

Supplementary data

Competing elimination and substitution reactions of simple acyclic disulfides

Steven M. Bachrach and Andrey Pereverzev

Department of Chemistry
Trinity University
1 Trinity Place
San Antonio TX, 78212

Electronic supplementary information (ESI) available: Coordinates of all MP2/aug-cc-pVDZ and B3LYP/aug-cc-pVDZ optimized structures, their absolute energies, and number of imaginary frequencies.

Supplementary Material for Organic & Biomolecular Chemistry
This journal is © The Royal Society of Chemistry 2005

CH₃SSH

S 1.360213 0.243610 -0.087320
S -0.495248 -0.720199 0.012995
C -1.629461 0.712148 -0.004314
H -2.649338 0.295984 -0.034597
H -1.454747 1.324025 -0.899611
H -1.505781 1.315569 0.905530
H 1.547195 0.416958 1.243763
E = -835.7050684 NIMAG = 0

CH₃SSCH₃

C -1.790079 0.823643 -0.400000
S -0.917206 -0.511890 0.494570
S 0.917203 -0.511894 -0.494570
C 1.790084 0.823641 0.399999
H -2.801294 0.882559 0.033482
H -1.857638 0.579607 -1.468789
H -1.279225 1.786257 -0.255681
H 2.801336 0.882491 -0.033409
H 1.857543 0.579655 1.468807
H 1.279292 1.786271 0.255586
E = -874.892090 NIMAG = 0

F⁻

E = -99.6659482

HO⁻

O 0.000000 0.000000 0.108143
H 0.000000 0.000000 -0.865141
E = -75.6370179 NIMAG = 0

CH₂CHCH₂⁻

C 0.000000 0.000000 0.393740
H 0.000000 0.000000 1.500129
C 0.000000 1.283495 -0.184076
C 0.000000 -1.283495 -0.184076
H 0.000000 1.426424 -1.272538
H 0.000000 -1.426424 -1.272538
H 0.000000 -2.178949 0.445710
H 0.000000 2.178949 0.445710
E = -116.892379 NIMAG = 0

H₂C=S

S 0.000000 0.000000 0.591715
C 0.000000 0.000000 -1.039402
H 0.000000 0.935522 -1.615513
H 0.000000 -0.935522 -1.615513
E = -436.8137351 NIMAG = 0

HF

F 0.000000 0.000000 0.092481
H 0.000000 0.000000 -0.832330
E = -100.2558045 NIMAG = 0

H₂O

O 0.000000 0.000000 0.119182
H 0.000000 0.760347 -0.476727
H 0.000000 -0.760347 -0.476727
E = -76.2609097 NIMAG = 0

CH₂=CHCH₃

C -1.303113 0.127311 0.000000
C 0.000000 0.482365 0.000000
C 1.149710 -0.490376 0.000000
H -1.602088 -0.925795 0.000000
H -2.096446 0.878776 0.000000
H 0.253859 1.550086 0.000000
H 1.788825 -0.344303 0.886863
H 0.787447 -1.530259 0.000000
H 1.788825 -0.344303 -0.886863
E = -117.520257 NIMAG = 0

HS⁻

H 0.000000 0.000000 0.079781
H 0.000000 0.000000 -1.276494
E = -398.2932553 NIMAG = 0

CH₃F⁻

C 0.000000 0.000000 -1.132358
S 0.000000 0.000000 0.713710
H 0.000000 1.028395 -1.541737
H 0.890616 -0.514198 -1.541737
H -0.890616 -0.514198 -1.541737
E = -437.462259 NIMAG = 0

CH₃SF

S 0.108022 -0.618776 0.000021
C -1.351490 0.432978 0.000060
H -1.392205 1.050495 -0.907420
H -1.392923 1.050044 0.907759
H -2.202812 -0.269643 -0.000827
F 1.263169 0.607961 -0.000022
E = -537.0663117 NIMAG = 0

CH₃SOH

S 0.073705 -0.624136 0.008913
C -1.374344 0.462112 0.002502
H -1.382788 1.078259 -0.907441
H -1.408402 1.093321 0.901861
H -2.250932 -0.207590 -0.003331
O 1.315548 0.561278 -0.117872
H 1.584514 0.759289 0.794268
E = -513.0776207 NIMAG = 0

Supplementary Material for Organic & Biomolecular Chemistry
This journal is © The Royal Society of Chemistry 2005

CH₂=CHCH₂SCH₃

C -1.197877 1.340320 0.065935
S -1.321511 -0.462425 -0.168884
H -0.333697 1.744321 -0.481695
H -2.121891 1.782161 -0.334512
H -1.115112 1.585652 1.136023
C 0.332929 -0.925127 0.493767
C 1.436046 -0.385971 -0.366932
C 2.288900 0.586054 0.028959
H 2.228930 1.013700 1.034875
H 3.067184 0.964733 -0.638124
H 1.507011 -0.793789 -1.382319
H 0.332383 -2.027310 0.505457
H 0.419385 -0.562325 1.532062
E = -554.378112 NIMAG = 0

1-IDn

S 2.145521 0.145826 -0.071447
S 0.177887 -0.631967 0.000586
C -0.881941 0.835067 -0.035954
H -1.969893 0.423860 -0.018087
H -0.687205 1.409713 -0.954513
H -0.686001 1.454434 0.853543
H 2.312614 0.388446 1.252280
F -3.428043 -0.100956 0.024030
E = -935.4017867 NIMAG = 0

1-TS

S 2.212708 0.121194 -0.070498
S 0.132996 -0.566808 -0.001543
C -0.961046 0.802659 -0.037726
H -2.241963 0.237745 -0.003144
F -3.348092 -0.123530 0.026767
H -0.883953 1.388243 -0.968475
H -0.869568 1.444992 0.854005
H 2.363309 0.354660 1.255723
E = -935.3982027 NIMAG = 1

1-IDx

S 2.454723 0.018858 -0.057002
S 0.015155 -0.433261 -0.029667
C -0.949709 0.943348 -0.032539
H -2.579048 0.030947 0.013357
F -3.506279 -0.246627 0.039059
H -1.103616 1.501927 -0.967961
H -1.079659 1.521981 0.894489
H 2.499045 0.135146 1.290522
E = -935.4027648 NIMAG = 0

2-IDn

C 1.181225 0.371796 0.707730
S 0.201825 -0.659035 -0.420130
S -1.760929 -0.471433 0.310904
C -2.198409 1.173466 -0.359910
H 2.274673 0.316425 0.321741
H 1.092749 -0.022881 1.731595
H 0.820008 1.412413 0.665470
H -3.226487 1.406465 -0.035385
H -2.146029 1.158355 -1.458232
H -1.511160 1.935484 0.036924
F 3.749447 0.289962 -0.177936
E = -974.5875328 NIMAG = 0

Supplementary Material for Organic & Biomolecular Chemistry
This journal is © The Royal Society of Chemistry 2005

2-TS

C 1.228795 0.406069 0.644344
S 0.245244 -0.640694 -0.362049
S -1.838792 -0.503155 0.263252
C -2.161446 1.198954 -0.317534
H 2.587469 0.272299 0.145088
H 1.233608 0.100569 1.704130
H 0.972811 1.474561 0.530079
H -3.167479 1.502640 0.017502
H -2.101682 1.247872 -1.415610
H -1.414567 1.878861 0.123478
F 3.664724 0.243849 -0.164974
E = -974.5828906 NIMAG = 1

2-IDx

S -2.089816 -0.539537 0.134118
S 0.366621 -0.710760 -0.149020
C 1.096906 0.701948 0.409218
H 2.852569 0.179802 0.013741
F 3.807266 0.097866 -0.116105
H 1.228176 0.869764 1.488801
H 1.118138 1.599134 -0.227760
C -2.059529 1.237462 -0.250502
H -2.892131 1.749457 0.258397
H -2.118962 1.426647 -1.335790
H -1.106321 1.662690 0.133688
E = -974.5849926 NIMAG = 0

3-IDn

S 2.172496 0.129477 -0.083245
S 0.191144 -0.619724 0.016568
C -0.856401 0.851484 -0.037807
H -1.953635 0.440838 -0.044518
H -0.647397 1.425620 -0.954068
H -0.680845 1.472052 0.855123
H 2.350959 0.394489 1.234575
O -3.475343 -0.082079 0.112335
H -3.946178 -0.341319 -0.696115
E = -911.3717993 NIMAG = 0

3-TS

S 2.187371 0.133857 -0.094659
S 0.181006 -0.604637 0.031895
C -0.906769 0.812816 -0.024686
H -2.065208 0.348047 -0.002318
H -0.755977 1.384268 -0.955161
H -0.755710 1.458250 0.856270
H 2.371076 0.415718 1.218644
O -3.438343 -0.076965 0.102282
H -3.740866 -0.334976 -0.783338
E = -911.3715069 NIMAG = 1

3-IDx

S 2.488571 -0.190856 -0.186372
S -0.055051 -0.213860 0.239985
C -0.851496 1.224842 -0.071036
H -2.777133 0.112140 0.037168
H -1.127342 1.503684 -1.099132
H -0.846903 2.038736 0.668958
H 2.711119 0.274264 1.064946
O -3.576712 -0.439579 -0.096332
H -3.173382 -1.285792 -0.332873
E = -911.3993226 NIMAG = 0

4-IDn

C 1.157870 0.374160 0.714541
S 0.185045 -0.650944 -0.420598
S -1.784973 -0.478734 0.301100
C -2.219735 1.174536 -0.350401
H 2.263153 0.290740 0.351869
H 1.046532 -0.007996 1.741334
H 0.823271 1.422739 0.655259
H -3.249587 1.403350 -0.028600
H -2.160965 1.174003 -1.448523
H -1.534437 1.930936 0.060398
O 3.796528 0.364985 -0.204049
H 4.409846 -0.350972 0.027785
E = -950.5575484 NIMAG = 0

4-TS

C 1.200986 0.411450 0.647814
S 0.204702 -0.636894 -0.408405
S -1.796174 -0.495461 0.300984
C -2.217413 1.168701 -0.328638
H 2.393527 0.315063 0.232486
H 1.140279 0.072741 1.695498
H 0.886182 1.466209 0.562987
H -3.238403 1.415012 0.008301
H -2.171518 1.181060 -1.427723
H -1.512016 1.907447 0.081957
O 3.738896 0.344084 -0.185544
H 4.152906 -0.473424 0.134528
E = -950.5569721 NIMAG = 0

4-IDx

C 0.904986 1.034946 0.277666
S 0.485017 -0.594593 0.288377
S -2.095783 -0.671261 -0.133451
C -2.167746 1.133525 -0.173334
H 0.865944 1.639274 1.194701
H 1.135820 1.560693 -0.660533
H -2.775810 1.543918 0.650036
H -2.549320 1.510366 -1.136723
H -1.116951 1.523016 -0.048134
H 3.035118 0.326456 0.034563
O 3.893214 -0.004784 -0.301006
H 3.608294 -0.822613 -0.730657
E = -950.5826811 NIMAG = 0

Supplementary Material for Organic & Biomolecular Chemistry
This journal is © The Royal Society of Chemistry 2005

5-IDn

S -3.076630 -0.372075 -0.112747
S -1.313700 0.766993 0.051018
C -0.011448 -0.508230 -0.069062
H 0.939955 0.059272 -0.016566
C 2.929454 1.247788 0.163564
C 3.310489 -0.007043 -0.353897
C 3.234909 -1.288487 0.217308
H -0.082722 -1.037020 -1.028138
H -0.089924 -1.208512 0.772831
H -3.199749 -0.731486 1.188866
H 3.097174 2.161442 -0.414759
H 2.635685 1.363498 1.215555
H 3.669801 0.012791 -1.398476
H 3.572209 -2.168675 -0.338483
H 2.922433 -1.434175 1.259343
E = -952.619354 NIMAG = 0

5-IDn B3LYP/aug-cc-pVDZ

S -2.985173 0.661107 0.206079
S -1.539730 -0.862947 -0.402634
C -0.024002 -0.456754 0.518743
H 0.783562 -1.137543 0.177294
C 3.268408 -1.043285 -0.019125
C 3.365939 0.315297 0.304930
C 3.036859 1.450937 -0.431807
H -0.170970 -0.593384 1.596625
H 0.332234 0.557134 0.294792
H -2.600607 1.636431 -0.661852
H 3.624093 -1.809252 0.671078
H 2.966065 -1.373772 -1.016853
H 3.737038 0.518150 1.321809
H 3.163393 2.449028 -0.011076
H 2.680409 1.385489 -1.463378
E = -954.2520469 NIMAG = 0

5-TS MP2/aug-cc-pVDZ

S 3.171015 -0.072822 -0.004343
S 0.431986 -0.238595 -0.045121
C -0.232562 1.349344 -0.160095
H -1.631787 1.249009 0.030221
H -0.177689 1.846668 -1.142999
H -0.018372 2.026162 0.682829
H 3.096516 0.039620 1.342939
C -2.901865 0.835628 0.033318
H -3.495836 1.478912 0.696483
C -2.648293 -0.519359 0.458961
H -2.737472 -0.747995 1.529247
C -1.910295 -1.385342 -0.326068
H -1.590699 -2.359790 0.052673
H -3.120045 0.983746 -1.034404
H -1.814539 -1.215293 -1.402251
E = -952.622843 NIMAG = 1

5-TS B3LYP/aug-cc-pVDZ

S -0.074627 0.056989 -3.147503
S -0.264416 0.041419 -0.670779
C 1.302401 -0.034744 0.078262
H 1.166230 -0.045448 1.421932
H 1.942877 0.845350 -0.079791
H 1.856054 -0.970488 -0.089108
H -0.079252 -1.296588 -3.262183
C 0.954098 0.079155 2.856055
H 1.696762 -0.502424 3.412708
C -0.403972 -0.390899 2.879309
H -0.549713 -1.444768 3.148157
C -1.489777 0.274551 2.390955
H -2.462417 -0.210385 2.308811
H 1.107574 1.162655 2.922107
H -1.429916 1.319178 2.082389
E = -954.2479375 NIMAG = 1

6-IDn

S 2.705796 -0.048187 -0.466032
S 0.896106 -1.003097 -0.017597
C -0.327910 0.243994 -0.556045
H -1.316992 -0.198605 -0.324995
C -3.227410 -0.946460 0.802673
C -3.684357 -0.003658 -0.139823
C -3.454867 1.380012 -0.232855
H -0.220508 0.433512 -1.632040
H -0.206996 1.171926 0.019188
H -3.538921 -1.993349 0.736765
H -2.695072 -0.634230 1.710943
H -4.270387 -0.431330 -0.973201
H -3.892309 1.965327 -1.047259
H -2.918824 1.926340 0.554022
C 2.832034 1.093610 0.958420
H 3.768618 1.663773 0.841830
H 1.981090 1.790324 0.961527
H 2.854918 0.521874 1.897058
E = -991.805798

Supplementary Material for Organic & Biomolecular Chemistry
This journal is © The Royal Society of Chemistry 2005

6-TS MP2/aug-cc-pVDZ

S 0.250125 0.225829 0.033882
S 0.033772 0.110357 2.676232
C 1.647057 0.038355 3.305447
H 1.589244 -0.152074 4.664361
H 2.244298 0.963279 3.229653
H 2.225973 -0.865276 3.044794
C 1.263069 -0.169368 6.002675
H 1.936942 -0.851359 6.537988
C -0.107762 -0.572163 5.819774
H -0.340334 -1.642724 5.901371
C -1.025002 0.237297 5.180158
H -2.014765 -0.135526 4.903979
H 1.447578 0.894781 6.208127
H -0.850966 1.312657 5.084812
C 1.347690 -1.236810 0.089349
H 1.899110 -1.339660 -0.860881
H 2.092502 -1.122528 0.900851
H 0.775382 -2.162651 0.272573
E = -991.801537

6-TS B3LYP/aug-cc-pVDZ

S 2.859359 -0.154274 -0.512967
S 0.601471 -0.456507 -0.424773
C -0.243786 1.067087 -0.165186
H -1.571201 0.940205 -0.145905
H -0.092649 1.795911 -0.975034
H -0.037855 1.522548 0.815749
C -3.075176 1.090523 -0.186570
H -3.261614 2.089449 0.227206
C -3.590655 -0.018344 0.571745
H -3.680719 0.153853 1.653867
C -3.867756 -1.286076 0.144971
H -4.141158 -2.074583 0.847488
H -3.215149 1.043186 -1.275087
H -3.802860 -1.561853 -0.910593
C 3.206190 0.065654 1.277233
H 4.274305 0.299521 1.398340
H 2.614691 0.900418 1.678776
H 2.968025 -0.849205 1.835884
E = -993.5577614 NIMAG = 1

7-TSn

S 1.955163 -0.242943 -0.065204
S -0.392688 -0.370894 -0.036065
C -0.392375 1.463745 -0.005138
H -1.445056 1.763586 0.109614
H 0.031149 1.869276 -0.936341
H 0.210370 1.824394 0.839999
H 2.308963 -0.169327 1.239752
F -2.638975 -0.472112 0.044235
E = -935.4000209 NIMAG = 1

7-INT

S 1.937589 -0.171036 -0.074292
S -0.374832 -0.399524 -0.010869
C -0.596910 1.418318 -0.011509
H -1.680379 1.577110 -0.094133
H -0.061575 1.864910 -0.862470
H -0.211243 1.855405 0.923247
H 2.129798 -0.018728 1.257543
F -2.399916 -0.517738 0.023049
E = -935.4066901 NIMAG = 0

7-TSx

F 2.888441 0.013510 -0.000051
S 1.262439 -0.519444 0.000004
C 0.428705 1.058397 0.000067
H 0.657287 1.628544 -0.911440
H 0.657332 1.628499 0.911591
H -0.655100 0.765771 0.000080
S -2.935483 -0.053743 -0.000048
H -2.459012 -1.323789 0.000523
E = -935.3810375 NIMAG = 1

7-IDx

F -2.909832 0.077463 0.032472
S -1.311474 -0.537035 -0.021964
C -0.394648 0.992958 -0.008879
H -0.565285 1.553882 0.920766
H -0.612725 1.597970 -0.900237
H 0.672756 0.642553 -0.044557
S 2.945427 -0.104272 -0.071558
H 2.918385 -0.188409 1.281405
E = -935.3816351 NIMAG = 0

8-TSn

S -1.604473 -0.541879 0.332353
S 0.449173 -0.507226 -0.172918
C 1.045466 0.839969 0.897801
H 2.124847 0.825744 0.596426
H 0.875022 0.586226 1.954872
H 0.545651 1.787571 0.640297
F 3.222190 0.003519 -0.487673
C -2.215695 0.853499 -0.682832
H -1.995190 0.667896 -1.744246
H -3.305990 0.933190 -0.534342
H -1.737868 1.792577 -0.364720
E = -974.5851692 NIMAG = 1

Supplementary Material for Organic & Biomolecular Chemistry
This journal is © The Royal Society of Chemistry 2005

E = -911.3713387 NIMAG = 1

8-INT

C -0.900661 1.345456 -0.413716
S -0.684358 -0.434124 -0.039578
S 1.494252 -0.385773 -0.576544
C 2.178132 0.318328 0.970013
H -1.977552 1.526614 -0.303448
H -0.553062 1.558819 -1.435461
H -0.335605 1.966538 0.300899
H 3.267288 0.453107 0.852522
H 1.983179 -0.356001 1.818528
H 1.724076 1.300097 1.181095
F -2.747939 -0.368169 0.456227
E = -974.5882478 NIMAG = 0

8-TSx

F 3.170835 0.102527 0.111153
S 1.549571 0.297130 -0.414041
C 0.742359 -0.916338 0.610092
H 0.803689 -0.652075 1.675371
H 1.136466 -1.923613 0.414129
H -0.336095 -0.879790 0.271448
S -2.523395 -0.509586 -0.291025
C -2.141874 1.147425 0.421007
H -2.367582 1.958368 -0.294768
H -2.725862 1.340917 1.339240
H -1.069850 1.246215 0.688658
E = -974.5537765 NIMAG = 1

8-IDx

F 3.151323 -0.031642 0.000434
S 1.492980 0.458135 -0.000457
C 0.720127 -1.147451 0.000118
H 0.979790 -1.707476 0.909904
H 0.979078 -1.707885 -0.909635
H -0.398113 -0.964747 0.000502
S -2.605541 -0.482372 -0.000090
C -1.886071 1.200053 0.000403
H -2.183216 1.780476 -0.891247
H -2.174373 1.776362 0.897609
H -0.768442 1.180227 -0.005404
E = -974.5557276 NIMAG = 0

9-TSn

S 2.116736 0.000246 -0.059258
S 0.061408 -0.525067 -0.025571
C -0.763747 1.090051 -0.040583
H -1.855432 0.782993 -0.084671
H -0.452803 1.661444 -0.928513
H -0.527015 1.643943 0.880790
H 2.302890 0.179668 1.272021
O -3.213158 -0.238247 0.101254
H -4.030190 -0.505239 -0.348909

9-INT

S 2.065031 -0.201382 -0.092485
S -0.512457 -0.387321 0.032945
C -0.546733 1.446578 -0.016752
H -1.600604 1.732312 0.120761
H -0.162557 1.817773 -0.978825
H 0.076811 1.855229 0.790600
H 2.230317 -0.074384 1.245464
O -2.434458 -0.485267 0.088840
H -2.629096 -0.709025 -0.835571
E = -911.3919077 NIMAG = 0

9-TSx

O -2.854505 -0.146047 0.055767
S -1.137677 -0.491580 0.030688
C -0.476976 1.186253 0.028796
H -0.798192 1.726822 0.931616
H -0.777026 1.726759 -0.882408
H 0.624475 1.026084 0.030919
S 2.815953 -0.140780 -0.097622
H -3.097630 -0.072420 -0.880460
H 2.893861 -0.238618 1.252378
E = -911.3868793 NIMAG = 1

9-IDx

O -2.988603 0.115415 0.045349
S -1.377325 -0.555812 0.020739
C -0.382398 0.944550 0.063719
H -0.586024 1.513806 0.982471
H -0.564474 1.560078 -0.830506
H 0.680060 0.598943 0.054643
S 3.047370 -0.086385 -0.102061
H -3.195652 0.281576 -0.887944
H 3.148579 -0.269880 1.237376
E = -911.3870842 NIMAG = 0

10-TSn

S -1.701829 -0.548581 0.222532
S 0.340139 -0.545191 -0.300583
C 1.057067 0.521789 0.985356
H 2.150451 0.511122 0.708982
H 0.864936 0.086172 1.977595
H 0.633064 1.536156 0.917428
O 3.465360 0.222486 -0.380989
H 4.385899 -0.052998 -0.515687
C -2.219556 1.061299 -0.477892
H -2.030952 1.076301 -1.561176
H -3.298030 1.185498 -0.281985
H -1.666272 1.879687 0.006774
E = -950.5568131 NIMAG = 1

Supplementary Material for Organic & Biomolecular Chemistry
This journal is © The Royal Society of Chemistry 2005

10-INT

C -0.829375 1.346965 -0.497575
S -0.812284 -0.405230 0.045029
S 1.569391 -0.476884 -0.554386
C 2.235525 0.383095 0.921367
H -1.813245 1.743716 -0.208425
H -0.682673 1.418302 -1.586117
H -0.029205 1.909970 0.006788
H 3.327111 0.515298 0.819754
H 2.032310 -0.193681 1.838973
H 1.782721 1.384387 1.034420
O -2.754994 -0.286056 0.496209
H -3.127674 -0.756075 -0.268104
E = -950.56998 NIMAG = 0

10-TSx

O 3.148465 0.293693 0.060213
S 1.486728 0.175314 -0.473875
C 0.770237 -0.776708 0.877037
H 0.878139 -0.235916 1.828870
H 1.226195 -1.776767 0.937577
H -0.307809 -0.874581 0.593108
S -2.461483 -0.526133 -0.341791
C -2.195998 1.134872 0.415431
H -2.305692 1.942398 -0.331145
H -2.919006 1.331784 1.228230
H -1.180230 1.233775 0.847542
H 3.571321 -0.506109 -0.290036
E = -950.5588782 NIMAG = 1

10-IDx

O 3.248669 -0.025912 0.023226
S 1.569753 0.471874 0.015139
C 0.742960 -1.125175 0.101164
H 1.011738 -1.643512 1.033325
H 0.996030 -1.738023 -0.777532
H -0.362855 -0.932459 0.085698
S -2.678415 -0.508236 -0.050866
C -2.029070 1.210287 0.032315
H -2.321160 1.802673 -0.853758
H -2.393604 1.742693 0.929505
H -0.918289 1.238116 0.078494
H 3.454030 -0.191080 -0.910789
E = -950.560011 NIMAG = 0

11-TS MP2/aug-cc-pVDZ

S -0.550885 0.049016 -0.999710
C -0.558529 -0.201830 0.804948
H 0.525071 -0.257189 1.003005
C 2.642386 0.229387 0.134698
C 2.746848 -0.372405 1.408959
C 2.289218 0.074077 2.657804
S -2.647272 0.160684 -1.431723
H -1.021824 0.652294 1.316603
H -1.059775 -1.144612 1.064634
H 3.116493 -0.235369 -0.735098
H 2.298873 1.266177 0.025192
H 3.194505 -1.382073 1.410414
H 2.426789 -0.536595 3.555142
H 1.856373 1.074239 2.785391
H -2.885532 -1.167466 -1.560798
E = -952.621687 NIMAG = 1

11-TS B3LYP/aug-cc-pVDZ

S -0.568553 0.058983 -0.976200
C -0.592825 -0.229036 0.833653
H 0.487197 -0.272754 1.021543
C 2.763846 0.241809 0.166117
C 2.818732 -0.367671 1.427107
C 2.386286 0.095898 2.666243
S -2.742818 0.151283 -1.490474
H -1.060561 0.604888 1.367262
H -1.076843 -1.180866 1.079729
H 3.183865 -0.252436 -0.709248
H 2.447587 1.280032 0.045553
H 3.223973 -1.390653 1.429427
H 2.484922 -0.518251 3.561701
H 1.976684 1.101000 2.793467
H -2.941129 -1.181220 -1.681362
E = -954.256787 NIMAG = 1

11-IDx MP2/aug-cc-pVDZ

C -0.250562 -0.066959 -0.493092
S -0.250562 -0.066959 1.329431
H 0.782210 -0.066959 -0.873082
H -0.774906 0.844157 -0.846508
H -0.789747 -0.955209 -0.860403
C 0.615989 -1.667059 1.607194
C 2.043552 -1.596922 1.154179
C 2.529427 -2.254104 0.076057
H 1.887610 -2.913550 -0.516597
H 3.568358 -2.134449 -0.242506
H 2.697475 -0.916267 1.713430
H 0.551513 -1.853463 2.692634

Supplementary Material for Organic & Biomolecular Chemistry
This journal is © The Royal Society of Chemistry 2005

H 0.072589 -2.469191 1.077446
S -1.905043 2.678130 -2.222608
H -3.135856 2.196475 -1.919612
E = -952.688691 NIMAG = 0

11-IDX B3LYP/aug-cc-pvDZ

C -0.314869 0.013191 -0.465643
S -0.216047 0.090727 1.361183
H 0.688995 -0.012475 -0.906725
H -0.856137 -0.909296 -0.748921
H -0.875740 0.876629 -0.847741
C 0.671626 1.696969 1.600124
C 2.102274 1.638881 1.163843
C 2.628688 2.343814 0.154263
H 2.025849 3.043557 -0.428516
H 3.675152 2.234026 -0.133237
H 2.731751 0.927456 1.706941
H 0.603871 1.890069 2.681185
H 0.128440 2.494194 1.072075
S -1.994316 -2.735688 -2.302921
H -3.282679 -2.381919 -2.042787
E = -954.3068466 NIMAG = 0

12-TS MP2/aug-cc-pVDZ

S -0.630066 -0.720497 -0.085357
C 0.282943 0.836988 -0.349874
H 1.314318 0.562245 -0.069994
H 0.220775 1.143530 -1.402713
H -0.097803 1.625864 0.315028
C 2.822366 -1.243514 0.259377
C 3.455907 -0.008479 0.510366
C 3.702218 1.076656 -0.347505
H 2.751587 -2.000636 1.046042
H 2.554271 -1.549012 -0.760346
H 3.745996 0.157259 1.563330
H 4.198085 1.979291 0.022047
H 3.494197 1.015814 -1.423299
S -2.610441 -0.127926 -0.538074
C -3.067705 0.685940 1.036308
H -2.987823 -0.030841 1.866203
H -2.410911 1.548560 1.223472
H -4.108948 1.037140 0.943094
E = -991.806904 NIMG = 1

12-TS B3LYP/aug-cc-pVDZ

S -0.610543 -0.677633 -0.141729
C 0.259942 0.930244 -0.302405
H 1.293794 0.657658 -0.049349
H 0.192915 1.311088 -1.326803
H -0.128630 1.662081 0.415130
C 3.020977 -1.193702 0.197906
C 3.561053 0.060023 0.506215
C 3.781849 1.176634 -0.300330
H 2.940332 -1.968742 0.959880
H 2.782304 -1.480215 -0.829188
H 3.813087 0.203055 1.568382
H 4.210156 2.090766 0.112094
H 3.595274 1.155507 -1.377301
S -2.686799 -0.164317 -0.547186
C -3.255553 0.405966 1.107544
H -3.113295 -0.385821 1.853208
H -2.711846 1.307203 1.418221
H -4.326230 0.643629 1.024779
E = -993.568704 NIMAG = 1

12-IDx B3LYP/aug-cc-pVDZ

C 0.127862 0.146932 -0.348384
S 0.384971 0.216828 1.462825
H 1.090970 0.117940 -0.872058
H -0.437468 -0.776179 -0.591960
H -0.456982 1.015944 -0.678021
C 1.323148 1.804771 1.628204
C 2.708063 1.719569 1.067568
C 3.152767 2.406729 0.007428
H 2.510727 3.111325 -0.525440
H 4.167163 2.277091 -0.372084
H 3.372326 1.002163 1.558958
H 1.354099 1.993854 2.711596
H 0.751736 2.614623 1.151781
S -1.937994 -2.427133 -1.841123
C -3.380244 -1.455870 -1.208949
H -3.057865 -0.579184 -0.617602
H -4.010341 -1.078874 -2.033158
H -4.025573 -2.066621 -0.554456
E = -993.6075926 NIMAG = 0

Supplementary Material for Organic & Biomolecular Chemistry
This journal is © The Royal Society of Chemistry 2005

H 4.115918 -0.203263 -0.001428
H 3.391095 1.157786 0.892249
H 3.389941 1.160007 -0.890764
E = -874.2949666 NIMAG = 1

13a-ID

S -1.765502 -1.531020 0.000000
C -1.090334 -0.037468 0.000000
S 2.104152 1.460503 0.000000
H 2.864854 0.338609 0.000000
H -1.741244 0.850673 0.000000
H 0.000000 0.163798 0.000000
E = -835.1249197 NIMAG = 0

13a-TS

S 2.265112 0.164837 -0.000013
S 0.736474 -0.431593 0.000040
S -2.358341 0.015205 -0.000014
H -3.305344 0.983866 0.000074
H 0.189084 -0.637570 -0.926335
H 0.189086 -0.637417 0.926451
E = -835.1247761 NIMAG = 0

13a-P

S 1.569426 -0.230669 -0.018088
C 0.082546 0.795992 0.043532
S -1.542657 -0.165141 -0.031394
H -0.962518 -1.316188 0.374945
H 0.028206 1.387623 0.972280
H 0.010738 1.485564 -0.816708
E = -835.1518216 NIMAG = 0

13b-ID

S -2.450036 0.523157 0.000000
C -0.965104 1.218005 0.000000
S 2.209052 -0.138507 0.000000
C 1.241264 -1.711570 0.000000
H -0.886082 2.316815 0.000000
H 0.000000 0.666854 0.000000
H 1.468091 -2.324049 0.891778
H 1.468091 -2.324049 -0.891778
H 0.148688 -1.528570 0.000000
E = -874.2957861 NIMAG = 0

13b-TS

S -2.912968 0.271912 -0.000026
C -1.427261 -0.426929 0.000085
S 1.650703 -0.353418 -0.000029
C 3.275488 0.515393 0.000015
H -0.895041 -0.670476 0.926455
H -0.895030 -0.670742 -0.926221

13b-P

S -1.775047 0.329286 -0.138629
C -0.510164 -0.841514 0.413395
S 1.241012 -0.576810 -0.229477
C 1.407618 1.188154 0.179722
H -0.417813 -0.859407 1.514628
H -0.714846 -1.872359 0.071384
H 2.229580 1.610852 -0.418975
H 1.616675 1.338086 1.252079
H 0.446242 1.663372 -0.088112
E = -874.3360349 NIMAG = 0