	-0.979433

C	-0.183056	-0.829379	-0.863985
C	-2.448979	1.004701	-0.501250
C	-1.008990	1.424655	-0.361208
C	-2.095068	-1.800608	0.388045
C	-2.909298	0.509454	0.885854
C	-2.023636	-0.633337	1.369980
C	-0.592545	-0.140436	1.466908
H	-2.170209	0.142498	-2.472850
H	-3.531734	-0.511324	-1.568241
H	-1.624956	-2.148657	-1.695567
H	0.216352	-0.453265	-1.806003
H	0.513186	-1.577029	-0.487212
H	-3.122364	-2.166674	0.316580
H	0.869628	0.638456	0.183612
H	-3.948441	0.180492	0.796979
H	-1.475897	-2.629391	0.740209
H	-2.893357	1.340385	1.597084
H	0.117605	-0.904196	1.781195
H	-2.340643	-0.953843	2.364812
H	-0.493822	0.716388	2.135570
B	3.006454	-0.235467	0.154491
N	-0.140785	0.307971	0.112550
O	-0.528481	2.489026	-0.562628
F	2.875289	-0.754580	-1.126872
F	2.318300	1.052751	0.162254
F	4.296781	-0.067918	0.546524
F	2.275047	-1.046151	1.053496
C	-3.290443	2.164656	-0.989718
H	-2.950247	2.514492	-1.964829
H	-4.331425	1.849449	-1.078443
H	-3.240415	3.006533	-0.298644

PBE0 Methanol

C	-2.643803	-0.188137	-1.451070
C	-1.793826	-1.366118	-0.991181
C	-0.338545	-0.945513	-0.982372
C	-2.481921	1.011883	-0.492260
C	-1.025696	1.355998	-0.462101
C	-2.208194	-1.801369	0.411525
C	-2.866347	0.555460	0.932622
C	-2.013628	-0.629308	1.369170
C	-0.557522	-0.211280	1.370214
H	-2.372322	0.111818	-2.466380
H	-3.701931	-0.459656	-1.460029
H	-1.896020	-2.193395	-1.695258
H	-0.002291	-0.595661	-1.958172
H	0.332547	-1.730513	-0.636640
H	-3.255368	-2.110791	0.410600
H	0.810145	0.511769	-0.033085
H	-3.923373	0.280158	0.914131
H	-1.611067	-2.657695	0.734604
H	-2.755577	1.390139	1.629459
H	0.120225	-1.017530	1.647005

H	-2.276494	-0.918962	2.387791
H	-0.372964	0.645441	2.017829
B	3.296725	-0.077298	0.299055
N	-0.177870	0.200343	-0.023963
O	-0.480957	2.378473	-0.726476
F	4.142538	-0.439323	-0.741196
F	2.444200	0.978736	-0.143022
F	4.024122	0.360346	1.398337
F	2.476055	-1.156709	0.657773
C	-3.301760	2.203106	-0.940407
H	-3.015122	2.523195	-1.942962
H	-4.356703	1.925789	-0.954602
H	-3.175333	3.046187	-0.259975

TPSS

C	-2.502535	-0.191716	-1.489910
C	-1.618335	-1.340470	-0.984289
C	-0.176811	-0.853976	-0.879095
C	-2.452421	1.014277	-0.508191
C	-1.007856	1.441746	-0.375887
C	-2.103654	-1.814893	0.396083
C	-2.913861	0.517985	0.894060
C	-2.025720	-0.636139	1.381435
C	-0.583463	-0.147759	1.480774
H	-2.182374	0.133043	-2.486257
H	-3.547664	-0.512999	-1.567668
H	-1.643544	-2.168796	-1.699712
H	0.220605	-0.475986	-1.822888
H	0.517527	-1.599792	-0.490213
H	-3.135334	-2.177185	0.328177
H	0.890439	0.635985	0.184233
H	-3.956333	0.191764	0.804441
H	-1.482145	-2.644590	0.749488
H	-2.889312	1.352539	1.604082
H	0.127581	-0.917019	1.785678
H	-2.345770	-0.953872	2.379210
H	-0.477408	0.715386	2.143013
B	3.024544	-0.224139	0.163756
N	-0.126768	0.304847	0.105318
O	-0.518822	2.513825	-0.583030
F	2.884696	-0.677674	-1.153711
F	2.344574	1.082905	0.238788
F	4.326238	-0.092501	0.569127
F	2.276068	-1.081979	1.027506
C	-3.307260	2.179874	-1.001274
H	-2.966560	2.527636	-1.979846
H	-4.348846	1.856496	-1.086992
H	-3.257557	3.022758	-0.307239

TPSSH

C	-2.519062	-0.197504	-1.484428

C	-1.601273	-1.319110	-0.990142
C	-0.171508	-0.802850	-0.917693
C	-2.473696	1.012902	-0.515077
C	-1.036561	1.461875	-0.422961
C	-2.046639	-1.792648	0.399290
C	-2.894762	0.520167	0.894796
C	-1.974975	-0.608185	1.371423
C	-0.545426	-0.089793	1.437380
H	-2.228108	0.125432	-2.487854
H	-3.555788	-0.541763	-1.537977
H	-1.620782	-2.151390	-1.697275
H	0.196786	-0.425871	-1.870922
H	0.542005	-1.531439	-0.538602
H	-3.068777	-2.177631	0.354822
H	0.867063	0.722870	0.128529
H	-3.929381	0.171936	0.829889
H	-1.400850	-2.603498	0.745135
H	-2.874474	1.358321	1.597176
H	0.187113	-0.839605	1.731983
H	-2.266408	-0.923811	2.375793
H	-0.444982	0.778721	2.089418
B	2.989037	-0.331674	0.254291
N	-0.129616	0.359974	0.053728
O	-0.569014	2.530591	-0.668982
F	2.817695	-0.586888	-1.110018
F	2.346020	0.956127	0.520744
F	4.297189	-0.281624	0.641024
F	2.248315	-1.290462	0.993883
C	-3.355860	2.156082	-0.998718
H	-3.044043	2.499632	-1.985761
H	-4.391379	1.815744	-1.058246
H	-3.305940	3.004954	-0.315679

3,5,7-Trimethyl-methyl-1-azatricyclo[3.3.1.1^{3,7}]decan-2-one, tetrafluoroboric acid salt (3)

C	-2.528094	-0.180593	-1.486210
C	-1.644485	-1.346410	-1.014312
C	-0.210981	-0.833255	-0.886138
C	-2.484239	1.011481	-0.494808
C	-1.039730	1.441492	-0.361157
C	-2.122486	-1.807737	0.374326
C	-2.936642	0.500510	0.899529
C	-2.056050	-0.658102	1.396018
C	-0.612886	-0.157023	1.469268
H	-2.210212	0.155452	-2.485878
H	-3.576464	-0.508756	-1.572315
H	0.185506	-0.444692	-1.833653
H	0.493606	-1.589867	-0.519069
H	-3.158421	-2.177329	0.304540
H	0.870226	0.630922	0.185880
H	-3.984114	0.169723	0.813206
H	-1.500349	-2.648599	0.720020

H	-2.917633	1.330353	1.624033
H	0.104073	-0.927613	1.780578
H	-0.511679	0.702695	2.146969
B	3.010291	-0.255962	0.136540
N	-0.159725	0.301826	0.107828
O	-0.552882	2.517638	-0.559907
F	2.876941	-0.712841	-1.182783
F	2.302135	1.050666	0.208791
F	4.311496	-0.089425	0.538989
F	2.278947	-1.121881	1.007898
C	-3.344608	2.174805	-0.973483
H	-3.008855	2.538472	-1.952927
H	-4.389352	1.847922	-1.062008
H	-3.300309	3.016500	-0.270730
C	-2.500498	-1.125137	2.781175
H	-3.538525	-1.484431	2.750025
H	-1.867697	-1.948220	3.141180
H	-2.446627	-0.307550	3.514388
C	-1.678303	-2.496683	-2.019073
H	-1.032816	-3.323741	-1.692544
H	-2.701146	-2.884415	-2.125095
H	-1.333796	-2.168784	-3.010122

PBE0

C	-2.520785	-0.181157	-1.475904
C	-1.641902	-1.338793	-1.006859
C	-0.218148	-0.826270	-0.876507
C	-2.476810	0.998942	-0.489259
C	-1.038760	1.421220	-0.350830
C	-2.117500	-1.799233	0.371531
C	-2.929293	0.493120	0.893387
C	-2.052942	-0.657188	1.386436
C	-0.618708	-0.157806	1.459064
H	-2.203658	0.153332	-2.468474
H	-3.561215	-0.508918	-1.564084
H	0.176584	-0.441621	-1.817919
H	0.479788	-1.579130	-0.511904
H	-3.146078	-2.167398	0.301201
H	0.839583	0.626120	0.180279
H	-3.969305	0.163329	0.808411
H	-1.498885	-2.634261	0.714872
H	-2.911219	1.317056	1.613797
H	0.091461	-0.924223	1.768655
H	-0.519606	0.694312	2.134833
B	2.977122	-0.247436	0.128983
N	-0.171623	0.298673	0.109303
O	-0.558415	2.487492	-0.541966
F	2.845361	-0.744416	-1.160782
F	2.290054	1.040311	0.159810
F	4.268287	-0.087879	0.523323
F	2.246992	-1.073948	1.015080
C	-3.323332	2.161273	-0.965158

H	-2.984768	2.522431	-1.936674
H	-4.363088	1.842936	-1.056785
H	-3.276293	2.995842	-0.265084
C	-2.492350	-1.121863	2.763293
H	-3.522999	-1.480891	2.733387
H	-1.861640	-1.938203	3.120991
H	-2.439982	-0.309158	3.491481
C	-1.670774	-2.481157	-2.006178
H	-1.030005	-3.302692	-1.679956
H	-2.686423	-2.866880	-2.115450
H	-1.325109	-2.154461	-2.989375

PBE0 Methanol

C	-2.638709	-0.189941	-1.471185
C	-1.785788	-1.381358	-1.040732
C	-0.335797	-0.929089	-0.999234
C	-2.497130	0.995149	-0.495540
C	-1.046453	1.356032	-0.451998
C	-2.200482	-1.814627	0.365068
C	-2.884002	0.515246	0.917598
C	-2.032059	-0.670735	1.364537
C	-0.577292	-0.232149	1.358220
H	-2.363276	0.126656	-2.481171
H	-3.693911	-0.474463	-1.493426
H	0.003494	-0.562412	-1.968520
H	0.339821	-1.714920	-0.662456
H	-3.246117	-2.134861	0.352809
H	0.793282	0.519330	-0.019291
H	-3.938527	0.228556	0.891193
H	-1.599953	-2.673502	0.680428
H	-2.786379	1.340399	1.628785
H	0.105896	-1.035830	1.631301
H	-0.406548	0.617465	2.020022
B	3.275019	-0.039795	0.361120
N	-0.193094	0.200399	-0.024415
O	-0.509102	2.386426	-0.698037
F	4.151028	-0.347830	-0.671129
F	2.414877	1.019103	-0.061287
F	3.968235	0.366815	1.493511
F	2.463462	-1.144718	0.657702
C	-3.329542	2.182724	-0.931629
H	-3.040789	2.520404	-1.927714
H	-4.380755	1.892506	-0.956176
H	-3.217488	3.017208	-0.238290
C	-2.410129	-1.108071	2.768437
H	-3.455050	-1.422772	2.792762
H	-1.793743	-1.948919	3.093489
H	-2.282864	-0.291272	3.482434
C	-1.917957	-2.525516	-2.029956
H	-1.298550	-3.373237	-1.729497

H	-2.955470	-2.861558	-2.076332
H	-1.614544	-2.215436	-3.032434

TPSS

C	-2.551502	-0.186038	-1.492543
C	-1.636492	-1.332021	-1.028522
C	-0.206708	-0.799486	-0.933632
C	-2.509237	1.015415	-0.507989
C	-1.072754	1.469914	-0.411076
C	-2.080858	-1.796276	0.371175
C	-2.929392	0.503250	0.898203
C	-2.018030	-0.637367	1.383684
C	-0.583166	-0.112398	1.435134
H	-2.259453	0.148611	-2.495200
H	-3.590606	-0.532377	-1.551759
H	0.162380	-0.410461	-1.885150
H	0.508054	-1.535376	-0.562457
H	-3.106756	-2.182436	0.321302
H	0.841510	0.712751	0.135676
H	-3.966720	0.153809	0.829533
H	-1.436295	-2.616764	0.708881
H	-2.909970	1.334048	1.614061
H	0.150767	-0.867441	1.723758
H	-0.484446	0.751116	2.098942
B	2.964432	-0.357643	0.250520
N	-0.162961	0.353715	0.054152
O	-0.602777	2.546670	-0.642722
F	2.804167	-0.613854	-1.120042
F	2.319558	0.941056	0.513002
F	4.273749	-0.307573	0.652015
F	2.212320	-1.317839	0.988722
C	-3.400662	2.163103	-0.979118
H	-3.091179	2.519218	-1.965060
H	-4.436689	1.817208	-1.040519
H	-3.353110	3.006255	-0.285137
C	-2.430698	-1.106222	2.782504
H	-3.457447	-1.485053	2.767685
H	-1.775274	-1.910031	3.131948
H	-2.380572	-0.284549	3.504848
C	-1.671207	-2.492868	-2.027883
H	-1.011812	-3.304201	-1.704570
H	-2.687767	-2.890165	-2.111407
H	-1.348783	-2.166293	-3.021990

TPSSH

C	-2.550016	-0.186566	-1.488023
C	-1.636649	-1.328998	-1.025689
C	-0.211233	-0.795573	-0.930607
C	-2.506875	1.010059	-0.506090
C	-1.072058	1.460910	-0.408819

C	-2.078801	-1.792144	0.370318
C	-2.925856	0.500791	0.895524
C	-2.016358	-0.636324	1.379823
C	-0.585093	-0.111764	1.429077
H	-2.259168	0.147001	-2.488844
H	-3.586519	-0.532759	-1.547643
H	0.156474	-0.407829	-1.880517
H	0.502198	-1.530630	-0.562702
H	-3.101947	-2.178754	0.321334
H	0.830298	0.709583	0.132902
H	-3.960832	0.151754	0.828526
H	-1.435089	-2.610529	0.707087
H	-2.906894	1.329699	1.610014
H	0.146539	-0.865088	1.718458
H	-0.486779	0.749061	2.092637
B	2.952491	-0.356537	0.250140
N	-0.168282	0.352053	0.053778
O	-0.604298	2.532905	-0.640049
F	2.790258	-0.610840	-1.115023
F	2.311690	0.933637	0.513489
F	4.258326	-0.309469	0.645973
F	2.205033	-1.313499	0.984870
C	-3.392406	2.157038	-0.975945
H	-3.081879	2.513044	-1.958985
H	-4.427035	1.814722	-1.039124
H	-3.344397	2.997852	-0.282869
C	-2.426056	-1.103341	2.775057
H	-3.450550	-1.481573	2.762115
H	-1.771858	-1.905237	3.123926
H	-2.375573	-0.283418	3.495815
C	-1.668742	-2.486530	-2.021894
H	-1.008984	-3.294713	-1.699371
H	-2.681924	-2.885993	-2.105672
H	-1.347544	-2.160595	-3.014029

Cationic fragments
PBE0
$(1)^{+}$

C	-2.492368	-0.190894	-1.487730
C	-1.608691	-1.328674	-0.981830
C	-0.176006	-0.836869	-0.872577
C	-2.449025	0.982715	-0.491295
C	-1.039857	1.442071	-0.377284
C	-2.089218	-1.804439	0.388260
C	-2.911538	0.508065	0.899203
C	-2.022056	-0.638696	1.373641

C	-0.588766	-0.148022	1.479562
H	-2.175974	0.140058	-2.479495
H	-3.527481	-0.525657	-1.575515
H	-1.620009	-2.153026	-1.697157
H	0.206413	-0.451565	-1.818952
H	-3.040551	1.827338	-0.842401
H	0.504815	-1.604735	-0.502249
H	-3.115000	-2.169801	0.315218
H	0.796576	0.697802	0.161940
H	-3.947859	0.175105	0.818702
H	-1.477558	-2.639191	0.740216
H	-2.894318	1.337564	1.609735
H	0.100155	-0.929610	1.803236
H	-2.333573	-0.962241	2.368459
H	-0.489140	0.709745	2.146385
N	-0.141299	0.298102	0.114221
O	-0.518261	2.478505	-0.586399

(2)$^+$

C	-2.484844	-0.180337	-1.483531
C	-1.610236	-1.324051	-0.979516
C	-0.175788	-0.841064	-0.870080
C	-2.458754	1.015203	-0.504478
C	-1.032443	1.443380	-0.380048
C	-2.094028	-1.797935	0.389051
C	-2.900674	0.519922	0.891431
C	-2.021496	-0.630754	1.370912
C	-0.586775	-0.148311	1.478774
H	-2.167396	0.147445	-2.476945
H	-3.522469	-0.509344	-1.572710
H	-1.628061	-2.146917	-1.696583
H	0.209049	-0.458711	-1.816656
H	0.501789	-1.610593	-0.497187
H	-3.121805	-2.157504	0.315230
H	0.796785	0.694176	0.159988
H	-3.939714	0.193125	0.810402
H	-1.486958	-2.635434	0.742374
H	-2.881819	1.350259	1.602269
H	0.099356	-0.932329	1.802578
H	-2.338897	-0.948851	2.365748
H	-0.483868	0.709675	2.144795
N	-0.141191	0.294597	0.113522
O	-0.494439	2.472898	-0.586944
C	-3.311329	2.168617	-0.993737
H	-2.979435	2.519732	-1.970947
H	-4.347765	1.840671	-1.079596
H	-3.272849	3.010506	-0.302301

(3)$^+$

C	-2.511817	-0.176649	-1.478843
C	-1.639275	-1.340281	-1.007457
C	-0.208921	-0.836776	-0.881084

C	-2.485460	1.008704	-0.491839
C	-1.061437	1.439279	-0.368812
C	-2.114532	-1.797141	0.372724
C	-2.920654	0.501731	0.898831
C	-2.051003	-0.656140	1.389364
C	-0.613092	-0.165303	1.471710
H	-2.197873	0.158585	-2.471814
H	-3.549645	-0.507213	-1.569150
H	0.171558	-0.446659	-1.826961
H	0.470507	-1.610298	-0.518490
H	-3.143158	-2.159846	0.299601
H	0.766660	0.685960	0.159050
H	-3.960274	0.173872	0.819455
H	-1.507020	-2.640064	0.717600
H	-2.901633	1.325534	1.618512
H	0.074155	-0.951667	1.789056
H	-0.510242	0.687363	2.145542
N	-0.171802	0.287664	0.111239
O	-0.524851	2.471420	-0.569063
C	-3.343572	2.163734	-0.969024
H	-3.016232	2.523463	-1.944644
H	-4.379333	1.833362	-1.053776
H	-3.305131	3.000312	-0.271157
C	-2.492322	-1.118892	2.767661
H	-3.524322	-1.470707	2.732951
H	-1.872072	-1.942497	3.126825
H	-2.440311	-0.308122	3.497339
C	-1.671611	-2.481923	-2.009457
H	-1.043329	-3.313430	-1.683997
H	-2.689990	-2.857555	-2.117907
H	-1.328157	-2.158965	-2.994450

Products of Hydrolysis
(4)

PBE

C	-0.738186	1.664980	-2.323863
C	-0.174001	0.398835	-1.634260
C	1.348209	0.330739	-1.506209
C	-0.771331	2.967361	-1.484899
C	-0.784024	0.237264	-0.236678

C	-1.073119	2.711336	0.012317
C	-0.386357	1.463528	0.594040
C	1.142959	1.532114	0.713146
H	-0.217306	1.843869	-3.273109
H	-1.781525	1.427894	-2.582174
H	-0.455672	-0.459647	-2.263011
H	1.872148	0.473469	-2.458314
H	1.649506	-0.636066	-1.079927
H	-1.880053	0.168325	-0.297424
H	-2.156503	2.560064	0.129144
H	-0.423893	-0.691867	0.232558
H	-0.814383	3.614120	0.581627
H	1.498137	0.702028	1.339291
H	-0.750712	1.345985	1.626463
H	1.482049	2.472027	1.167076
B	4.564336	2.524963	-1.664554
F	3.918948	1.754021	-2.659683
F	3.792451	3.729684	-1.475457
F	5.873400	2.801712	-1.948942
F	4.456699	1.769024	-0.416694
N	1.859098	1.403217	-0.597598
H	1.804742	2.277677	-1.147257
H	2.902643	1.318781	-0.438240
H	-1.600864	3.582198	-1.870469
C	0.424302	3.918840	-1.602757
O	0.535685	4.932505	-0.947710
O	1.363261	3.485137	-2.486089
H	2.216397	3.976823	-2.343428

PBE0

C	-0.742711	1.664462	-2.316940
C	-0.166989	0.414892	-1.631545
C	1.346823	0.355769	-1.517135
C	-0.776034	2.959846	-1.487375
C	-0.758038	0.254561	-0.236823
C	-1.055543	2.710610	0.004034
C	-0.360626	1.477082	0.580889
C	1.160105	1.548735	0.688501
H	-0.236863	1.841832	-3.266442
H	-1.780088	1.421408	-2.561557
H	-0.445105	-0.442514	-2.250093
H	1.857385	0.500163	-2.467265
H	1.648614	-0.608403	-1.103640
H	-1.846945	0.178027	-0.284562
H	-2.129657	2.553676	0.132373
H	-0.387934	-0.664842	0.226786
H	-0.800178	3.611161	0.564328
H	1.512155	0.730248	1.319100
H	-0.713524	1.362965	1.609644
H	1.498680	2.485906	1.131498
B	4.539214	2.487391	-1.608030
F	3.907617	1.769844	-2.632837
F	3.742991	3.634071	-1.340231

F	5.822802	2.816709	-1.896646
F	4.472674	1.664200	-0.428261
N	1.866885	1.408544	-0.611623
H	1.847709	2.281653	-1.144816
H	2.891017	1.284551	-0.448811
H	-1.605505	3.566441	-1.864066
C	0.403204	3.909982	-1.624608
O	0.503350	4.925074	-0.995106
O	1.333327	3.484475	-2.491869
H	2.148227	4.012422	-2.389955

(5)

PBE

C	-0.761078	1.618285	-2.333195
C	-0.084664	0.426599	-1.626551
C	1.433169	0.503819	-1.462289
C	-0.835020	2.938970	-1.528220
C	-0.721076	0.206444	-0.250015
C	-1.162938	2.666681	-0.042127
C	-0.446148	1.457528	0.590670
C	1.067170	1.590631	0.814616
H	-0.294204	1.804242	-3.308414
H	-1.800010	1.310723	-2.534531
H	-0.256902	-0.458107	-2.259292
H	1.965996	0.750347	-2.387712
H	1.810040	-0.463442	-1.102172
H	-1.805188	0.049968	-0.349011
H	-2.243068	2.462273	0.026218
H	-0.302000	-0.691282	0.231664
H	-0.969043	3.580305	0.534876
H	1.410887	0.759740	1.445879
H	-0.869522	1.327142	1.598994
H	1.330838	2.535700	1.304553
B	4.555326	2.359676	-1.770349
F	4.085320	1.520195	-2.795475
F	3.611689	3.449831	-1.621746
F	5.826119	2.825388	-1.975918
F	4.485642	1.605823	-0.515348
N	1.871981	1.525636	-0.449117
H	1.916993	2.457642	-0.886211
H	2.903579	1.378011	-0.256419
C	0.450634	3.775059	-1.604587
O	0.838499	4.503506	-0.707367
O	1.129722	3.609262	-2.761699
H	2.024618	4.010017	-2.640501
C	-1.928800	3.844147	-2.137976
H	-1.713045	4.067518	-3.191270
H	-2.900741	3.334381	-2.084045
H	-2.001482	4.792190	-1.588631

PBE0

C	-0.750444	1.621875	-2.325217
C	-0.077572	0.440412	-1.620826
C	1.431197	0.521350	-1.455445
C	-0.827306	2.932737	-1.524674
C	-0.712302	0.221418	-0.254692
C	-1.152986	2.664069	-0.048837
C	-0.439788	1.464123	0.581362
C	1.064205	1.596669	0.805494
H	-0.284592	1.807483	-3.293076
H	-1.781139	1.315478	-2.528670
H	-0.244303	-0.439201	-2.248811
H	1.955622	0.770871	-2.376124
H	1.805942	-0.443276	-1.108545
H	-1.789111	0.066685	-0.355327
H	-2.225969	2.460221	0.020276
H	-0.298181	-0.671722	0.223149
H	-0.962560	3.571683	0.524883
H	1.400484	0.774499	1.439814
H	-0.860731	1.334569	1.582502
H	1.323407	2.537228	1.290370
B	4.530570	2.347394	-1.767131
F	4.092302	1.519898	-2.794859
F	3.570690	3.398385	-1.614819
F	5.777315	2.846094	-1.963674
F	4.475345	1.589586	-0.541823
N	1.867477	1.525757	-0.443527
H	1.937882	2.450534	-0.870513
H	2.878355	1.359286	-0.244220
C	0.449676	3.759836	-1.605022
O	0.849242	4.459606	-0.708059
O	1.103416	3.620940	-2.757418
H	1.985149	4.021805	-2.655061
C	-1.911650	3.832476	-2.133449
H	-1.691523	4.057268	-3.178147
H	-2.877575	3.326092	-2.086952
H	-1.987252	4.772720	-1.585650

(6)

PBE

C	-2.554297	-0.113331	-1.491501
C	-1.666605	-1.282906	-1.039539
C	-0.216555	-0.813666	-0.934743
C	-2.478158	1.065653	-0.493935
C	-1.005651	1.533003	-0.411394
C	-2.138691	-1.781163	0.335938
C	-2.905821	0.548255	0.898555
C	-2.022235	-0.626588	1.342953
C	-0.571410	-0.158444	1.412732
H	-2.282492	0.212330	-2.512092
H	-3.604391	-0.436165	-1.557626
H	-1.712750	-2.096500	-1.777716
H	0.199880	-0.450461	-1.881409

H	0.465614	-1.588364	-0.565068
H	-3.181560	-2.127642	0.275667
H	0.847654	0.680105	0.125034
H	-3.957529	0.228154	0.837581
H	-1.525642	-2.635430	0.660220
H	-2.855622	1.369664	1.626887
H	0.134548	-0.950555	1.690457
H	-2.323919	-0.962555	2.345588
H	-0.440817	0.683882	2.100156
B	3.026981	0.051357	0.066068
N	-0.151830	0.313557	0.050459
O	-0.852889	2.524297	0.537968
F	2.800259	-0.199278	-1.298646
F	2.252136	1.282364	0.394423
F	4.347914	0.250592	0.380825
F	2.426517	-0.981641	0.838151
O	-0.458887	1.993435	-1.607067
H	0.031747	2.918908	0.414204
H	-0.814379	1.487491	-2.355857
C	-3.369765	2.224032	-0.940064
H	-3.079653	2.601416	-1.929686
H	-4.412471	1.882932	-0.997693
H	-3.315287	3.057388	-0.229181

PBE0

C	-2.546629	-0.113458	-1.481777
C	-1.663829	-1.274715	-1.032350
C	-0.224237	-0.804421	-0.924314
C	-2.467563	1.056273	-0.490978
C	-1.003528	1.514048	-0.402980
C	-2.134029	-1.768954	0.334159
C	-2.896642	0.546390	0.891766
C	-2.019977	-0.621509	1.334423
C	-0.578107	-0.154994	1.402477
H	-2.279452	0.210006	-2.495718
H	-3.589340	-0.435115	-1.546139
H	-1.705770	-2.083495	-1.765017
H	0.191788	-0.448008	-1.865387
H	0.453442	-1.572685	-0.555874
H	-3.169622	-2.112932	0.273531
H	0.819651	0.672948	0.124168
H	-3.942268	0.231418	0.832526
H	-1.525783	-2.617408	0.658613
H	-2.842420	1.363611	1.613972
H	0.122059	-0.942686	1.677995
H	-2.318448	-0.955073	2.330573
H	-0.449817	0.680340	2.087364
B	2.986443	0.075444	0.050580
N	-0.164741	0.314591	0.051680
O	-0.857222	2.496359	0.536495
F	2.742848	-0.154739	-1.301401
F	2.238589	1.280858	0.401485
F	4.302592	0.249662	0.343295

F	2.395630	-0.958235	0.801525
O	-0.462911	1.977015	-1.582502
H	0.009645	2.902942	0.414970
H	-0.726829	1.428162	-2.323357
C	-3.343769	2.213293	-0.936837
H	-3.053040	2.580218	-1.922031
H	-4.383244	1.884789	-0.989946
H	-3.279527	3.044189	-0.234339

(7)

PBE

C	-2.566373	-0.113445	-1.480074
C	-1.676215	-1.296174	-1.057617
C	-0.230953	-0.803420	-0.943840
C	-2.490126	1.060600	-0.481005
C	-1.021484	1.536845	-0.408842
C	-2.132713	-1.773102	0.333403
C	-2.903645	0.537784	0.910484
C	-2.022782	-0.638539	1.367455
C	-0.571254	-0.156793	1.404188
H	-2.301899	0.214925	-2.502616
H	-3.615356	-0.443117	-1.543069
H	0.178659	-0.438686	-1.893811
H	0.455986	-1.578431	-0.581901
H	-3.176553	-2.123595	0.279640
H	0.836828	0.685044	0.111746
H	-3.954742	0.211387	0.858697
H	-1.517332	-2.630123	0.651471
H	-2.852646	1.356232	1.643231
H	0.139519	-0.946944	1.677619
H	-0.440785	0.684171	2.094354
B	3.018833	0.054184	0.027422
N	-0.163483	0.318971	0.042726
O	-0.865935	2.526800	0.541596
F	2.784222	-0.192475	-1.336508
F	2.245905	1.283328	0.364844
F	4.341760	0.252870	0.334894
F	2.424397	-0.982305	0.800175
O	-0.486174	2.004775	-1.607033
H	0.015212	2.926552	0.410407
H	-0.827662	1.485010	-2.352943
C	-3.392899	2.214670	-0.917163
H	-3.112218	2.596343	-1.907777
H	-4.433895	1.867332	-0.967490
H	-3.338220	3.046411	-0.204355
C	-1.746663	-2.428025	-2.080088
H	-1.104203	-3.268207	-1.781730
H	-2.776108	-2.802346	-2.170105
H	-1.419534	-2.088544	-3.073651
C	-2.433205	-1.119242	2.757326
H	-3.474944	-1.469721	2.750818

H	-1.797921	-1.951520	3.092233
H	-2.352561	-0.309902	3.497062

PBE0

C	-2.560034	-0.116445	-1.469882
C	-1.673043	-1.288534	-1.049529
C	-0.238827	-0.793180	-0.935644
C	-2.480045	1.049815	-0.478986
C	-1.019559	1.516301	-0.400918
C	-2.126136	-1.762627	0.331992
C	-2.894696	0.534770	0.903301
C	-2.020301	-0.634336	1.357991
C	-0.577759	-0.155115	1.393866
H	-2.303215	0.207113	-2.487730
H	-3.601671	-0.445187	-1.528172
H	0.163681	-0.429563	-1.880411
H	0.446619	-1.561014	-0.579188
H	-3.161443	-2.114685	0.278371
H	0.809341	0.675920	0.111112
H	-3.939928	0.214413	0.853424
H	-1.512924	-2.611955	0.650387
H	-2.839617	1.349403	1.629820
H	0.126054	-0.942347	1.664020
H	-0.448745	0.677872	2.082564
B	2.980480	0.067399	0.016664
N	-0.176470	0.319077	0.044166
O	-0.871169	2.496974	0.540790
F	2.738175	-0.167930	-1.334011
F	2.234409	1.274303	0.364226
F	4.297158	0.241318	0.309975
F	2.389277	-0.963737	0.772081
O	-0.488162	1.982004	-1.583317
H	-0.007913	2.909190	0.413926
H	-0.792467	1.460912	-2.328689
C	-3.368029	2.202494	-0.914337
H	-3.091379	2.572495	-1.902616
H	-4.406118	1.868138	-0.956514
H	-3.300717	3.033166	-0.211867
C	-1.738741	-2.414954	-2.063577
H	-1.102103	-3.249310	-1.762896
H	-2.761061	-2.787111	-2.156213
H	-1.410823	-2.081485	-3.051070
C	-2.426976	-1.112914	2.739277
H	-3.461225	-1.462997	2.731916
H	-1.794249	-1.939148	3.071056
H	-2.348811	-0.308924	3.474815

Transition state
PBE
(8)

C	-0.836487	1.726841	-2.207647

C	-0.585126	0.353918	-1.544529
C	0.839981	-0.185842	-1.719272
C	-0.481529	2.998837	-1.373664
C	-0.908893	0.409261	-0.048320
C	-0.236300	2.815056	0.163574
C	0.076696	1.381428	0.608468
C	1.516405	0.920722	0.359795
H	-0.330934	1.782196	-3.179552
H	-1.914746	1.797784	-2.407105
H	-1.262197	-0.355390	-2.044651
H	1.098258	-0.256264	-2.786062
H	0.878711	-1.208882	-1.293984
H	-1.948377	0.733811	0.120649
H	-1.174567	3.118214	0.649501
H	-0.805474	-0.594456	0.390370
H	0.547734	3.502404	0.499169
H	1.665822	-0.026799	0.915184
H	-0.067930	1.372945	1.700155
H	2.237315	1.655853	0.734069
B	3.880879	3.702846	-0.738434
F	3.926266	4.024441	-2.143113
F	2.503703	3.887686	-0.318621
F	4.711923	4.530122	-0.016572
F	4.203548	2.336630	-0.580115
N	1.788984	0.722919	-1.073036
H	1.957391	1.888988	-2.206257
H	2.755465	0.407117	-1.176241
H	-1.346983	3.683200	-1.459431
C	0.518338	3.893781	-1.983313
O	0.786640	4.962338	-2.301540
O	1.957476	2.514386	-3.024299
H	2.745049	3.104847	-2.858260

(9)

PBE

C	-2.456162	0.095310	-0.995207
C	-1.543915	-1.070229	-0.580094
C	-0.108257	-0.549981	-0.527486
C	-2.362697	1.272426	-0.008479
C	-0.917180	1.752325	0.141744
C	-1.942416	-1.537934	0.831611
C	-2.731426	0.764361	1.411224
C	-1.815779	-0.392385	1.852153
C	-0.369175	0.110577	1.844552
H	-2.192631	0.428428	-2.012874
H	-3.503429	-0.244703	-1.035487
H	0.238519	-0.164555	-1.492830
H	0.610317	-1.308423	-0.194111
H	-2.980698	-1.908234	0.820749
H	1.012175	0.925833	0.493651
H	-3.779099	0.424914	1.390939
H	-1.300624	-2.379825	1.136294
H	-2.665015	1.598492	2.125620
H	0.365197	-0.662519	2.101615

H	-0.228879	0.970938	2.510851
B	3.148906	-0.060018	0.396871
N	-0.009935	0.577414	0.458161
O	-0.631132	2.839281	0.795400
F	2.924720	-0.348570	-0.958874
F	2.472231	1.236206	0.669971
F	4.477323	0.050635	0.726413
F	2.466331	-1.019110	1.201114
O	-0.241329	2.288820	-1.296536
H	-0.110339	3.076810	-0.407394
H	-0.968045	2.601733	-1.869752
C	-3.271805	2.429628	-0.415619
H	-3.079243	2.763258	-1.447917
H	-4.320768	2.107285	-0.379144
H	-3.140769	3.286612	0.255461
C	-1.628420	-2.216596	-1.585227
H	-0.961693	-3.041083	-1.297493
H	-2.653435	-2.609655	-1.637705
H	-1.338771	-1.884038	-2.592283
C	-2.177353	-0.864396	3.258983
H	-3.214291	-1.227036	3.288508
H	-1.521864	-1.686198	3.579146
H	-2.081753	-0.048073	3.988924

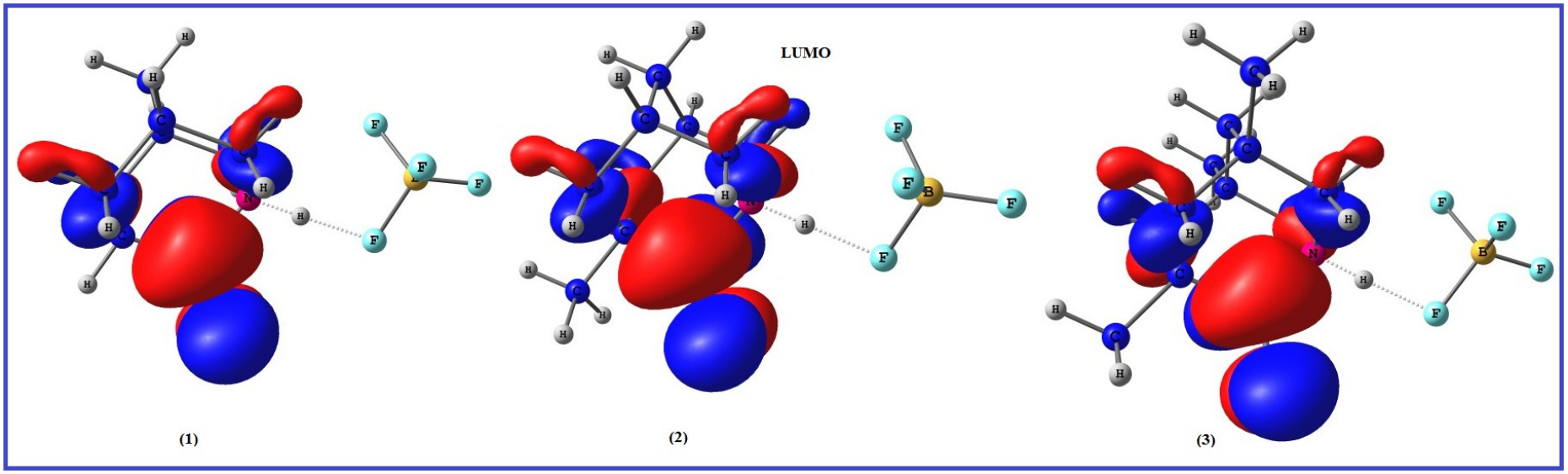

Figure S1. LUMO of the Tetrafluoroboric Acid Salts of Twisted Amides (**1-3**)

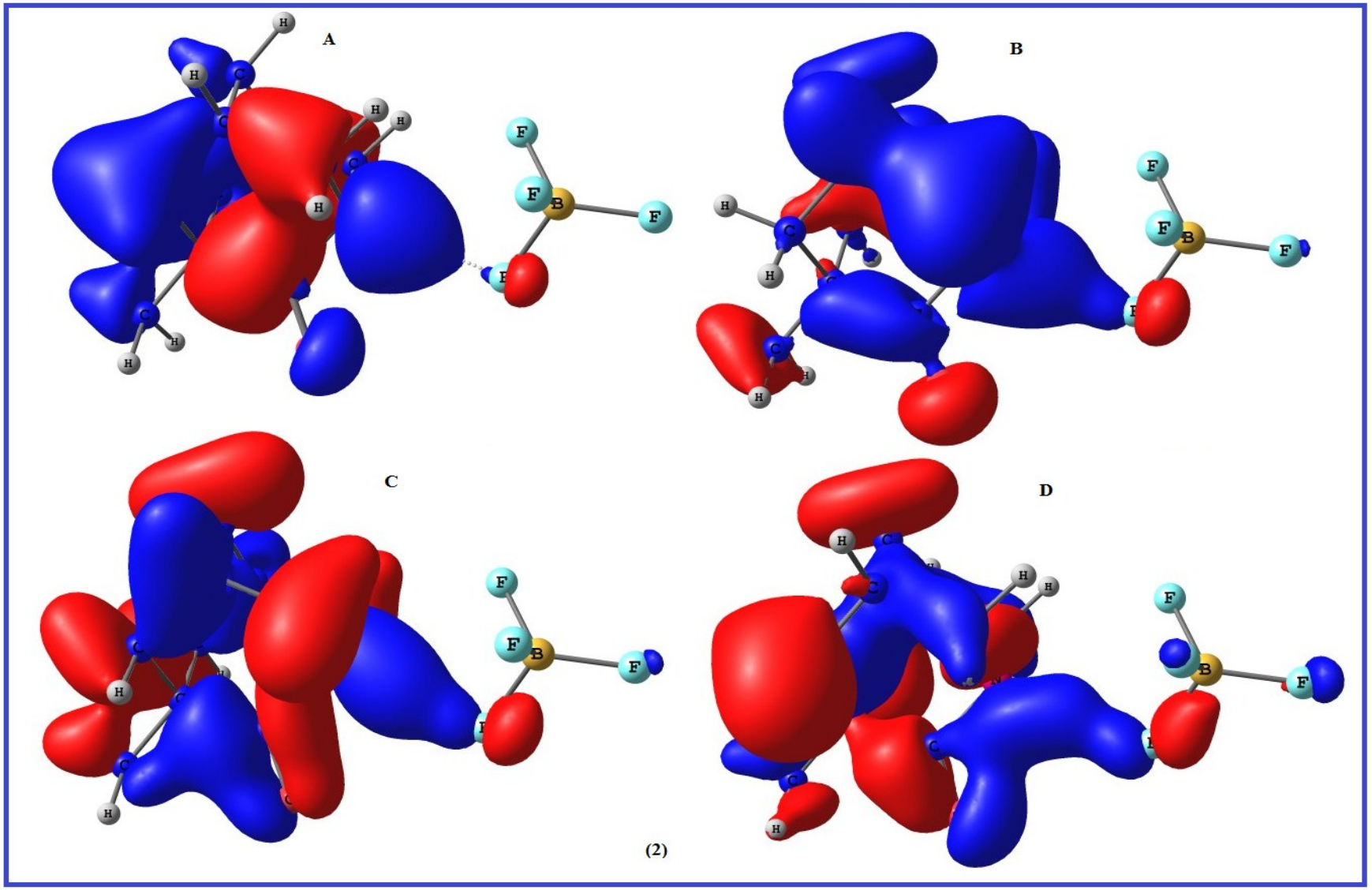
A
B
C
D
(2)

Figure S2. Important Molecular Orbitals of Salt (**2**)

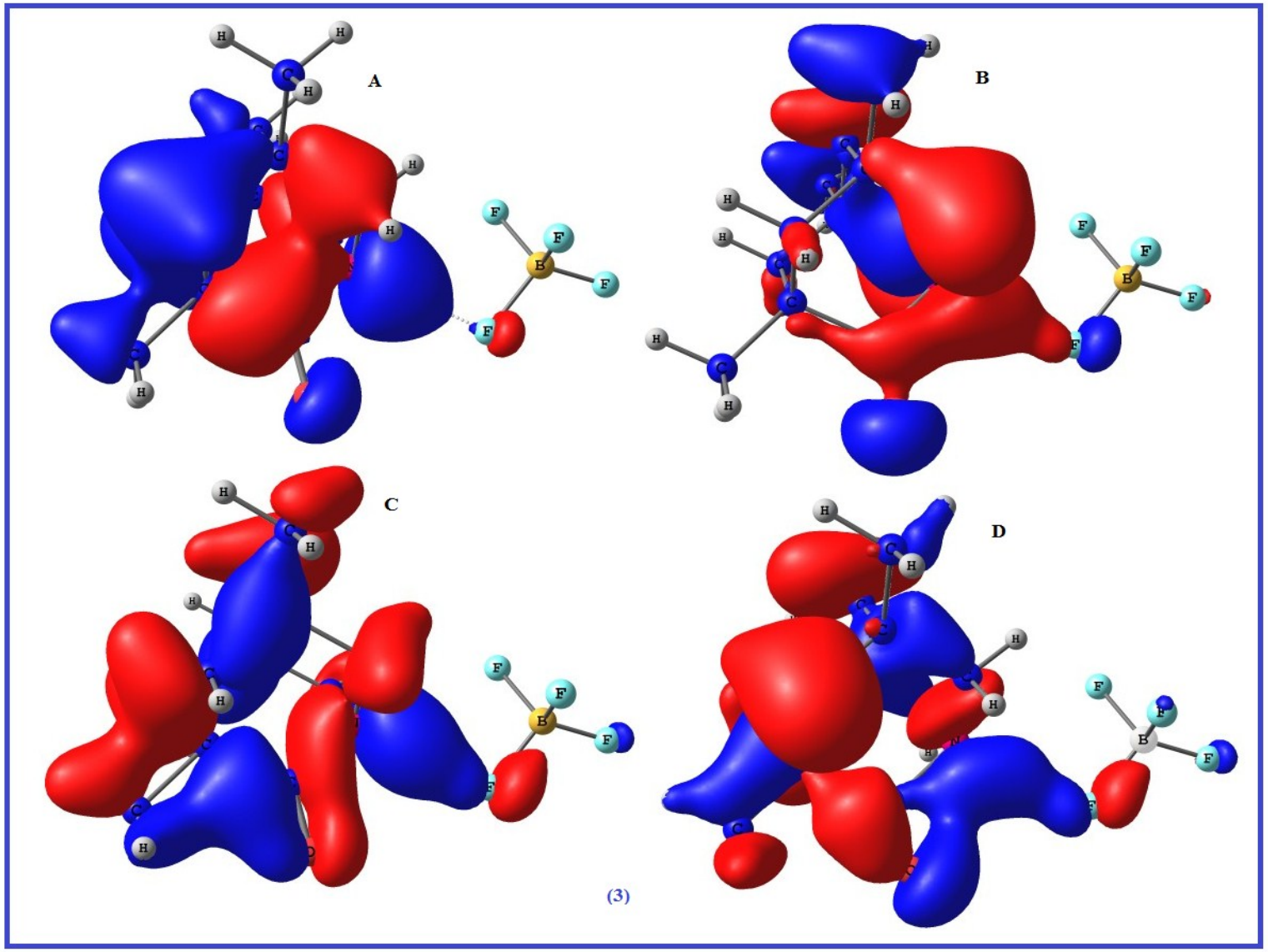
A
B
C
D
(3)

Figure S3. Important Molecular Orbitals of Salt (**3**)