

Supporting Information

Regional Electrophilic and Nucleophilic Fukui Functions Efficiently Highlight the Lewis Acidic/Basic Regions in Ionic Liquids.

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Complete Reference 27 S2

Cartesian coordinates, total energy and number of imaginary frequencies of the ionic pairs calculated at the B3LYP/6-311++G(d,p) level of theory S2

Cartesian coordinates, total energy and number of imaginary frequencies of the ionic pairs calculated at the B3LYP/AUG-cc-pVTZ level of theory S10

Complete Reference 27

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J., Gaussian 09, Revision B.01. Wallingford CT, 2009.

Cartesian coordinates, total energy and number of imaginary frequencies of the ionic pairs calculated at the B3LYP/6-311++G(d,p) level of theory

C₄mimBF₄

C	1.17714421	-0.80725143	0.60937247
C	0.43738563	-2.68172848	-0.28589965
C	1.74488472	-2.53983860	-0.63320979
N	2.18869774	-1.35957595	-0.06406008
H	1.20502867	0.14279054	1.11749111
H	-0.27326660	-3.45154908	-0.53034991
H	2.38607239	-3.16388039	-1.23103985
C	3.51723638	-0.75362302	-0.21639698
H	4.22890305	-1.23685763	0.45446218
H	3.83929842	-0.87428707	-1.24995318
H	3.42957023	0.30845901	0.00831073
N	0.10314776	-1.58973365	0.49476168
C	-1.24629074	-1.23167910	0.98353201

C	-2.18515172	-0.84808645	-0.16168693
H	-1.11087111	-0.38337569	1.65367732
H	-1.62533829	-2.08133932	1.55746813
C	-3.54142402	-0.36414644	0.36492010
H	-1.70597114	-0.05792004	-0.74593830
H	-2.33238259	-1.70862391	-0.82602981
C	-4.50351376	0.01828149	-0.76298205
H	-3.99865380	-1.14287469	0.98885077
H	-3.37911318	0.50257710	1.01450052
H	-5.45778703	0.37019071	-0.36291240
H	-4.08461705	0.81807098	-1.37963864
H	-4.71078403	-0.83517029	-1.41645086
F	0.33122157	3.51183401	-0.38459491
B	0.60356740	2.20585420	-0.05307172
F	0.28905408	1.31100965	-1.11293490
F	1.98636364	2.01977378	0.27159017
F	-0.14802464	1.78606212	1.09395172

E(B3LYP) = -848.10071026 a.u.

NIMAG = 0

C₄mimCF₃CO₂

C	1.21978002	-1.40262663	-0.09952078
C	3.39965531	-1.15934586	-0.39472548
C	3.18082147	-2.43143399	0.03587928
N	1.81432971	-2.56048762	0.21494333
H	0.12360946	-1.23985647	-0.04862186
H	4.31475677	-0.65463089	-0.65182836
H	3.86665477	-3.23984802	0.22199568
C	1.08753756	-3.75210588	0.66442437
H	1.25602496	-4.57234808	-0.03407266
H	1.42725825	-4.03756949	1.66050159
H	0.02656787	-3.50759054	0.69441179
N	2.16597434	-0.53697309	-0.47526202
C	1.90340453	0.86636211	-0.86787873
C	2.28933244	1.85514938	0.23286709
H	0.83119088	0.92628562	-1.07284020
H	2.46245013	1.05313787	-1.78818306
C	1.96500711	3.29796438	-0.17317484
H	1.73500022	1.59845026	1.14203012
H	3.35701527	1.76614071	0.47051001
C	2.32423168	4.31231197	0.91586982
H	2.50260092	3.54676712	-1.09645526
H	0.89774127	3.36727020	-0.40602183
H	2.08088423	5.32983780	0.60022617

H	1.77229187	4.11119657	1.83870097
H	3.39281940	4.28361998	1.15219403
F	-3.67128305	0.61688044	1.27763338
C	-3.46667032	0.17684839	0.00574369
F	-4.27253954	-0.89117100	-0.17358654
F	-3.90913976	1.14573965	-0.81947066
C	-1.95213752	-0.16142340	-0.20664848
O	-1.61802188	-1.31569392	0.15368260
O	-1.24924090	0.75295784	-0.66599761

E(B3LYP) = -949.87075963 a.u.

NIMAG = 0

C₄mimCl

C	-1.36084280	0.19539023	-0.09794277
C	-1.20844716	-1.99463627	-0.40363524
C	-2.45591055	-1.73011274	0.07010911
N	-2.52864544	-0.35800164	0.25528622
H	-1.03798435	1.26785630	-0.06563174
H	-0.74640557	-2.92726672	-0.67797977
H	-3.28272884	-2.38598349	0.28187737
C	-3.68347107	0.39452386	0.74766448
H	-4.52488406	0.27535421	0.06398441
H	-3.96037999	0.03983435	1.74102172
H	-3.40711618	1.44580379	0.80262060
N	-0.54682266	-0.78420840	-0.50399159
C	0.85481017	-0.56117078	-0.92499866
C	1.83980536	-0.73758789	0.23061968
H	0.90039033	0.46571408	-1.29497928
H	1.05716702	-1.25585879	-1.74375493
C	3.28050047	-0.46435939	-0.21614086
H	1.56594290	-0.03087538	1.02018388
H	1.76041448	-1.75061571	0.64523958
C	4.28817990	-0.61105579	0.92719845
H	3.54965008	-1.14701815	-1.03211154
H	3.33396272	0.55027343	-0.62352849
H	5.30559407	-0.40831581	0.58317714
H	4.06556403	0.08999241	1.73651049
H	4.27333701	-1.62275061	1.34562736
Cl	0.19694178	2.84961049	-0.17873861

E(B3LYP) = -883.73509748 a.u.

NIMAG = 0

C₄mimDCA

C	-1.17307642	-0.67383526	-0.15852827
C	-0.34607769	-2.69896166	-0.43457570
C	-1.64090721	-2.82767503	-0.03573904
N	-2.14047540	-1.55061846	0.13319338
H	-1.29980485	0.39836463	-0.10494326
H	0.39287812	-3.44408027	-0.67272134
H	-2.24159324	-3.70418148	0.13532279
C	-3.50499493	-1.19108961	0.55311035
H	-4.21614247	-1.56663454	-0.18317523
H	-3.70612991	-1.63751360	1.52719813
H	-3.56540950	-0.10242914	0.61735935
N	-0.07211310	-1.34620575	-0.50886161
C	1.23642582	-0.74269286	-0.85874566
C	2.23946489	-0.82900961	0.29221961
H	1.06032621	0.30348739	-1.11776417
H	1.59752261	-1.26826324	-1.74584835
C	3.57909773	-0.18818019	-0.09215410
H	1.82194404	-0.30586180	1.15911990
H	2.39108422	-1.87532003	0.58646122
C	4.59497888	-0.22504268	1.05231870
H	3.99300748	-0.70718718	-0.96587813
H	3.39334593	0.84643965	-0.39423282
H	5.53945813	0.23454194	0.75079139
H	4.22501624	0.32343737	1.92351697
H	4.80999947	-1.25125072	1.36838410
N	1.20509747	2.52788025	-0.71067129
C	0.17937521	2.98117877	-0.37308637
N	-0.95471725	3.51667281	0.00161664
C	-1.93694696	2.70383274	0.26080659
N	-2.83201111	1.98159999	0.49653019

E(B3LYP) = -663.98716140 a.u.

NIMAG = 0

C₄mimCH₃SO₃

C	0.98524813	-1.26032029	0.63713735
C	-0.04809904	-2.96138013	-0.31985219
C	1.26976398	-3.02892220	-0.65349051
N	1.89701736	-1.95472308	-0.04953999
H	1.13442002	-0.32399883	1.16756134
H	-0.87398121	-3.59430470	-0.59266952
H	1.80512996	-3.73329998	-1.26592269
C	3.30078172	-1.54679409	-0.19645547
H	3.88882623	-1.91366686	0.64596720
H	3.68520624	-1.96731908	-1.12427358

H	3.31903040	-0.45620900	-0.24929805
N	-0.20377610	-1.84954010	0.48722302
C	-1.47534405	-1.27713807	0.98239005
C	-2.34572791	-0.74763908	-0.15888494
H	-1.19417683	-0.45827173	1.64600901
H	-1.98373575	-2.05112330	1.56383995
C	-3.61525430	-0.07415414	0.37499617
H	-1.75788502	-0.02174548	-0.72967298
H	-2.62014812	-1.56926402	-0.83255668
C	-4.49749331	0.47653681	-0.74884190
H	-4.19160293	-0.78477198	0.98173281
H	-3.32524876	0.74454445	1.04237387
H	-5.39013119	0.96328886	-0.34703761
H	-3.95108341	1.21266946	-1.34425309
H	-4.82802907	-0.32109629	-1.42210406
H	0.17064379	4.20829266	0.35942301
C	1.10783892	3.74988069	0.04718462
S	0.85236220	1.96536748	-0.05270870
H	1.89438470	3.94222921	0.77511238
H	1.39916052	4.10224712	-0.94125921
O	2.16949337	1.37955239	-0.45320327
O	0.46325923	1.52699334	1.33249424
O	-0.22794575	1.74662360	-1.04660518

E(B3LYP) = -1087.33921078 a.u.

NIMAG = 0

C₄mimNTf₂

C	2.15852088	-1.52396698	0.12216798
C	4.13222290	-1.40107456	-0.85703219
C	3.66101543	-2.66531922	-1.02758072
N	2.42627716	-2.72158664	-0.40790041
H	1.25137137	-1.25206036	0.64670540
H	5.04439694	-0.93997596	-1.19319574
H	4.08808846	-3.51496462	-1.53112039
C	1.54439216	-3.89508746	-0.34142887
H	1.54611834	-4.38694819	-1.31342375
H	1.90330769	-4.58432813	0.42419854
H	0.53191786	-3.56231382	-0.11465207
N	3.18406374	-0.70623943	-0.13086289
C	3.21798189	0.74219226	0.17332301
C	2.75551325	1.06571694	1.59287062
H	2.58482237	1.23369791	-0.56722827
H	4.25172065	1.05816505	0.01925888
C	2.86192815	2.56790404	1.88501932

H	1.71633878	0.74904087	1.72260106
H	3.36291983	0.50270833	2.31145998
C	2.38837907	2.92381067	3.29672875
H	3.90054963	2.89552138	1.75258742
H	2.26526281	3.11976183	1.15100973
H	2.47306754	3.99783992	3.47954467
H	1.34213374	2.64165918	3.44272611
H	2.98334205	2.40853490	4.05724166
O	-1.29307636	0.85457839	-3.12389999
S	-0.81166318	0.68700595	-1.76452143
C	-0.81871393	2.43623998	-1.04562884
O	0.56998528	0.22020441	-1.54332745
N	-1.91084582	-0.06231274	-0.86601815
F	0.06558252	3.19436576	-1.71355055
F	-0.45845218	2.41714409	0.24633571
F	-2.02331715	2.99303605	-1.14653448
S	-1.54539019	-1.07092034	0.32305477
O	-0.53691594	-0.59496721	1.29368015
O	-1.38842563	-2.46904473	-0.10356687
C	-3.19514630	-0.99860562	1.23603211
F	-3.11818170	-1.82719295	2.28508208
F	-3.43494985	0.23468693	1.67976999
F	-4.19491135	-1.38868122	0.45104370

E(B3LYP) = -2251.01809202 a.u.

NIMAG = 0

C₄mimOAc

C	0.54048683	0.91346259	-0.18274395
C	-0.95958462	2.55040944	-0.31028890
C	0.21465758	3.08860810	0.11626977
N	1.13249911	2.05401895	0.18986933
H	0.98084855	-0.12929599	-0.23984853
H	-1.91465642	3.00878806	-0.50058157
H	0.47284421	4.10371982	0.36453751
C	2.54207119	2.15818326	0.59807084
H	3.06696581	2.82252455	-0.08995008
H	2.59234991	2.55985367	1.61104838
H	2.96963689	1.14905760	0.56210266
N	-0.73263955	1.19675234	-0.49313393
C	-1.70926421	0.17521852	-0.90981392
C	-2.66032114	-0.22450662	0.21997316
H	-1.12529860	-0.68455427	-1.24226105
H	-2.25791994	0.57138972	-1.76826959
C	-3.64954498	-1.30874477	-0.22320961

H	-2.06594979	-0.58931136	1.06413311
H	-3.21029029	0.65655656	0.57241950
C	-4.60212118	-1.73430594	0.89732480
H	-4.23086789	-0.94556672	-1.07959832
H	-3.08912723	-2.18073045	-0.57778906
H	-5.29250593	-2.50880870	0.55413484
H	-4.05027239	-2.13628538	1.75196987
H	-5.20021477	-0.88977291	1.25380453
H	3.11073142	-3.60753519	-1.09028717
C	3.18255453	-3.20440055	-0.07629730
C	2.55991981	-1.80779966	-0.03456850
H	2.61771073	-3.87569999	0.57681696
H	4.22615239	-3.17912916	0.23756143
O	3.26445899	-0.84408798	0.34819228
O	1.34150719	-1.72307891	-0.39886629

E(B3LYP) = -652.04719298 a.u.

NIMAG = 0

C₄mimOTf

C	1.10997997	-1.57995657	-0.54304487
C	3.08192354	-1.66324378	0.44409401
C	2.40486188	-2.79873380	0.76791239
N	1.17289915	-2.72455426	0.14290802
H	0.23901243	-1.24139638	-1.08674327
H	4.06527351	-1.32919112	0.72566870
H	2.68921951	-3.63732945	1.37956826
C	0.07530880	-3.69833089	0.21938154
H	-0.81780534	-3.22568406	-0.18886283
H	0.33153748	-4.59149795	-0.35168379
H	-0.09525190	-3.95966190	1.26343449
N	2.25585721	-0.91619473	-0.37698428
C	2.51715647	0.44305789	-0.90043689
C	2.40619276	1.51127148	0.18782988
H	1.76788276	0.62282098	-1.67034587
H	3.50864254	0.42959932	-1.35994161
C	2.61391600	2.91751663	-0.38622002
H	1.40923076	1.44191063	0.63097084
H	3.14062570	1.31941298	0.97984576
C	2.49390548	4.00900133	0.68074155
H	3.59847303	2.97982514	-0.86686166
H	1.86884714	3.09066078	-1.16951030
H	2.63938160	5.00077104	0.24542870
H	1.50513462	3.99233225	1.14721553
H	3.24046716	3.87938942	1.47087886

O	-1.79873538	-1.26878818	-0.97842280
S	-1.92773451	0.21531958	-0.92671637
C	-2.31653373	0.52115863	0.89400051
O	-0.61242636	0.88799488	-1.09014112
O	-3.05538741	0.79224608	-1.64886233
F	-2.42214270	1.82994626	1.15992213
F	-3.45724726	-0.07617454	1.26168451
F	-1.32461903	0.02468347	1.67514868

E(B3LYP) = -1385.14695304 a.u.
NIMAG = 0

C₄mimPF₆

C	0.51618806	1.74194673	0.65153044
C	2.39440481	2.24524774	-0.38732017
C	1.47436772	3.19577232	-0.70296223
N	0.30526278	2.86216628	-0.04279562
H	-0.22621481	1.21159788	1.22326518
H	3.41830299	2.13015592	-0.69688410
H	1.54758627	4.06417758	-1.33421936
C	-0.98283085	3.56045746	-0.13318862
H	-0.96528492	4.46018473	0.48323514
H	-1.16584521	3.82443542	-1.17397549
H	-1.76278414	2.87855860	0.20017241
N	1.77625805	1.34716780	0.46430329
C	2.33929206	0.07188291	0.95905068
C	2.50850389	-0.95515541	-0.16264422
H	1.63981075	-0.30100343	1.70627753
H	3.28871225	0.30019220	1.45005679
C	2.98088137	-2.30812299	0.38239777
H	1.54875099	-1.07342811	-0.67148518
H	3.22852257	-0.58167269	-0.90110736
C	3.14633922	-3.35529068	-0.72247776
H	3.93074607	-2.18274397	0.91759388
H	2.25178255	-2.66821012	1.11599989
H	3.47609232	-4.31194049	-0.30970363
H	2.20014702	-3.52418448	-1.24318447
H	3.88725881	-3.03895593	-1.46361378
F	-2.92606761	-1.52204712	0.98047389
P	-1.87028967	-0.83876711	-0.03489342
F	-0.68303924	-0.91792514	1.14505067
F	-0.74894509	-0.08370155	-1.01267116
F	-2.26278785	0.67434539	0.56783629
F	-1.39486519	-2.27996071	-0.60694514
F	-2.99282437	-0.67642452	-1.18884432

E(B3LYP) = -1364.30835069 a.u.

NIMAG = 0

Cartesian coordinates, total energy and number of imaginary frequencies of the ionic pairs
calculated at the B3LYP/AUG-cc-pVTZ level of theory

C₄mimBF₄

C	1.14936187	-0.82734323	0.60573491
C	0.38871297	-2.68629052	-0.29111787
C	1.69642425	-2.56373941	-0.63100577
N	2.15346565	-1.39274848	-0.06119247
H	1.19003020	0.12018409	1.11379587
H	-0.32995895	-3.44465602	-0.53814733
H	2.32975152	-3.19542147	-1.22515699
C	3.48852746	-0.80982111	-0.20622302
H	4.19296080	-1.32127092	0.44714843
H	3.80417692	-0.91199571	-1.24126991
H	3.42381173	0.24556206	0.04441702
N	0.06711343	-1.59186994	0.48581858
C	-1.27400534	-1.22099236	0.97416081
C	-2.20358932	-0.80819442	-0.16370098
H	-1.12961351	-0.38715295	1.65644809
H	-1.66834505	-2.07106693	1.53213006
C	-3.55362896	-0.32218798	0.36590384
H	-1.71677006	-0.01437669	-0.73185531
H	-2.35579974	-1.65315872	-0.84226073
C	-4.50654595	0.08968814	-0.75428555
H	-4.01859743	-1.10613603	0.97256799
H	-3.38524264	0.52811942	1.03108017
H	-5.45703084	0.44036543	-0.35147424
H	-4.07999204	0.89594206	-1.35230611
H	-4.71756967	-0.74687601	-1.42367889
F	0.42009001	3.50366087	-0.39272149
B	0.65698096	2.19557281	-0.05183291
F	0.37281596	1.31343010	-1.12406508
F	2.01734909	1.99306462	0.32607532
F	-0.14606721	1.79314251	1.05721677

E(B3LYP) = -848.18284868 u.a.

NIMAG = 0

C₄mimCF₃CO₂

C	1.16318874	-1.42068481	-0.08909228
C	3.34148074	-1.26988675	-0.41781031

C	3.07567184	-2.53083623	0.00778896
N	1.71130631	-2.60203544	0.20779362
H	0.07610892	-1.21116554	-0.01710248
H	4.27154310	-0.80485214	-0.68648683
H	3.72776479	-3.36728343	0.17769984
C	0.94431521	-3.76135431	0.66136202
H	1.06889835	-4.58347245	-0.04040215
H	1.28586156	-4.06658216	1.64832257
H	-0.10290963	-3.47502973	0.70817992
N	2.13760197	-0.59603774	-0.47385653
C	1.93046983	0.81389683	-0.85855199
C	2.38329474	1.78344216	0.22879666
H	0.86012205	0.92301371	-1.03757794
H	2.47567638	0.97800158	-1.78848469
C	2.12644744	3.23588448	-0.17690025
H	1.83360499	1.55875244	1.14604499
H	3.44639490	1.64146390	0.44817450
C	2.55175355	4.23260306	0.89923249
H	2.65990574	3.45325727	-1.10728540
H	1.06315255	3.35771484	-0.39360892
H	2.35663849	5.25758499	0.58343961
H	2.00563681	4.06334836	1.82875878
H	3.61821928	4.15008845	1.11959036
F	-3.88523153	0.15844519	1.28416501
C	-3.47766715	0.26897709	-0.00227070
F	-4.22684402	-0.59026970	-0.72994868
F	-3.79549524	1.50870445	-0.40890161
C	-1.95141519	-0.05512439	-0.13564136
O	-1.65143625	-1.22452250	0.20564304
O	-1.21682350	0.85430322	-0.54765982

E(B3LYP) = -949.95842012 u.a.

NIMAG = 0

C₄mimCl

C	-1.36122063	0.18195178	-0.07555117
C	-1.15743712	-1.99136437	-0.42695132
C	-2.41154539	-1.76586183	0.03933639
N	-2.51662253	-0.40353205	0.25339811
H	-1.06747116	1.26030547	-0.02864066
H	-0.67388183	-2.90541064	-0.71749979
H	-3.22315089	-2.44334471	0.22950364
C	-3.68911368	0.30978671	0.75010558
H	-4.52527777	0.17208368	0.06733410
H	-3.95773199	-0.06022778	1.73757361

H	-3.44418399	1.36577473	0.81380952
N	-0.52381986	-0.76752609	-0.49427695
C	0.86799939	-0.50255910	-0.90779034
C	1.86215357	-0.73170926	0.22588672
H	0.89528641	0.54326659	-1.21659384
H	1.07675611	-1.14507765	-1.76349853
C	3.29295254	-0.41945817	-0.21430091
H	1.58763229	-0.07717680	1.05582715
H	1.79785272	-1.76449867	0.58351687
C	4.30957506	-0.61602159	0.90841160
H	3.56119355	-1.05260710	-1.06595772
H	3.33243340	0.61307460	-0.56780031
H	5.31965272	-0.38590515	0.56855809
H	4.08772068	0.03645714	1.75427656
H	4.30759859	-1.64611008	1.27159600
Cl	0.11344026	2.87636569	-0.16651356

E(B3LYP) = -883.78486862 u.a.

NIMAG = 0

C₄mimDCA

C	-1.17438190	-0.66996539	-0.14832362
C	-0.34240308	-2.68560841	-0.43434551
C	-1.63394906	-2.82076874	-0.03909879
N	-2.13681403	-1.54950084	0.13613667
H	-1.30668786	0.39976695	-0.09095234
H	0.39740153	-3.42557653	-0.67571913
H	-2.23033235	-3.69858013	0.12608336
C	-3.49881837	-1.19819964	0.55574248
H	-4.20821910	-1.58808791	-0.17117296
H	-3.69444303	-1.63533180	1.53258621
H	-3.56904971	-0.11192681	0.60770398
N	-0.07326459	-1.33484538	-0.49986930
C	1.22815531	-0.72785050	-0.85124511
C	2.23622368	-0.81694490	0.29043523
H	1.04941246	0.31722218	-1.10235453
H	1.58732113	-1.24710885	-1.73982473
C	3.57734033	-0.19585062	-0.10589736
H	1.83120464	-0.28494501	1.15455733
H	2.37782833	-1.86053164	0.58936957
C	4.59757820	-0.23469117	1.02956143
H	3.97858263	-0.72514164	-0.97600023
H	3.40211123	0.83587939	-0.41444315
H	5.54388100	0.20838471	0.71884760
H	4.24048939	0.32505718	1.89557958

H	4.80022768	-1.25813955	1.35338616
N	1.22521202	2.53707735	-0.65203157
C	0.18594918	2.97414495	-0.34668571
N	-0.96269671	3.49872153	-0.00824511
C	-1.94753368	2.68808390	0.23782866
N	-2.84796316	1.97354274	0.46179764

E(B3LYP) = -664.05130194 u.a.

NIMAG = 0

C₄mimCH₃SO₃

C	-0.74082486	1.37581534	0.59626846
C	0.52405375	2.95249472	-0.28281508
C	-0.76503578	3.21444486	-0.61792027
N	-1.53844950	2.21563762	-0.06341872
H	-1.02606675	0.45009330	1.09095923
H	1.43016872	3.47549382	-0.52369550
H	-1.19093351	4.00902990	-1.20134295
C	-2.98481898	2.03497598	-0.21018232
H	-3.50824090	2.52126236	0.61110447
H	-3.29352776	2.47718083	-1.15342701
H	-3.18285034	0.96397468	-0.22567875
N	0.51627591	1.80120399	0.47696756
C	1.68909092	1.05420998	0.96748048
C	2.45683079	0.38028318	-0.16656171
H	1.30259573	0.30420230	1.65479018
H	2.31526106	1.75223393	1.52482953
C	3.62931665	-0.44482640	0.36565513
H	1.76613701	-0.26896227	-0.70857627
H	2.82677808	1.13785280	-0.86465552
C	4.40677593	-1.13772526	-0.75183440
H	4.30570360	0.19450545	0.94268799
H	3.24470692	-1.19683383	1.05903132
H	5.23019055	-1.72933273	-0.35038625
H	3.75702512	-1.80592161	-1.31797574
H	4.82887046	-0.41141203	-1.44970489
H	-0.88030964	-4.14295779	0.38834255
C	-1.72090346	-3.54998875	0.03809865
S	-1.19747573	-1.83059767	-0.04325177
H	-2.55718238	-3.62006028	0.72829818
H	-2.01793647	-3.85684594	-0.96122878
O	-2.38103039	-1.05909323	-0.50185689
O	-0.80942317	-1.45541048	1.34934060
O	-0.05985524	-1.78048776	-0.98189844

E(B3LYP) = -1087.44502909 u.a.

NIMAG = 0

C₄mimNTf₂

C	2.14321284	-1.52167934	-0.00982629
C	4.12803763	-1.38230993	-0.95153002
C	3.67285524	-2.64810085	-1.12781166
N	2.43045290	-2.71426177	-0.53198136
H	1.22827120	-1.25754422	0.50137798
H	5.04034715	-0.91455693	-1.27060220
H	4.11509343	-3.49234494	-1.62248549
C	1.55771155	-3.89012854	-0.48427074
H	1.53443781	-4.34917287	-1.46942468
H	1.93894195	-4.60234344	0.24509956
H	0.55421686	-3.56942331	-0.21700024
N	3.16217009	-0.69598821	-0.24771898
C	3.18423361	0.74205838	0.08485146
C	2.92484944	1.01508897	1.56245298
H	2.43317922	1.22197452	-0.54022065
H	4.16719199	1.10521949	-0.21143806
C	2.99292333	2.51143077	1.87425003
H	1.93705385	0.63726435	1.83348169
H	3.65848332	0.47423119	2.16717187
C	2.72116965	2.81559656	3.34602320
H	3.97781586	2.89871761	1.59572659
H	2.26529773	3.03885803	1.25317534
H	2.77321158	3.88689738	3.54031274
H	1.72839767	2.47186948	3.63969646
H	3.44983508	2.32435550	3.99391025
O	-1.49794574	0.93166470	-3.05292833
S	-0.94199530	0.74293205	-1.73226490
C	-0.90747971	2.48122163	-0.99782720
O	0.44280282	0.27880815	-1.60509196
N	-1.98082051	-0.02349071	-0.79167245
F	-0.08233786	3.24824447	-1.72358745
F	-0.45343082	2.45737426	0.26275820
F	-2.12000101	3.02840943	-1.00525421
S	-1.53205492	-1.04848323	0.34149554
O	-0.51297225	-0.56636042	1.28320773
O	-1.34127171	-2.41778915	-0.13408558
C	-3.14000656	-1.07791342	1.31932090
F	-2.98251706	-1.92752337	2.34026839
F	-3.42034667	0.12953783	1.80502148
F	-4.15131455	-1.49506173	0.56418550

E(B3LYP) = -2251.01806932 u.a.

NIMAG = 0

C₄mimOAc

C	0.53843785	0.91337052	-0.17707435
C	-0.94878200	2.55354376	-0.31315598
C	0.22417906	3.08578441	0.11308518
N	1.13413003	2.04920291	0.19211674
H	0.97466829	-0.12950131	-0.23130761
H	-1.89888959	3.01556471	-0.50699096
H	0.48622499	4.09829311	0.35825882
C	2.53881993	2.14758120	0.60300594
H	3.06671657	2.81230455	-0.07853625
H	2.58900710	2.54603103	1.61472828
H	2.96310366	1.13979011	0.56445591
N	-0.72936077	1.20151864	-0.49045735
C	-1.70807727	0.18839451	-0.90768292
C	-2.64562959	-0.22611373	0.22336519
H	-1.13124655	-0.66621511	-1.25716745
H	-2.26634921	0.59476824	-1.75179524
C	-3.64134326	-1.29680759	-0.22498024
H	-2.04453610	-0.60587990	1.05266902
H	-3.18666994	0.64907929	0.59532811
C	-4.58177643	-1.73527433	0.89579918
H	-4.22837282	-0.91888772	-1.06754419
H	-3.08945373	-2.16294903	-0.59858520
H	-5.27778475	-2.49912687	0.54864727
H	-4.02386433	-2.15187970	1.73597919
H	-5.17018714	-0.89560551	1.27113826
H	3.08875045	-3.60604079	-1.09480793
C	3.16273261	-3.20629024	-0.08235586
C	2.54360528	-1.81032701	-0.03688154
H	2.59857092	-3.87690281	0.56769236
H	4.20450533	-3.18532265	0.22884482
O	3.25307639	-0.84971790	0.33878986
O	1.32435179	-1.72474952	-0.39146152

E(B3LYP) = -652.10809622 u.a.

NIMAG = 0

C₄mimOTf

C	-1.35578439	-1.40335002	0.32626476
C	-3.48631338	-1.25621916	-0.21128460
C	-3.03582056	-2.46893043	-0.62383013
N	-1.70074499	-2.53867705	-0.28021047

H	-0.36248959	-1.16739782	0.68219361
H	-4.45990956	-0.80908820	-0.28609650
H	-3.54298615	-3.27394873	-1.12204733
C	-0.77840703	-3.64993393	-0.52739816
H	0.21663141	-3.33221220	-0.22557715
H	-1.08750264	-4.51866728	0.05020834
H	-0.78275211	-3.89170020	-1.58778364
N	-2.42238188	-0.60784791	0.38225754
C	-2.40660870	0.76569037	0.92136321
C	-2.23367728	1.81488693	-0.17281871
H	-1.57239675	0.81388784	1.61705825
H	-3.33806861	0.90609274	1.46966492
C	-2.18549622	3.22860988	0.40883705
H	-1.30285926	1.60744416	-0.70366233
H	-3.05007765	1.73703014	-0.89730258
C	-1.98808876	4.29745426	-0.66423757
H	-3.10846548	3.42985123	0.96155475
H	-1.36949432	3.28363902	1.13287747
H	-1.95448230	5.29367964	-0.22301911
H	-1.05265103	4.14145439	-1.20322577
H	-2.80068223	4.28406608	-1.39359887
O	1.62749098	-1.64056907	0.58719836
S	1.99451086	-0.23803504	0.88702490
C	2.52404054	0.41472362	-0.79658692
O	0.80739907	0.58778998	1.19388102
O	3.15587711	-0.04492133	1.73570561
F	2.85450379	1.71027282	-0.73328938
F	3.57220573	-0.26426741	-1.27551667
F	1.51425657	0.29334094	-1.68831620

E(B3LYP) = -1385.28064080 u.a.

NIMAG = 0

C₄mimPF₆

C	0.64121254	1.68268311	0.61507277
C	2.57714771	2.10919785	-0.33914070
C	1.72412192	3.11388320	-0.65984275
N	0.51751312	2.82749511	-0.05361412
H	-0.14846809	1.17885557	1.14337529
H	3.60288742	1.94773529	-0.61226337
H	1.86731675	3.99209888	-1.26102674
C	-0.72089658	3.59991345	-0.16676492
H	-0.65496533	4.50135684	0.43940709
H	-0.87593281	3.86537733	-1.20931977
H	-1.54390585	2.97432063	0.16523401

N	1.88168498	1.22607617	0.46186537
C	2.36163763	-0.08027936	0.94953396
C	2.45205709	-1.11595809	-0.16846464
H	1.65239671	-0.40609485	1.70615000
H	3.32834868	0.08429476	1.42631525
C	2.87285566	-2.48465546	0.36865821
H	1.47731101	-1.19053610	-0.65139550
H	3.16758781	-0.77926113	-0.92474994
C	2.95696574	-3.54072127	-0.73182726
H	3.83970641	-2.40258483	0.87546184
H	2.15076473	-2.80539932	1.12338086
H	3.25256203	-4.50785037	-0.32478836
H	1.99193853	-3.66610029	-1.22391395
H	3.68836807	-3.26263862	-1.49346308
F	-3.03046634	-1.31713329	0.99898875
P	-1.95118076	-0.71487454	-0.02886821
F	-0.76190623	-0.88970359	1.12030634
F	-0.80844049	-0.05063062	-1.02623238
F	-2.22214756	0.80884795	0.57871776
F	-1.60262177	-2.17882541	-0.60781881
F	-3.07588456	-0.47031422	-1.15357095

E(B3LYP) = -1364.44359887 u.a.

NIMAG = 0