

Quantum chemical investigation into the electrophilic bromination of substituted stilbenes and stilbazoles

Supporting Information

Table S1: Cartesian coordinates for the optimised geometries of stilbenes and stilbazoles calculated at the MP2/6-31G(d,p) level of theory.

Stilbene 1

C,0.0191068147,-0.6757871238,0.1264603123
C,-0.0191177354,0.6757899412,0.1264603123
C,-2.1763349241,-3.6857814405,0.6768357463
C,-1.0743183965,-2.8432068989,0.6531629196
C,-1.1553322527,-1.5474259521,0.1085655696
C,-2.3809694746,-1.1463107913,-0.4427604285
C,-3.5013226269,-1.9783253694,-0.4179754131
C,-3.3996264525,-3.2560890133,0.1447330726
C,1.155321332,1.5474287695,0.1085655696
C,1.0743074758,2.8432097163,0.6531629196
C,2.1763240034,3.6857842579,0.6768357463
C,3.3996155318,3.2560918307,0.1447330726
C,3.5013117062,1.9783281868,-0.4179754131
C,2.3809585539,1.1463136087,-0.4427604285
O,4.4231539492,4.1646952989,0.2176112074
C,5.6776119194,3.7536853967,-0.3124721248
O,-4.4231648699,-4.1646924815,0.2176112074
C,-5.6776228401,-3.7536825793,-0.3124721248
H,-0.9849959851,1.1707891966,0.1808354572
H,0.9849850643,-1.1707863792,0.1808354572
H,0.1349442065,3.183737816,1.0740804607
H,2.4593438614,0.1758210097,-0.9178196129
H,4.4248831794,1.6322872573,-0.8589917198
H,2.1198752589,4.680314213,1.0995500374
H,-0.1349551272,-3.1837349986,1.0740804607
H,-2.4593547821,-0.1758181923,-0.9178196129
H,-4.4248941001,-1.6322844399,-0.8589917198
H,-2.1198861796,-4.6803113956,1.0995500374
H,6.3499223526,4.5908449612,-0.1531358874
H,6.0597726423,2.8732098624,0.2076404071
H,5.6077203563,3.5393990161,-1.380684574
H,-6.3499332733,-4.5908421438,-0.1531358874
H,-6.059783563,-2.8732070449,0.2076404071
H,-5.607731277,-3.5393961987,-1.380684574

Stilbene 3

C,-0.5956491099,-0.5172975489,0.0324585983
C,0.5374470806,-1.2540080609,0.0552671075
C,0.5863816914,-2.7165787437,0.0052948544
C,-0.6459926204,0.9444710787,0.0549610021
C,-1.7797981156,1.5976941064,0.5742892349
C,0.4005051689,1.7400810136,-0.4334762017

Stilbene 2

C,-0.3195961385,-1.5097167547,0.5977391331
C,0.5614299761,-1.6171293901,-0.4221287145
C,2.008155759,-1.7719976906,-0.2671864481
C,-1.7685601618,-1.3822303984,0.4439173718
C,-2.525057597,-0.74220462,1.4440060662
C,-2.4531753362,-1.8846823631,-0.6722350107
C,-3.8316754808,-1.7226501478,-0.8182332019
C,-3.8972510433,-0.5809871065,1.3177451685
C,-4.5592708406,-1.0670971345,0.1821025799
C,2.8670478743,-1.3518292949,-1.2962931411
C,2.5854866528,-2.3443968663,0.8796577439
C,3.9682334469,-2.4450248144,1.0055737202
C,4.8249610695,-2.0114300712,-0.0153054282
C,4.2493528035,-1.462897641,-1.1679994756
H,0.0603540621,-1.4760287076,1.6152136188
H,0.1919873782,-1.5447040966,-1.4414294174
H,-2.0225516005,-0.3563975338,2.3238596685
H,-1.9062262427,-2.4295994911,-1.4322253199
H,-4.3209908601,-2.1304016068,-1.6908797317
H,-4.4818022815,-0.0846783658,2.0812327361
H,2.4427805352,-0.9226847407,-2.1973680798
H,1.9459270876,-2.7302662476,1.6643503231
H,4.390310826,-2.8963726817,1.8968875516
H,4.8901048546,-1.1295923059,-1.9769536399
O,-5.9132210252,-0.8568934345,0.1569240858
C,-6.6109183989,-1.3384572192,-0.9854996647
H,-7.65068298,-1.07051179,-0.8264910902
H,-6.2474813614,-0.8676596357,-1.9009444295
H,-6.5230107286,-2.4226819737,-1.0780647101
C,6.3195491387,-2.0975541441,0.1402470028
H,6.6010804624,-2.9530238538,0.7533287896
H,6.8092928311,-2.1993373408,-0.827524791
H,6.7175883189,-1.201764537,0.6201357344

Stilbene 4

C,-0.8594189567,-1.4345644624,0.5676415454
C,0.0174948525,-1.3681680471,-0.4591853892
C,1.4711105245,-1.2914746478,-0.3091268226
C,-2.3110717558,-1.537280923,0.42682635
C,-3.1472760959,-1.0644886537,1.4559985707
C,-2.9183826109,-2.102149808,-0.7040566586

C,0.3493082255,3.1334091902,-0.371885442
C,-1.8493611332,2.9819994009,0.6346973091
C,-0.781835442,3.7593797047,0.1652447032
C,1.67909658,-3.3923019678,0.5744088256
C,-0.4280575792,-3.4786486246,-0.6004995219
C,-0.3681760051,-4.8706212538,-0.5993983096
C,0.7166690507,-5.5296483426,-0.0154539879
C,1.7433759237,-4.7844365057,0.5679252016
H,-1.553077499,-1.0312306666,0.0356240272
H,1.4911077863,-0.7438149928,0.1589476922
H,-2.608912833,1.0063199617,0.946202763
H,1.2623932188,1.267001001,-0.8884809219
H,1.1745410016,3.7092307616,-0.7650823669
H,-2.7163077841,3.4883840796,1.0382977868
H,2.4746637209,-2.816594027,1.0340775188
H,-1.2516422535,-2.9750393283,-1.0917628
H,-1.1572946642,-5.4418493253,-1.0724864965
H,0.7654890591,-6.6111072612,-0.0241802949
H,2.59164719,-5.2866036627,1.016147045
O,-0.9523830506,5.1149352787,0.2698410307
C,0.1166340816,5.9290714143,-0.1975361514
H,-0.1981918842,6.9528253301,-0.0215654711
H,1.0380633933,5.72971177,0.3528850941
H,0.2940193802,5.779521346,-1.2642935463

Stilbene 5

C,0.183204,0.59845,-0.098072
C,-0.749474,-0.37895,-0.038922
C,-2.195067,-0.171363,-0.07732
C,1.627353,0.369065,-0.077437
C,2.483441,1.374709,0.405571
C,2.202412,-0.830216,-0.536774
C,3.575563,-1.042588,-0.474458
C,3.861227,1.19082,0.46539
C,4.382715,-0.023248,0.02613
C,-3.047701,-1.146561,0.458433
C,-2.781995,0.979474,-0.639922
C,-4.156903,1.156065,-0.628909
C,-4.992947,0.176478,-0.07194
C,-4.433979,-0.985411,0.471103
H,-0.138428,1.635369,-0.118035
H,-0.41891,-1.406812,0.086123
H,2.058255,2.310337,0.749448
H,1.568061,-1.596656,-0.963638
H,4.026322,-1.958837,-0.825906
H,4.523995,1.956229,0.840825
H,-2.619546,-2.046272,0.886269
H,-2.156272,1.729078,-1.108681

C,-4.3063768026,-2.1605512808,-0.83418718
C,-4.5286655067,-1.122103838,1.3440681494
C,-5.1177455863,-1.6673389416,0.1948783773
C,2.2407334396,-0.6824340286,-1.3151757129
C,2.1357695374,-1.8082063796,0.8175161798
C,3.5152608947,-1.6893877597,0.9505084904
C,4.2577691512,-1.0637995766,-0.0551886023
C,3.6224678101,-0.5682474752,-1.1962622055
H,-0.4795545064,-1.3691506916,1.5837578738
H,-0.3645861365,-1.3253145877,-1.4749760834
H,-2.7026108933,-0.6354241178,2.3468256981
H,-2.3007131492,-2.5236409278,-1.4879956801
H,-4.7345642329,-2.6099703502,-1.7183534968
H,-5.1761562834,-0.7548212896,2.1293415045
H,1.7444871857,-0.2868403893,-2.193796061
H,1.5683694729,-2.3250863033,1.581231144
H,4.0169597266,-2.0858983691,1.823084419
H,4.2029051921,-0.0876130725,-1.9721096642
O,-6.4867320738,-1.6776520379,0.1863906985
C,-7.1138305569,-2.2246287742,-0.9682942438
H,-8.1806442709,-2.1334839788,-0.7907618952
H,-6.8433909541,-1.6685770282,-1.8678328156
H,-6.8537826728,-3.2764006818,-1.1013562115
C,5.7480784605,-1.011757434,0.0500713788
F,6.1597052376,-0.9169914713,1.3369282252
F,6.3261249678,-2.1248910275,-0.4652487524
F,6.266126592,0.0452893547,-0.61928313

Stilbene 6

C,-0.4208626264,-1.5066320158,-0.3954773716
C,0.5166450565,-1.50973054,0.5792435463
C,1.9582133528,-1.5801193404,0.3444108401
C,-1.8631057923,-1.4171309304,-0.1803988742
C,-2.4232632031,-0.8601535646,0.986431391
C,-3.7968484755,-0.8219653825,1.1695441055
C,-4.6577854823,-1.3218228818,0.1807658596
C,-4.1250551789,-1.8577836107,-0.9966688562
C,-2.7399504621,-1.8952232644,-1.1640899147
C,2.7974958308,-2.1171508212,1.3366418371
C,4.1699594438,-2.2253257713,1.1427459556
C,4.7342177255,-1.7841588127,-0.063821214
C,3.916100283,-1.2294866546,-1.0609742377
C,2.5472842549,-1.1183347074,-0.8470394286
H,-0.0990130645,-1.6175558348,-1.4276711259
H,0.1989534703,-1.5045688857,1.6176236476
H,-1.7766161691,-0.4345650703,1.7439827984
H,-4.2352982982,-0.3895692336,2.059376222
H,-4.7636602146,-2.241839432,-1.7786769675
H,-2.332371525,-2.3174515438,-2.075935229
H,1.9279844937,-0.6507399621,-1.6021056004
H,4.361184302,-0.8700907055,-1.9798777239

H,-4.61615,2.033427,-1.065188
H,-5.053306,-1.760312,0.898678
N,5.834421,-0.233285,0.083077
O,6.534285,0.692345,0.527908
O,6.275788,-1.324502,-0.315637
O,-6.331842,0.453766,-0.123414
C,-7.207816,-0.525226,0.425302
H,-8.208655,-0.127119,0.292589
H,-7.119189,-1.476833,-0.101943
H,-7.013177,-0.680451,1.488024

Stilbene 7

C,0.4622768227,-1.6440779851,-0.4931039275
C,-0.4623095697,-1.644070369,0.4931054777
C,-1.9106088698,-1.6536839259,0.2844394447
C,1.9105760198,-1.6537060531,-0.2844378508
C,2.7592143465,-1.1322094988,-1.2748900868
C,2.500342782,-2.1834462504,0.8764392355
C,3.8806125718,-2.1463401948,1.0533900506
C,4.1399995016,-1.1049938711,-1.0952789963
C,4.7256626981,-1.61161665,0.0714274607
C,-2.759241576,-1.1321729026,1.2748888777
C,-2.5003813392,-2.1834239846,-0.8764348054
C,-3.8806507271,-2.1463039828,-1.0533858306
C,-4.7256950904,-1.6115660525,-0.0714261149
C,-4.140026436,-1.1049433372,1.0952776299
H,0.1261526748,-1.5918808186,-1.5250214186
H,-0.1261848624,-1.5918713262,1.5250226915
H,2.3268084956,-0.7337563926,-2.1861129413
H,1.8749929393,-2.6444752982,1.6314578569
H,4.3134694557,-2.5674180146,1.954278346
H,4.7728100921,-0.6954996272,-1.8749462476
H,-2.3268314324,-0.7337195761,2.1861095988
H,-1.8750364646,-2.6444638301,-1.6314509484
H,-4.3135121481,-2.5673819632,-1.954271871
H,-4.7728326136,-0.695438083,1.87494268
C,6.2145643709,-1.5490979303,0.282682115
H,6.7471346773,-1.5840047006,-0.66700526
H,6.5016611177,-0.6261792029,0.7895831593
H,6.558891157,-2.3823185624,0.8943341568
C,-6.2145960868,-1.549032399,-0.2826811167
H,-6.5589318631,-2.3822526109,-0.8943286697
H,-6.7471667766,-1.5839283013,0.6670064427
H,-6.5016828672,-0.6261133048,-0.789587138

Stilbene 9

C,-1.62976,0.457291,0.010648
C,-0.722989,-0.545078,0.02319
C,0.728197,-0.355108,0.026149
C,-3.081377,0.276004,0.025329
C,-3.910433,1.277844,-0.505482

H,4.8057769449,-2.6458430775,1.9110913072
H,2.3616095777,-2.4642655172,2.2662687108
C,6.1491173316,-1.8898056309,-0.2754268763
N,7.316570016,-1.9780204788,-0.4505877011
O,-5.9926585991,-1.2249722952,0.4656696813
C,-6.8930429185,-1.7150630566,-0.5221514261
H,-7.8864541063,-1.5532162985,-0.1162701753
H,-6.7874934137,-1.1686695443,-1.46116591
H,-6.7406955535,-2.7804661353,-0.7040762697

Stilbene 8

C,0.6043334444,-1.600061396,-0.4263711949
C,-0.3061016883,-1.8340008632,0.5434602601
C,-1.7143270831,-2.1675374145,0.3149174028
C,2.0118462907,-1.2646838396,-0.2020567585
C,2.9536118024,-1.5318572867,-1.2091578104
C,2.4698330354,-0.6710882115,0.9869794659
C,3.8211865898,-0.3911994056,1.1673890403
C,4.304007828,-1.244682508,-1.0245336392
C,4.7632395856,-0.6756302203,0.1692259431
C,-2.6598641394,-1.8791657052,1.3133496418
C,-2.1593982935,-2.7854038187,-0.8669048949
C,-3.5105948109,-3.0661115752,-1.0566859685
C,-4.4424445398,-2.7573748321,-0.0622697539
C,-4.0110766026,-2.165173737,1.1260682416
H,0.2964187843,-1.6832922196,-1.4649601052
H,-0.0002315331,-1.7497473193,1.5824239522
H,2.6213184038,-1.9813214424,-2.1384973521
H,1.7622723688,-0.410453474,1.7647554011
H,4.1509637414,0.0660445454,2.0939422229
H,5.0117419065,-1.4705556445,-1.8145146609
H,-2.3287633744,-1.4151940239,2.2357240009
H,-1.4416461392,-3.063517052,-1.6288337805
H,-3.8352581246,-3.5445157797,-1.972383694
H,-5.4908029201,-2.9837904044,-0.2093280625
H,-4.7245946327,-1.9292907803,1.9057057806
C,6.2151330151,-0.3247886251,0.3546353854
H,6.8543214781,-0.9775829718,-0.238601445
H,6.4148027362,0.7031684306,0.047167191
H,6.5107998711,-0.4200374254,1.3989091908

Stilbene 10

C,0.279511,-0.534729,0.078817
C,1.189408,0.460557,-0.017537
C,2.640206,0.276852,0.004724
C,-1.170116,-0.339538,0.071481
C,-2.00789

C,-3.691048,-0.868336,0.568033
C,-5.074503,-1.017984,0.536048
C,-5.294314,1.124133,-0.528586
C,-5.901248,-0.025562,-0.008217
C,1.558781,-1.353403,-0.511115
C,1.330286,0.802334,0.551218
C,2.710273,0.971538,0.50935
C,3.515024,-0.027346,-0.046313
C,2.941105,-1.197652,-0.548457
H,-1.275046,1.482148,-0.057919
H,-1.07355,-1.572337,-0.013869
H,-3.461222,2.176315,-0.914025
H,-3.079911,-1.63074,1.035964
H,-5.524008,-1.905604,0.967452
H,-5.912761,1.911233,-0.945429
H,1.110493,-2.255251,-0.911619
H,0.713033,1.561914,1.014253
H,3.164149,1.867303,0.911709
H,3.569551,-1.967937,-0.974532
C,-7.393998,-0.208448,-0.065314
H,-7.907768,0.751793,-0.041962
H,-7.692015,-0.721559,-0.981242
H,-7.748433,-0.802532,0.776239
C,5.002518,0.119441,-0.014997
F,5.383451,1.41489,-0.12011
F,5.528079,-0.350986,1.142988
F,5.599404,-0.560875,-1.022202

Stilbene 11

C,-0.199652,0.479393,0.199333
C,0.723635,-0.432264,-0.177523
C,2.173272,-0.240889,-0.123825
C,-1.647952,0.279727,0.138356
C,-2.494981,1.398544,0.051851
C,-2.236068,-0.997494,0.1856
C,-3.61416,-1.156395,0.103282
C,-3.876216,1.257276,-0.023392
C,-4.441271,-0.026485,-0.000727
C,3.013731,-1.365407,-0.080614
C,2.771792,1.030978,-0.137916
C,4.154934,1.164892,-0.064116
C,4.993234,0.042968,-0.002914
C,4.397426,-1.223917,-0.010644
H,0.131685,1.452004,0.550707
H,0.387439,-1.402585,-0.532714
H,-2.059157,2.390644,0.029842
H,-1.609313,-1.872294,0.303818
H,-4.058096,-2.142806,0.142043
H,-4.517911,2.125754,-0.096765
H,2.573678,-2.356521,-0.087289
H,2.154438,1.916719,-0.226232

7,-1.378095,-0.371928
C,-1.76687,0.858615,0.504996
C,-3.145459,1.036701,0.456501
C,-3.390372,-1.228116,-0.417859
C,-3.93451,-0.014877,-0.004714
C,3.468451,1.234968,-0.602726
C,3.249678,-0.825827,0.628084
C,4.632652,-0.980056,0.601476
C,5.458911,-0.032738,-0.018754
C,4.85181,1.076519,-0.620381
H,0.626282,-1.562925,0.121336
H,0.837493,1.478005,-0.166074
H,-1.565066,-2.31275,-0.695543
H,-1.145166,1.651558,0.900934
H,-3.613248,1.951663,0.788482
H,-4.039772,-2.018853,-0.762911
H,3.019152,2.101693,-1.074768
H,2.639618,-1.550207,1.154238
H,5.082387,-1.834192,1.095598
H,5.46986,1.829038,-1.097258
N,-5.391687,0.159336,-0.046965
O,-6.074886,-0.794387,-0.456818
O,-5.853409,1.250339,0.328393
C,6.950974,-0.222708,-0.068431
H,7.308103,-0.752477,0.813911
H,7.243633,-0.804083,-0.944419
H,7.466621,0.735399,-0.119855

Stilbene 12

C,0.4773246324,-1.7942148284,0.478263148
C,-0.4771961814,-1.7942622162,-0.4782565942
C,-1.9191536938,-1.8038215831,-0.2224556175
C,1.9192827084,-1.8036974818,0.2224624738
C,2.794226179,-1.2569154058,1.1762278182
C,2.4665056681,-2.3492491876,-0.9520175327
C,3.8405276643,-2.3115505711,-1.1794099925
C,4.1693815139,-1.2261407318,0.9520831213
C,4.6976263455,-1.7498167865,-0.2296302514
C,-2.7941299987,-1.2571296653,-1.1762425229
C,-2.4663439107,-2.3493599916,0.9520458225
C,-3.8403681889,-2.3117351162,1.1794366976
C,-4.6975006033,-1.7500902628,0.2296348039
C,-4.1692872001,-1.2264289271,-0.9520991382
H,0.1741871751,-1.7416922505,1.5202652168
H,-0.1740618485,-1.7417621367,-1.5202607064
H,2.3862789749,-0.844141559,2.0920826941
H,1.8134165552,-2.8231390073,-1.6746207561
H,4.2457602144,-2.7386596751,-2.0883205139
H,4.8270625764,-0.7958633989,1.6969825447
H,5.7657637665,-1.7298498228,-0.4047363436
H,-2.3862075696,-0.8443673158,-2.0921136154

H,4.595108,2.155765,-0.083884
H,5.023948,-2.108157,0.024793
C,-5.864957,-0.185643,-0.075985
N,-7.03975,-0.317166,-0.138725
C,6.485972,0.198576,0.107584
H,6.826708,1.090989,-0.416124
H,6.795119,0.288742,1.150312
H,7.002173,-0.661244,-0.317527

Stilbene 13

C,-0.2482726865,-1.5973440741,-0.5682072101
C,-1.1299265452,-1.8423566573,0.4263136529
C,-2.5393869225,-2.1869427824,0.230766694
C,1.1642922462,-1.270382591,-0.3670653105
C,1.8428742455,-0.5071920754,-1.3324591928
C,1.8758064268,-1.6949930772,0.7692042039
C,3.208477075,-1.3404604009,0.9510119913
C,3.1787254556,-0.1556222209,-1.1639839886
C,3.8578534707,-0.5653044956,-0.014166041
C,-3.4694068826,-1.8852413733,1.2397696202
C,-2.9989655943,-2.8178493128,-0.9384824306
C,-4.3525825288,-3.1015394765,-1.105520044
C,-5.2697395222,-2.7808510471,-0.1013216029
C,-4.8224241551,-2.1751610537,1.0745874696
H,-0.6010174414,-1.5959062867,-1.595412492
H,-0.7989528389,-1.7401186346,1.4561968171
H,1.3104866498,-0.1799252707,-2.2179682053
H,1.3861584338,-2.3248561567,1.5012524374
H,3.7467399408,-1.6679806249,1.830371505
H,3.6878081382,0.4416147048,-1.9082599411
H,-3.1253287687,-1.4099850593,2.1514942848
H,-2.2894236884,-3.1065789302,-1.7042939308
H,-4.6904218917,-3.5907390896,-2.0105648716
H,-6.3198033334,-3.0101349969,-0.2303504407
H,-5.5255404987,-1.9306082019,1.8608269896
C,5.3120914443,-0.2554062258,0.1428502813
F,5.6547609352,0.8946465664,-0.4843231834
F,5.6620001709,-0.126376422,1.4448128243
F,6.0918036657,-1.2348897336,-0.377620886

Stilbene 15

C,-0.3313766861,-1.6412642648,0.5405702505
C,0.5681920147,-1.8446007276,-0.4477765088
C,1.988675722,-2.1316092585,-0.2423222927
C,-1.74672707,-1.3385239942,0.3285937314
C,-2.6839930694,-1.6770193096,1.3204092207
C,-2.2108928702,-0.707147225,-0.8398160898
C,-3.5653004132,-0.4617055046,-1.032459402
C,-4.0410988679,-1.429364101,1.1472225757
C,-4.487049878,-0.8226155621,-0.0367305714
C,2.6963611852,-2.8449804237,-1.2244413071

H,-1.8132263454,-2.8231820901,1.674667739
H,-4.2455751003,-2.7388328295,2.0883640023
H,-5.7656392368,-1.730180692,0.4047400343
H,-4.8269940964,-0.796220467,-1.6970155315

Stilbene 14

C,0.0132714023,-1.6134463631,0.578858766
C,-0.8771437042,-1.8470975988,-0.4109381693
C,-2.2948539579,-2.1499355647,-0.2090251485
C,1.4326169152,-1.3268879616,0.3700055402
C,2.1374774314,-0.5779241006,1.3287308507
C,2.1302601779,-1.7852478227,-0.7625276859
C,3.4710274519,-1.4718807664,-0.9592817842
C,3.4819271386,-0.2620721356,1.1598212954
C,4.124435798,-0.7140708577,0.0102068887
C,-3.2161718996,-1.8409334371,-1.2239205232
C,-2.7708662972,-2.7469590631,0.9714998085
C,-4.1315972028,-2.9908976803,1.1426774654
C,-5.0398719934,-2.6631050092,0.1326537029
C,-4.576453795,-2.0908460514,-1.0537260286
H,-0.3367322512,-1.5880834553,1.6065508051
H,-0.5458168933,-1.7672601609,-1.4428052102
H,1.6182160329,-0.2297196785,2.2138857322
H,1.6213998443,-2.4087216027,-1.4866800723
H,4.0160908638,-1.8202155259,-1.8240096812
H,4.0285876281,0.3178380398,1.8884549535
H,-2.8594077574,-1.3916970464,-2.1438988974
H,-2.0696738722,-3.0415776697,1.742757091
H,-4.4825585469,-3.4545522636,2.0561014081
H,-6.0957342527,-2.8614006038,0.2654154406
H,-5.2728162944,-1.841289132,-1.8443444683
N,5.5433051157,-0.3894087525,-0.1828115351
O,6.1060127559,0.2826118651,0.6981058822
O,6.0947631622,-0.8052286012,-1.2159184262

Stilbene 16

C,0.893982,-0.482359,0.096035
C,0.000791,0.528569,0.00801
C,-1.452604,0.360815,0.037438
C,2.346971,-0.313129,0.07986
C,3.161444,-1.366163,-0.372518
C,2.966884,0.87335,0.51269
C,4.348153,1.025655,0.456631
C,4.545955,-1.240617,-0.427409
C,5.114394,-0.038747,-0.013696
C,-2.270884,1.317253,-0.587645

C,2.6767908848,-1.7123918032,0.9098058749
C,4.0210037682,-2.0317108641,1.0874537826
C,4.7090338719,-2.7566291797,0.1108925864
C,4.0426260938,-3.1586988487,-1.0484093683
H,-0.0119455412,-1.7488292089,1.5729614496
H,0.2236385668,-1.841138479,-1.4783499059
H,-2.3407041484,-2.151255889,2.2324868102
H,-1.5009483624,-0.3889167791,-1.5928213988
H,-3.9142401205,0.0263318361,-1.9333706711
H,-4.7551159777,-1.6993283974,1.9144855682
H,2.1797030674,-3.1628644262,-2.1230474209
H,2.1622387179,-1.1153034392,1.6527852719
H,4.5381519659,-1.6987516948,1.9786294102
H,4.5707214876,-3.7138448622,-1.8134009388
C,-5.8847172117,-0.5606748965,-0.2263370683
N,-7.0381765242,-0.3454287004,-0.3832104145
H,5.7557553948,-2.9961489965,0.248037826

Stilbene 17

C,0.929628,0.489626,-0.011135
C,0.026244,-0.512713,0.077831
C,-1.42465,-0.328647,0.070657
C,2.380518,0.3082,0.010108
C,3.205111,1.264324,-0.608788
C,2.988383,-0.793993,0.638828
C,4.367906,-0.95941,0.615107
C,4.58712,1.116396,-0.633676
C,5.173718,-0.002674,-0.023105
C,-2.252075,-1.373188,-0.378253
C,-2.029962,0.863581,0.508705
C,-3.409893,1.029434,0.461176
C,-4.189415,-0.026686,-0.006169
C,-3.635474,-1.233638,-0.424842
H,0.574939,1.506327,-0.154069
H,0.380194,-1.538957,0.11285
H,2.751993,2.125915,-1.085103
H,2.376382,-1.513583,1.168011
H,4.829456,-1.8081,1.103105
H,5.213656,1.854183,-1.1178
H,-1.801304,-2.302812,-0.705237
H,-1.415543,1.660211,0.908717
H,-3.885979,1.938725,0.796881
H,-4.278503,-2.027805,-0.773898
C,6.598896,-0.164841,-0.040757
N,7.775069,-0.299403,-0.056188
N,-5.648649,0.135837,-0.048587
O,-6.118204,1.221809,0.331136

C,-2.066666,-0.725184,0.686546
C,-3.449223,-0.875659,0.669791
C,-4.243405,0.079665,0.028728
C,-3.655279,1.178338,-0.602393
H,0.529286,-1.504527,0.13797
H,0.365108,1.54107,-0.140823
H,2.699483,-2.291633,-0.695654
H,2.362534,1.676489,0.914989
H,4.835106,1.930686,0.788228
H,5.178884,-2.041651,-0.779215
H,-1.812414,2.169203,-1.076049
H,-1.458404,-1.441636,1.224262
H,-3.914926,-1.70891,1.178519
H,-4.276355,1.919717,-1.086417
N,6.574802,0.10913,-0.06492
O,7.236967,-0.85596,-0.482162
O,7.057724,1.190637,0.310824
C,-5.725165,-0.114386,-0.040494
F,-6.080483,-0.849676,-1.121974
F,-6.199326,-0.762735,1.049347
F,-6.384805,1.064129,-0.130717

Stilbene 18

C,-0.447557,0.524305,-0.041203
C,0.443895,-0.49155,-0.042589
C,1.897985,-0.324527,-0.037071
C,-1.901411,0.356226,-0.061528
C,-2.721107,1.358595,0.484418
C,-2.514707,-0.776385,-0.625886
C,-3.897492,-0.924803,-0.601501
C,-4.105778,1.222342,0.505654
C,-4.692841,0.07814,-0.039652
C,2.707383,-1.33394,0.511289
C,2.520676,0.820905,-0.564082
C,3.902921,0.967232,-0.514627
C,4.687354,-0.041588,0.052121
C,4.091642,-1.199568,0.55739
H,-0.081914,1.544982,0.024536
H,0.077098,-1.513156,-0.001848
H,-2.263439,2.245755,0.906405
H,-1.904983,-1.532774,-1.103903
H,-4.362212,-1.795024,-1.045072
H,-4.727673,1.999639,0.928424
H,2.241899,-2.226324,0.913251
H,1.919085,1.588088,-1.035199
H,4.37416,1.853107,-0.918776
H,4.704943,-1.977249,0.991867
C,-6.174712,-0.108999,0.040137
F,-6.834151,1.07326,0.034902
F,-6.646652,-0.841243,-0.996387
F,-6.534495,-0.756261,1.175291

O,-6.322616,-0.822281,-0.462908

C,6.177858,0.081473,0.030401
F,6.577304,1.371209,0.132309
F,6.755833,-0.603606,1.044806
F,6.70198,-0.402714,-1.121957

Stilbene 19

C,-1.371188,-0.474438,-0.047089
C,-0.475197,0.537918,-0.049511
C,0.977674,0.364024,-0.06642
C,-2.82366,-0.301628,-0.04396
C,-3.63912,-1.312449,0.494474
C,-3.442011,0.846627,-0.571497
C,-4.822384,1.001199,-0.525542
C,-5.02195,-1.176182,0.539861
C,-5.61861,-0.01223,0.031795
C,1.799994,1.368302,0.472239
C,1.587446,-0.775842,-0.620114
C,2.969599,-0.928772,-0.592487
C,3.767704,0.076022,-0.037785
C,3.184054,1.227007,0.496829
H,-1.008851,-1.497272,0.000403
H,-0.836401,1.560598,0.010544
H,-3.178105,-2.209107,0.892008
H,-2.837011,1.612943,-1.039577
H,-5.291742,1.886092,-0.935589
H,-5.641199,-1.957028,0.96187
H,1.344956,2.260729,0.885868
H,0.975954,-1.534152,-1.092824
H,3.431906,-1.804345,-1.027951
H,3.80819,2.005559,0.913917
C,-7.044673,0.138791,0.071431
N,-8.221408,0.263985,0.10503
C,5.24896,-0.115903,0.045722
F,5.719358,-0.857735,-0.984517
F,5.912358,1.063911,0.032463
F,5.604098,-0.755797,1.186328

Stilbene 21

C,0.5433631058,0.4023712015,0.0088983102
C,-0.5434272021,-0.4024065578,0.0088983102
C,-0.4977840716,-1.8640434152,0.0162295004
C,0.4977199753,1.8640080589,0.0162295004
C,1.5759695466,2.5916135693,-0.5175331737
C,-0.5921700809,2.5764095015,0.5491988794
C,-0.6253133848,3.9652159671,0.5131034186
C,1.5608237871,3.9812683142,-0.5532492374
C,0.4535949989,4.6737544694,-0.0398641083
C,-1.5760336429,-2.5916489256,-0.5175331737
C,0.5921059846,-2.5764448578,0.5491988794
C,0.6252492885,-3.9652513234,0.5131034186
C,-0.4536590952,-4.6737898257,-0.0398641083

Stilbene 20

C,0.4504091642,-1.4533558658,-0.5043215702
C,-0.4503832007,-1.4533529881,0.5043265868
C,-1.9017155533,-1.4602929361,0.3245406197
C,1.901741561,-1.4602845149,-0.324535524
C,2.7253413741,-0.9235791812,-1.3301142736
C,2.5113236199,-1.996913867,0.8245687856
C,3.8916784562,-1.9620777779,0.9892391913
C,4.1090409012,-0.8873719183,-1.1914404156
C,4.6674275556,-1.4060399496,-0.0259961887
C,-2.725318787,-0.9235813902,1.330113252
C,-2.5112941921,-1.9969392703,-0.8245575735
C,-3.8916492504,-1.9621138554,-0.9892283763
C,-4.6674018936,-1.4060693999,0.0260006662
C,-4.1090185448,-0.8873845264,1.1914389813
H,0.0934360594,-1.3992699132,-1.5287254533
H,-0.0934104407,-1.3992530846,1.5287298534
H,2.2711932095,-0.5197061042,-2.2272931394
H,1.9000538691,-2.4636721782,1.5865597071
H,4.3710740695,-2.3729438953,1.8653335203
H,4.7491746173,-0.4716313244,-1.9552623879
H,-2.2711731964,-0.519695193,2.2272875145
H,-1.9000214665,-2.4637023707,-1.586543175
H,-4.3710422451,-2.3729930136,-1.8653180222
H,-4.7491549105,-0.4716393065,1.9552562151
N,6.1270662799,-1.3758221543,0.1348922186
O,6.7975104759,-0.8809383952,-0.7868543259
O,6.6004846818,-1.8457087183,1.1833381645
N,-6.1270408105,-1.3758627409,-0.1348880854
O,-6.6004562176,-1.845764272,-1.1833286756
O,-6.7974881605,-0.8809727489,0.7868528185

Stilbazole 22

C,-0.5638017781,-0.4937464829,0.
C,0.5446817729,-1.2674651073,0.
C,0.5704897607,-2.7296253023,0.
C,-0.610968593,0.9669523762,0.
C,-1.8678018292,1.6028753096,0.
C,0.530071792,1.7846829738,0.
C,0.4319210943,3.1752922079,0.
C,-1.9819368833,2.9852569186,0.
C,-0.8304770262,3.7828148151,0.
C,1.8049029231,-3.3966696081,0.
C,-0.5749248554,-3.5429312183,0.
C,-0.4335734498,-4.9271329462,0.
N,0.75038,-5.5696987792,0.

C,-1.5608878834,-3.9813036705,-0.5532492374
H,1.5308323144,-0.04684077,-0.0453836035
H,-1.5308964107,0.0468054137,-0.0453836035
H,2.4288327065,2.056867882,-0.9190640899
H,-1.4082803761,2.0376770684,1.0140790871
H,-1.4655709665,4.5072611,0.9273455433
H,2.3925866782,4.5329123708,-0.9717093072
H,-2.4288968028,-2.0569032383,-0.9190640899
H,1.4082162798,-2.0377124247,1.0140790871
H,1.4655068702,-4.5072964563,0.9273455433
H,-2.3926507745,-4.5329477271,-0.9717093072
C,0.4276517416,6.1077557392,-0.0694925009
N,0.4056164985,7.291162981,-0.0948617849
C,-0.4277158379,-6.1077910955,-0.0694925009
N,-0.4056805948,-7.2911983373,-0.0948617849

Stilbazole 23

C,-0.2977594579,0.375146321,0.
C,-0.4825133281,-0.9637660031,0.
C,-1.7731204418,-1.6521076396,0.
C,0.9842248208,1.0785988729,0.
C,0.9806663219,2.482992933,0.
C,2.2317319213,0.4260980776,0.
C,3.4143487877,1.1561322912,0.
C,2.1703345212,3.2088381435,0.
C,3.4086823653,2.5596517528,0.
C,-1.8050754198,-3.0547517197,0.
C,-3.0181071018,-1.0016022616,0.
C,-4.1865207097,-1.7571809082,0.
N,-4.2199024887,-3.1038254699,0.
C,-3.0269782068,-3.7237127963,0.
H,-1.1703640191,1.0219580606,0.
H,0.3838295213,-1.6177581847,0.
H,0.0320057772,3.0085433534,0.
H,2.2817376235,-0.6556752093,0.
H,4.3626389277,0.6295625339,0.
H,2.1353070836,4.2923929974,0.
H,-0.8807402791,-3.6201640536,0.
H,-3.0882279673,0.0780938256,0.
H,-5.1514482677,-1.2624178861,0.
H,-3.0556770047,-4.8077446895,0.
C,4.701767147,3.3295512369,0.
H,4.5184350245,4.4028793673,0.
H,5.3008499247,3.0904135274,0.8793790012
H,5.3008499247,3.0904135274,-0.8793790012

C,1.8449071465,-4.7890712672,0.
H,-1.5361218921,-0.9779837818,0.
H,1.5213698227,-0.7935524764,0.
H,-2.7668992799,0.9968531563,0.
H,1.5178102183,1.3406119483,0.
H,1.3366158389,3.7657447626,0.
H,-2.9475723441,3.4733883443,0.
H,2.729032344,-2.8308726992,0.
H,-1.5684597024,-3.1144814703,0.
H,-1.3132643267,-5.5612217797,0.
H,2.7973700018,-5.3075668281,0.
O,-1.0496780201,5.1336745766,0.
C,0.1032784167,5.9686446565,0.
H,-0.274566294,6.9860386966,0.
H,0.7124800688,5.8044904988,0.8906991876
H,0.7124800688,5.8044904988,-0.8906991876

Stilbene 24

C,-0.2921500277,-0.6107770443,0.
C,0.2912270334,0.6103549713,0.
C,-0.3880627375,1.9030692166,0.
C,0.3871408037,-1.9034910371,0.
C,-0.3840232628,-3.0791108421,0.
C,1.7863633913,-2.0573130386,0.
C,2.3774642,-3.3136380587,0.
C,0.1970878705,-4.34197569,0.
C,1.5938765631,-4.4818715411,0.
C,0.3831007392,3.0786886506,0.
C,-1.7872859852,2.0568906605,0.
C,-2.3783866305,3.3132151613,0.
C,-1.5947988567,4.4814493735,0.
C,-0.1980107756,4.34155391,0.
H,-1.3769894635,-0.6699789511,0.
H,1.3760665666,0.6695558427,0.
H,-1.465772747,-2.9985722743,0.
H,2.4287897024,-1.1852628182,0.
H,3.4586659764,-3.3995140851,0.
H,-0.4292664023,-5.2272033757,0.
H,1.4648503107,2.9981509974,0.
H,-2.4297111601,1.1848396394,0.
H,-3.4595883468,3.3990922892,0.
H,0.4283443821,5.2267809446,0.
N,2.184669613,-5.7270146041,0.
H,1.6296462584,-6.5606310333,0.
H,3.1813734255,-5.8244285989,0.
N,-2.185594048,5.7265914153,0.
H,-3.1822971593,5.8240029727,0.
H,-1.6305722331,6.5602099477,0.

Table S2: Cartesian coordinates for the optimised geometries of the cationic intermediates of the electrophilic bromination of substituted stilbenes and stilbazole calculated at the MP2/6-31G(d,p) level of theory.

Stilbene 1

C,-0.5384809018,1.3388380429,0.4884749325
C,0.4502400982,0.8464090429,-0.4826020675
C,1.6939490982,0.2899190429,-0.2186940675
C,2.2720000982,0.2330710429,1.0905439325
C,3.5180420982,-0.3059349571,1.2676239325
C,4.2443220982,-0.8138799571,0.1542649325
C,3.6931240982,-0.7676519571,-1.1510680675
C,2.4403140982,-0.2286869571,-1.3224820675
C,-1.5666819018,0.2420950429,0.4058819325
C,-2.4885139018,0.1669020429,-0.6495700675
C,-3.3851599018,-0.8940209571,-0.7331190675
C,-3.3335179018,-1.9236349571,0.2215379325
C,-2.3962869018,-1.8611819571,1.2712969325
C,-1.5094579018,-0.8026609571,1.3494049325
H,-0.1593289018,1.4588220429,1.4993549325
H,0.1170130982,0.8820340429,-1.5168750675
H,2.0029230982,-0.1874649571,-2.3130470675
H,4.2398330982,-1.1487789571,-2.0001860675
H,3.9870040982,-0.3578029571,2.2406689325
H,1.7361270982,0.6254910429,1.9438179325
H,-0.7979849018,-0.7602729571,2.1666249325
H,-2.3895499018,-2.6607059571,1.9998219325
H,-4.1054409018,-0.9137869571,-1.5373260675
H,-2.5530249018,0.9784660429,-1.3637700675
O,5.4344780982,-1.3064679571,0.4513529325
C,6.2673980982,-1.8445589571,-0.6050240675
H,5.7696350982,-2.6874269571,-1.0791820675
H,6.4984250982,-1.0669979571,-1.3295950675
H,7.1683360982,-2.1719919571,-0.1018880675
O,-4.1439059018,-3.0033699571,0.2414309325
C,-5.1458949018,-3.1008609571,-0.7789620675
H,-5.8326259018,-2.2560699571,-0.7291410675
H,-5.6774169018,-4.0214929571,-0.5676940675
H,-4.6899189018,-3.1547689571,-1.7675800675
Br,-1.1694559018,3.0993280429,-0.0837520675

Stilbene 3

C,-0.7538829218,-0.5232872415,0.802109523
C,0.3093257656,-1.3578310703,1.3953271652
C,0.4460110779,-2.6407086877,0.6297155114
C,-0.6850138243,0.8046073768,0.4287505712
C,-1.8531618079,1.4105893513,-0.1487446697
C,0.492172644,1.6046208511,0.5992822238
C,0.5040340024,2.9246427269,0.2277142076
C,-1.8448756851,2.7242912523,-0.5266245596

Stilbene 2

C,-0.189196,0.423784,0.594483
C,0.780452,0.751833,-0.467629
C,1.98127,-0.132382,-0.301395
C,-1.507698,0.034521,0.455119
C,-2.256172,-0.270972,1.642779
C,-2.16321,-0.064034,-0.815335
C,-3.481258,-0.434746,-0.898866
C,-3.569086,-0.644617,1.564964
C,-4.200483,-0.730744,0.293843
C,2.148899,-1.202124,-1.190487
C,2.870403,0.02597,0.771116
C,3.927519,-0.865195,0.927317
C,4.111186,-1.939916,0.043878
C,3.211619,-2.086509,-1.020846
H,0.217907,0.481608,1.60109
H,0.374638,0.684041,-1.473302
H,-1.764872,-0.19864,2.605389
H,-1.623115,0.164168,-1.724061
H,-3.962983,-0.498722,-1.862791
H,-4.157054,-0.878434,2.441621
H,1.466187,-1.330793,-2.023275
H,2.76801,0.872006,1.440265
H,4.620124,-0.728359,1.749279
H,3.341276,-2.903902,-1.720093
O,-5.466263,-1.095074,0.327395
C,-6.219678,-1.213032,-0.907555
H,-7.209187,-1.518498,-0.59246
H,-6.260758,-0.24965,-1.410004
H,-5.771713,-1.972276,-1.544067
C,5.281712,-2.870627,0.199208
H,5.547105,-2.993911,1.247765
H,5.060142,-3.852229,-0.215743
H,6.156119,-2.477827,-0.321203
Br,1.15916,2.670707,-0.176032

Stilbene 4

C,-1.077492,0.437673,0.589954
C,-0.208467,0.999243,-0.46532
C,1.190213,0.46928,-0.34402
C,-2.333993,-0.115543,0.449138
C,-2.995083,-0.610874,1.626199
C,-3.009781,-0.212962,-0.812396
C,-4.264279,-0.759125,-0.896413
C,-4.242278,-1.163729,1.547015

C,-0.6671739081,3.5002624521,-0.3430678569
C,1.5748161983,-2.8103513218,-0.1823021081
C,-0.5606215569,-3.6163250585,0.6495338824
C,-0.4264386661,-4.7605035888,-0.1334599975
C,0.6993407147,-4.9305364488,-0.9448464187
C,1.7015809624,-3.9586610638,-0.9635180905
H,-1.6935478346,-1.0463174189,0.641237814
H,1.2654211986,-0.850683164,1.4919865474
H,-2.7450440929,0.8100891401,-0.2797872174
H,1.3825780541,1.1743839718,1.037085167
H,1.3960398643,3.516175084,0.3681330219
H,-2.7086171278,3.2065059524,-0.9628724773
H,2.3564032532,-2.0589810743,-0.1916025039
H,-1.4112949575,-3.5044157218,1.3110772783
H,-1.1950458294,-5.5215791133,-0.1068449061
H,0.8012753047,-5.8236666534,-1.54690249
H,2.5797164074,-4.0950240465,-1.580697799
O,-0.7631718702,4.7537200589,-0.735086085
C,0.3719853892,5.6479636987,-0.5940750325
H,0.0206548122,6.5940664488,-0.9853726028
H,0.6383111798,5.7452549097,0.4555595951
H,1.2088096658,5.2796797135,-1.1824984
Br,-0.3426014291,-1.6123182868,3.2501707067

Stilbene 5

C,0.208922,0.918353,0.491297
C,-0.764304,0.349333,-0.465233
C,-2.046454,-0.087973,-0.202468
C,1.565399,0.29919,0.32219
C,2.029563,-0.57244,1.316353
C,2.333256,0.520033,-0.830619
C,3.554946,-0.124892,-0.993222
C,3.251527,-1.224519,1.168941
C,3.985407,-0.991127,0.009954
C,-2.811297,-0.611403,-1.299142
C,-2.649546,-0.044992,1.101227
C,-3.929091,-0.49026,1.278295
C,-4.667184,-1.010851,0.173535
C,-4.092617,-1.067028,-1.125901
H,-0.118626,0.872192,1.526402
H,-0.403555,0.281823,-1.488896
H,1.444053,-0.736734,2.213486
H,1.998423,1.228948,-1.578056
H,4.172011,0.034408,-1.865199
H,3.636721,-1.894322,1.923529
H,-2.356698,-0.642493,-2.282287
H,-2.104434,0.354607,1.945111
H,-4.417581,-0.467329,2.242761

C,-4.895344,-1.245606,0.28541
C,1.643373,-0.439662,-1.308187
C,2.010974,0.810183,0.740303
C,3.274537,0.240732,0.859214
C,3.71777,-0.670037,-0.104957
C,2.908822,-1.010494,-1.19047
H,-0.650722,0.476676,1.589414
H,-0.595228,0.862787,-1.471589
H,-2.489121,-0.539235,2.581248
H,-2.539084,0.160795,-1.711536
H,-4.763497,-0.819332,-1.851672
H,-4.762818,-1.544728,2.41466
H,1.01627,-0.693805,-2.154958
H,1.681751,1.550653,1.459135
H,3.921327,0.512466,1.682192
H,3.270796,-1.701216,-1.939357
O,-6.092243,-1.790038,0.316426
C,-6.863988,-1.926179,-0.90716
H,-7.787305,-2.39518,-0.592425
H,-7.060012,-0.944447,-1.33103
H,-6.332771,-2.563358,-1.60981
C,5.054961,-1.333458,0.066019
F,5.937341,-0.512244,0.671893
F,4.942275,-2.443531,0.829034
F,5.577692,-1.706468,-1.120497
Br,-0.335631,2.945765,-0.109301

Stilbene 6

C,-0.411325,0.306758,-0.473683
C,0.599099,0.817069,0.473376
C,1.898715,0.089668,0.304645
C,-1.709438,-0.067078,-0.200528
C,-2.29674,0.001444,1.107347
C,-3.593997,-0.378716,1.295006
C,-4.368193,-0.854394,0.19694
C,-3.809601,-0.934447,-1.106326
C,-2.509555,-0.545501,-1.290196
C,2.277127,-0.831695,1.287697
C,3.436986,-1.58279,1.135335
C,4.220668,-1.417392,-0.014634
C,3.847815,-0.490764,-1.000384
C,2.688444,0.256212,-0.840067
H,-0.063259,0.223924,-1.499572
H,0.272863,0.806866,1.508726
H,-1.723779,0.367,1.946911
H,-4.070688,-0.335043,2.263526
H,-4.392836,-1.291973,-1.93995
H,-2.066781,-0.596143,-2.276815
H,2.420921,0.999975,-1.579177
H,4.469628,-0.359689,-1.874851
H,3.740234,-2.289076,1.895332

H,-4.64932,-1.457904,-1.964003
N,5.278496,-1.679451,-0.157927
O,5.642728,-2.431605,0.75921
O,5.90456,-1.45951,-1.206381
O,-5.883143,-1.41269,0.469813
C,-6.741424,-1.959872,-0.568117
H,-7.662864,-2.203365,-0.055186
H,-6.917146,-1.208648,-1.334008
H,-6.28839,-2.855305,-0.986184
Br,0.172633,2.84204,0.01041

Stilbene 7

C,-0.542471,0.056631,0.494829
C,0.441919,0.496181,-0.503382
C,1.79278,-0.101959,-0.297664
C,-1.87419,-0.295181,0.284925
C,-2.636603,-0.70061,1.420906
C,-2.489987,-0.274796,-1.001709
C,-3.812498,-0.643311,-1.124788
C,-3.956886,-1.074367,1.271041
C,-4.567935,-1.04882,0.000939
C,2.285328,-0.978097,-1.272513
C,2.532364,0.128224,0.870937
C,3.75446,-0.51181,1.04921
C,4.259799,-1.398679,0.085486
C,3.510181,-1.6136,-1.078299
H,-0.157516,0.00078,1.510495
H,0.106097,0.413024,-1.533115
H,-2.165867,-0.711482,2.396824
H,-1.93465,0.042954,-1.873688
H,-4.28893,-0.621375,-2.09671
H,-4.534961,-1.381036,2.133065
H,1.72125,-1.156896,-2.181067
H,2.182048,0.84244,1.607318
H,4.327668,-0.321042,1.948632
H,3.886552,-2.286885,-1.838949
C,-5.989436,-1.479542,-0.169853
H,-6.54384,-1.401665,0.762327
H,-6.489011,-0.884924,-0.932595
H,-6.01813,-2.522643,-0.49377
C,5.601259,-2.051419,0.272205
H,6.397535,-1.403863,-0.096884
H,5.796191,-2.250767,1.324498
H,5.658138,-2.992808,-0.271023
Br,0.348826,2.445232,-0.062257

Stilbene 9

C,0.528345,0.768335,0.51398
C,1.408215,0.132433,-0.480472
C,-0.908952,0.383531,0.359786
C,-1.502983,-0.374176,1.376628

H,1.674294,-0.955638,2.178734
C,5.414784,-2.19142,-0.180319
N,6.396351,-2.83599,-0.3199
O,-5.599415,-1.193763,0.502261
C,-6.492709,-1.689935,-0.528556
H,-7.420702,-1.887667,-0.010012
H,-6.635923,-0.928275,-1.28939
H,-6.091518,-2.604909,-0.954459
Br,0.707313,2.72373,-0.03262

Stilbene 8

C,-0.3467935938,0.4526977987,0.6617293716
C,-0.5866631892,-0.9003041864,1.1841789645
C,-1.7522191454,-1.5850102992,0.5491611132
C,0.8772961068,1.053214323,0.3767383474
C,0.85526497,2.3850785313,-0.1355126555
C,2.1288650745,0.3936643109,0.5617766403
C,3.2956301268,1.0557132983,0.2456667843
C,2.0365566806,3.0235712678,-0.4547885847
C,3.2739486597,2.3746875233,-0.2670391879
C,-1.5041673093,-2.7274066715,-0.2221266644
C,-3.0522750422,-1.0703250202,0.6527622146
C,-4.0971662245,-1.7023396599,-0.0166025842
C,-3.8505169587,-2.8390860008,-0.7928260858
C,-2.5564507673,-3.3532253648,-0.8905020883
H,-1.2497896545,1.0311623243,0.480035545
H,0.2960912746,-1.5325952357,1.2151236481
H,-0.0972308299,2.883614172,-0.2709872856
H,2.1693770973,-0.6093379409,0.964414245
H,4.2494472641,0.5650185575,0.3924452481
H,2.0193839943,4.03354989,-0.8432791215
H,-0.5000466471,-3.1295664852,-0.2935160973
H,-3.2521500852,-0.2178520517,1.2913938364
H,-5.103571273,-1.315548274,0.0732903088
H,-4.6668188192,-3.3291392597,-1.3065670864
H,-2.3666343348,-4.2400950248,-1.480241089
C,4.5539834711,3.0524181851,-0.6372882906
H,4.4414804472,4.1337896187,-0.6552668513
H,5.3507674412,2.7880480155,0.0556712421
H,4.8630305326,2.7282718428,-1.633933793
Br,-0.9175862482,-0.3436316051,3.0754751981

Stilbene 10

C,0.16297,0.664503,-0.522966
C,1.077817,0.108596,0.48929
C,2.370567,-0.36739,0.297652
C,-1.255872,0.223701,-0.342882

C,-2.817267,-0.816207,1.239287
C,-3.533227,-0.495056,0.08501
C,-2.948952,0.268845,-0.930559
C,-1.636884,0.709253,-0.7935
C,2.678471,-0.39796,-0.278331
C,3.32874,-0.399589,0.992774
C,4.584548,-0.954408,1.109082
C,5.237527,-1.530692,-0.007318
C,4.592596,-1.533744,-1.261538
C,3.339646,-0.974235,-1.405673
H,0.869639,0.669245,1.540547
H,0.992595,0.084106,-1.484579
H,-0.946499,-0.613609,2.275285
H,-3.286961,-1.391238,2.025129
H,-3.52466,0.530504,-1.807786
H,-1.1977,1.341491,-1.555904
H,2.844144,-0.967648,-2.369315
H,5.093206,-1.970772,-2.115718
H,5.088117,-0.950608,2.067441
H,2.854097,0.04716,1.855874
C,6.582666,-2.159966,0.15895
H,6.463496,-3.175303,0.54516
H,7.114337,-2.220605,-0.787574
H,7.187783,-1.605909,0.874356
C,-4.927945,-1.023941,-0.100905
F,-5.537562,-1.237052,1.082982
F,-4.905406,-2.198982,-0.767464
F,-5.685956,-0.165808,-0.814121
Br,0.902327,2.657864,-0.001105

Stilbene 11

C,-0.219773,0.586380,-0.505453
C,0.725847,0.061666,0.491176
C,2.038041,-0.346248,0.285951
C,-1.608963,0.066590,-0.326068
C,-2.125526,-0.790707,-1.303984
C,-2.361521,0.362084,0.817848
C,-3.619838,-0.199713,0.985582
C,-3.385096,-1.356957,-1.142910
C,-4.131352,-1.066108,0.006889
C,2.761983,-0.831065,1.415871
C,2.673242,-0.310777,-0.990584
C,3.974527,-0.742396,-1.109710
C,4.690262,-1.228334,0.009409
C,4.060720,-1.268037,1.269169
H,0.119319,0.498166,-1.532645
H,0.326052,-0.005321,1.499597
H,-1.550628,-1.011735,-2.194550
H,-1.985078,1.063639,1.551107
H,-4.212918,0.031289,1.859262
H,-3.793731,-2.014848,-1.896880

C,-1.820503,-0.60845,-1.318734
C,-1.994273,0.571373,0.798026
C,-3.286512,0.08647,0.969266
C,-3.114015,-1.100823,-1.161239
C,-3.817124,-0.74664,-0.014014
C,3.065654,-0.866979,1.441622
C,3.012862,-0.387314,-0.977751
C,4.293219,-0.885226,-1.082151
C,4.979737,-1.385764,0.050863
C,4.343084,-1.370976,1.309488
H,0.501512,0.536403,-1.547285
H,0.672028,0.081026,1.498241
H,-1.256511,-0.868796,-2.206775
H,-1.57914,1.254912,1.528903
H,-3.882858,0.344977,1.831862
H,-3.576577,-1.738434,-1.900125
H,2.57624,-0.846527,2.408193
H,2.512641,0.002629,-1.853861
H,4.790566,-0.89446,-2.043715
H,4.869265,-1.749876,2.175967
N,-5.186901,-1.264318,0.163216
O,-5.638175,-1.988491,-0.737238
O,-5.783048,-0.939943,1.201738
C,6.352403,-1.955552,-0.101403
H,6.925959,-1.401259,-0.842194
H,6.891811,-1.954757,0.842662
H,6.279547,-2.989492,-0.44802
Br,0.449529,2.589262,-0.09465

Stilbene 12

C,-0.4902521128,0.14558199,-0.5112250711
C,0.545968117,-0.1664295369,0.474631103
C,1.8992662507,-0.4590899764,0.2347345149
C,-1.8658228413,-0.3293449659,-0.2187515881
C,-2.4939434718,-1.1362862868,-1.1759336322
C,-2.5059013547,-0.0399108976,0.9952226606
C,-3.7670647166,-0.5715948291,1.2492517398
C,-3.75605466,-1.6677121136,-0.9105892968
C,-4.3903029381,-1.3897698866,0.3011220658
C,2.696456882,-0.8011085215,1.3618163374
C,2.464166351,-0.476077753,-1.0700103988
C,3.7931761039,-0.8270808335,-1.2258972163
C,4.5677133509,-1.1754177054,-0.1054565373
C,4.022296496,-1.1632936968,1.1848190296
H,-0.1978597297,0.0126203373,-1.5484507074
H,0.1927526693,-0.2184090918,1.5017749013
H,-2.002374335,-1.3481746096,-2.1184040218
H,-2.0482052189,0.6336947369,1.7105907896
H,-4.2691486848,-0.3408081382,2.1793099679
H,-4.2429361416,-2.2898765039,-1.6494908941

H,2.277648,-0.852638,2.383852
H,2.150042,0.069299,-1.856316
H,4.466199,-0.709453,-2.072556
H,4.608883,-1.636015,2.125425
C,-5.429099,-1.647688,0.180198
N,-6.497775,-2.132492,0.326042
C,6.087167,-1.725523,-0.159298
H,6.629261,-1.128275,-0.888682
H,6.629601,-1.718883,0.781700
H,6.064259,-2.752830,-0.528147
Br,-0.029377,2.506173,-0.030228

Stilbene 13

C,4.8607148409,-1.9367872965,-1.2222733248
C,3.6332220708,-1.3118705053,-1.3635506159
C,3.0061987873,-0.7158715385,-0.2308918023
C,3.6455550415,-0.7528834231,1.0415429913
C,4.8770082227,-1.3699686972,1.1595524953
C,5.4790433972,-1.9644496106,0.0355406507
C,1.7423614173,-0.147830468,-0.4278369282
C,0.8779808609,0.4891032331,0.572727587
Br,1.4773256255,2.3254713614,0.0257112724
C,-0.5844150507,0.2623048074,0.393360765
C,-1.2785718154,-0.3890648992,1.4203903994
C,-2.6304090378,-0.6894212055,1.2647862993
C,-3.2831614549,-0.328910216,0.0851642975
C,-2.5982834452,0.3335545085,-0.9390905919
C,-1.2488895842,0.6316363736,-0.7851131427
C,-4.7246305886,-0.7058116336,-0.1181037929
F,-4.8185915093,-1.8910289828,-0.7587891385
F,-5.3748364264,-0.8219348559,1.0572017591
F,-5.3687997157,0.214117516,-0.8651804824
H,1.2011462048,0.3637665843,1.6019542729
H,1.3207801643,-0.1869989247,-1.429819909
H,-0.7696976193,-0.6596729114,2.3381220455
H,-0.7298316988,1.1890095481,-1.5559138627
H,-3.1246586755,0.6295504873,-1.8361543491
H,-3.1761303255,-1.1840719176,2.0561341096
H,3.1375225176,-1.2727247128,-2.3261380777
H,3.1899417799,-0.2840171094,1.9031487472
H,5.379165524,-1.4020337592,2.1166181265
H,6.4414498624,-2.4487175357,0.144716726
H,5.34179663,-2.3974002167,-2.0738535265

Stilbene 15

C,-0.4444533489,-0.3454565551,1.0876910221
C,0.6034960647,-1.2133740813,0.5419429312
C,0.4979022589,-2.5609552854,0.1858437779
C,-0.4016784421,1.072016401,0.6345457897
C,-1.4971805278,1.566100426,-0.082294989
C,0.7195901279,1.8826557691,0.854794029

H,-5.3723352958,-1.7964809104,0.5025183186
H,2.2551344689,-0.7795560141,2.3510707886
H,1.8748876899,-0.1937728373,-1.9320361558
H,4.2388010856,-0.8393879982,-2.2110504167
H,5.6051496963,-1.4530171368,-0.243263272
H,4.6335530029,-1.4315256143,2.0352891127
Br,-0.2053136633,2.1088117935,-0.1055451213

Stilbene 14

C,0.52185,0.436509,-0.553032
C,1.412792,-0.150984,0.456599
C,2.690432,-0.685129,0.263374
C,-0.931184,0.159512,-0.355336
C,-1.60474,-0.56566,-1.347417
C,-1.605213,0.553739,0.810262
C,-2.941764,0.21569,0.991968
C,-2.943695,-0.910898,-1.178493
C,-3.581658,-0.516596,-0.006664
C,3.346815,-1.227852,1.407213
C,3.320128,-0.737659,-1.014138
C,4.57016,-1.316959,-1.125931
C,5.200851,-1.858637,0.009326
C,4.592934,-1.815518,1.272106
H,0.839837,0.288793,-1.580985
H,1.003059,-0.171584,1.46413
H,-1.089436,-0.859696,-2.254255
H,-1.103453,1.161083,1.554179
H,-3.49034,0.512764,1.87365
H,-3.489421,-1.465361,-1.92767
H,2.85823,-1.177316,2.372914
H,2.84191,-0.309279,-1.884509
H,5.06537,-1.360083,-2.086174
H,6.177914,-2.313847,-0.095117
H,5.096655,-2.235377,2.131625
N,-4.999709,-0.877506,0.181947
O,-5.546831,-1.512482,-0.732377
O,-5.535744,-0.521581,1.242573
Br,1.047486,2.310503,-0.0772

Stilbene 16

C,-0.847696,0.570537,-0.585815
C,0.145621,0.380677,0.469553
C,1.530114,0.121297,0.305307
C,-2.239801,0.124257,-0.364858
C,-2.84011,-0.650535,-1.368069
C,-2.937697,0.414049,0.818961

C,0.7502576725,3.1753926631,0.3506221064
C,-1.4724114668,2.8599002694,-0.5910169336
C,-0.3448329359,3.6642215841,-0.3792530484
C,1.6556221063,-3.1778686275,-0.3670221474
C,-0.7111285837,-3.2997502404,0.3160145182
C,-0.7436889963,-4.6165524634,-0.0984940659
C,0.4032236879,-5.2093670855,-0.653709964
C,1.5993988367,-4.4939275216,-0.7886687229
H,-1.4443502996,-0.7659924198,1.0642849094
H,1.5603532078,-0.7223608092,0.3854959405
H,-2.3699908832,0.9457239082,-0.2423487707
H,1.5451737413,1.5232616229,1.4557919548
H,1.6058844139,3.8127590989,0.5238871922
H,-2.3156282207,3.2504777279,-1.1429457798
H,2.5701033577,-2.6055742909,-0.4558692942
H,-1.5891968697,-2.8493448497,0.7562577172
H,-1.6516010703,-5.193878802,-0.0013798445
H,2.4703993956,-4.9690942093,-1.2155711859
C,-0.3125968176,4.9982678561,-0.9003592903
N,-0.2833716025,6.0978258029,-1.3345809767
H,0.3609522576,-6.240457421,-0.9786671824
Br,0.2269993929,-0.6060071053,2.9543953073

Stilbene 17

C,-0.873114,0.198255,0.460871
C,0.11165,0.407716,-0.595803
C,1.528902,0.08171,-0.37062
C,-2.240241,-0.15899,0.290573
C,-2.947704,-0.557373,1.448038
C,-2.877169,-0.184027,-0.972014
C,-4.187582,-0.61086,-1.069026
C,-4.255757,-1.000185,1.347396
C,-4.877905,-1.027572,0.087904
C,2.199951,-0.618681,-1.382264
C,2.191134,0.408173,0.823025
C,3.506388,0.011679,1.017387
C,4.140522,-0.703744,0.003379
C,3.516872,-1.026118,-1.195822
H,-0.464263,0.134378,1.464875
H,-0.238724,0.246601,-1.60953
H,-2.458907,-0.526857,2.413475
H,-2.365443,0.157243,-1.861445
H,-4.691506,-0.631675,-2.024999
H,-4.80249,-1.318394,2.223646
H,1.694904,-0.855175,-2.310136
H,1.701481,1.005841,1.581585
H,4.046955,0.252537,1.919759

C,-4.218316,-0.089304,1.012103
C,-4.121656,-1.164101,-1.184066
C,-4.781514,-0.87405,0.005836
C,2.264975,-0.199035,1.474003
C,2.168267,0.112696,-0.960934
C,3.508461,-0.220442,-1.043746
C,4.218481,-0.556296,0.12179
C,3.604343,-0.548435,1.378454
H,-0.489044,0.434145,-1.60138
H,-0.26105,0.308039,1.475154
H,-2.308316,-0.860571,-2.288508
H,-2.505414,1.064449,1.570379
H,-4.78508,0.121067,1.907169
H,-4.608954,-1.766308,-1.936735
H,1.772548,-0.179686,2.438973
H,1.631444,0.392069,-1.857984
H,4.016237,-0.220726,-1.998683
H,4.174823,-0.800668,2.261128
N,-6.141875,-1.409776,0.208795
O,-6.621435,-2.090581,-0.710154
O,-6.69794,-1.139005,1.284031
C,5.661289,-0.982835,-0.01227
F,6.291397,-0.230211,-0.933427
F,6.31606,-0.866388,1.155934
F,5.721165,-2.268219,-0.407756
Br,-0.535292,2.539023,-0.135781

Stilbene 18

C,0.5983553681,-0.4926952528,0.8348231587
C,-0.4761585049,0.4921550906,0.90468535
C,-0.3211301826,1.8929569489,0.5609128656
C,0.3999853906,-1.8937172582,0.5150655821
C,1.4767423771,-2.5700110992,-0.0867278593
C,-0.818257344,-2.562488008,0.7468662118
C,-0.9607208221,-3.8824064407,0.3459224009
C,1.3234839893,-3.8896124031,-0.5012880545
C,0.1075493724,-4.5392066525,-0.2817011995
C,-1.4670508901,2.5688987741,0.1038543672
C,0.9168856437,2.5618283438,0.6318273262
C,1.0059251273,3.8814749841,0.2148845884
C,-0.1349401452,4.5379057885,-0.2688757384
C,-1.3690795315,3.8882188336,-0.3279930386
H,1.5905386256,-0.0928596332,0.6471287611
H,-1.4843102258,0.092238814,0.8479193578
H,2.4187403298,-2.05857574,-0.245416115
H,-1.6311840937,-2.0748899423,1.2713001438
H,-1.8847340963,-4.4134706603,0.5295185137
H,2.1416494704,-4.4159087271,-0.9723641362
H,-2.4216653611,2.0573992287,0.0693919342
H,1.7911464494,2.0745423985,1.0463791349
H,1.9459469728,4.4126206865,0.2763698757

H,4.058185,-1.571086,-1.953783
C,-6.231164,-1.47494,-0.024929
N,-7.351509,-1.845472,-0.119809
N,5.538069,-1.126119,0.208903
O,6.061476,-0.82535,1.291362
O,6.077824,-1.750054,-0.715601
Br,-0.37512,2.34402,-0.122336

Stilbene 19

C,-1.226812,0.30904,-0.520317
C,-0.23311,0.388513,0.544006
C,1.182287,0.154244,0.355711
C,-2.598713,-0.115877,-0.31445
C,-3.244158,-0.743586,-1.393481
C,-3.265281,0.039956,0.914931
C,-4.548923,-0.455199,1.068937
C,-4.526168,-1.253139,-1.237379
C,-5.179797,-1.110131,-0.005104
C,1.906614,-0.304291,1.469317
C,1.823012,0.324921,-0.886173
C,3.164926,0.00646,-1.01109
C,3.871357,-0.480063,0.09671
C,3.249421,-0.637635,1.334372
H,-0.831549,0.183408,-1.522965
H,-0.613674,0.259041,1.551963
H,-2.73641,-0.847488,-2.343933
H,-2.805447,0.580216,1.732466
H,-5.075672,-0.336719,2.005258
H,-5.026052,-1.749061,-2.057225
H,1.415338,-0.415426,2.427576
H,1.294132,0.742729,-1.733035
H,3.674573,0.145553,-1.95372
H,3.813207,-0.999496,2.181243
C,-6.50517,-1.624105,0.162108
N,-7.600227,-2.049472,0.302262
C,5.311442,-0.878824,-0.085074
F,5.950253,-0.003276,-0.883672
F,5.960436,-0.931271,1.090981
F,5.385976,-2.093745,-0.660663
Br,-0.876069,2.351899,-0.036612

Stilbene 21

C,0.5695460879,0.4553183574,0.7418319868
C,-0.5696102257,-0.4553537174,0.7418319868
C,-0.4833037411,-1.8631044043,0.41193467
C,0.4832396033,1.8630690443,0.41193467
C,1.6331855895,2.4664197029,-0.1270032572
C,-0.6991097739,2.6102807883,0.5711819301

H,-2.2415953397,4.4142385762,-0.6889842394
C,-0.0931801113,-5.9506492533,-0.7699782862
F,1.081184584,-6.5937340945,-0.9098022144
F,-0.8598145561,-6.6501408447,0.0900499039
F,-0.7131747052,-5.9455337296,-1.9669454949
C,0.000505487,5.9490161896,-0.7800497529
F,0.8724720437,6.6490436242,-0.0275198288
F,0.4595251036,5.9430816754,-2.0474943279
F,-1.1820972121,6.5920592553,-0.7663443268
Br,0.19266828,0.0003986951,2.8839703715

Stilbene 20

C,0.097976137,0.7234757134,0.7974354269
C,-0.0980047358,-0.7235150936,0.7974335581
C,-1.3504265811,-1.3768929711,0.4649444376
C,1.3503978556,1.3768544669,0.4649475506
C,1.2722186267,2.6780440009,-0.0681748894
C,2.602587512,0.7474870948,0.618165884
C,3.7580876351,1.3983589952,0.2122840762
C,2.4246146735,3.3326830016,-0.4899259554
C,3.6436283064,2.6769069416,-0.3396853746
C,-1.2722475553,-2.6780811006,-0.0681814603
C,-2.6026161791,-0.7475260027,0.6181649062
C,-3.7581164569,-1.3983968338,0.2122818238
C,-3.6436573384,-2.676943326,-0.339691039
C,-2.4246437628,-3.3327189901,-0.4899338119
H,-0.8017281056,1.3191900729,0.6736726331
H,0.8016994596,-1.319229127,0.6736688521
H,0.3103718616,3.1666334752,-0.1694281485
H,2.683695362,-0.22629527,1.0859873656
H,4.734556756,0.9490407147,0.3193956814
H,2.3964564594,4.3257267528,-0.914093293
H,-0.3104008288,-3.1666703081,-0.169436373
H,-2.6837238509,0.2262551296,1.0859889842
H,-4.7345855369,-0.9490788355,0.3193949848
H,-2.3964857103,-4.3257616238,-0.9141037765
N,4.8749896387,3.3663446198,-0.7752820656
O,4.7419782666,4.5045652941,-1.2491961244
O,5.9419931757,2.7500216144,-0.6323669568
N,-4.8750188367,-3.3663798566,-0.7752890773
O,-5.9420223193,-2.7500572277,-0.6323719382
O,-4.7420076452,-4.5045992823,-1.2492061855
Br,-0.0000139157,-0.0000223439,2.811985329

Stilbazole 22

C,0.121631,0.074962,0.612012
C,1.127206,0.324894,-0.44283
C,2.336749,-0.544514,-0.253969
C,-1.238193,-0.101578,0.460615
C,-2.028915,-0.338681,1.638506
C,-1.897009,-0.054983,-0.813199

C,-0.7359517654,3.9334058349,0.1663222459
C,1.5942519541,3.7889360224,-0.5467924395
C,0.4088258637,4.5239938387,-0.4011285102
C,-1.6332497273,-2.4664550629,-0.1270032572
C,0.6990456361,-2.6103161483,0.5711819301
C,0.7358876276,-3.9334411949,0.1663222459
C,-0.4088900015,-4.5240291987,-0.4011285102
C,-1.5943160919,-3.7889713824,-0.5467924395
H,1.5419420924,-0.0090600295,0.6143765657
H,-1.5420062302,0.0090246695,0.6143765657
H,2.5467359306,1.8952791179,-0.2328950162
H,-1.5709269699,2.1784353183,1.0455462521
H,-1.634582723,4.5214024483,0.2885215026
H,2.4688881989,4.2578054777,-0.9747526891
H,-2.5468000684,-1.8953144779,-0.2328950163
H,1.5708628321,-2.1784706783,1.0455462521
H,1.6345185852,-4.5214378083,0.2885215026
H,-2.4689523366,-4.2578408377,-0.9747526891
C,0.3621547847,5.8909763101,-0.8223913714
N,0.3216330422,7.0208339099,-1.1712220811
C,-0.3622189224,-5.8910116701,-0.8223913714
N,-0.3216971799,-7.0208692699,-1.1712220811
Br,-0.0000320689,-0.00001768,2.7523254214

Stilbazole 23

C,-0.225551,-0.055985,0.514531
C,0.815288,0.254111,-0.480741
C,2.097837,-0.479919,-0.237583
C,-1.586216,-0.238781,0.293029
C,-2.404001,-0.540546,1.425053
C,-2.183653,-0.152233,-1.001269
C,-3.539029,-0.35918,-1.135318
C,-3.757153,-0.755153,1.263389
C,-4.348304,-0.664861,-0.014072
C,2.488853,-1.470645,-1.14192
C,2.883265,-0.25826,0.898197
C,4.021146,-1.043356,1.077524
N,4.408724,-2.005214,0.220436
C,3.647822,-2.2001,-0.868624
H,0.139237,-0.143934,1.535678
H,0.487142,0.170138,-1.513015
H,-1.947337,-0.601316,2.405837
H,-1.586828,0.094002,-1.86903
H,-4.000985,-0.285555,-2.111638
H,-4.37639,-0.98482,2.120707
H,1.917888,-1.671414,-2.040322
H,2.645497,0.52842,1.603209
H,4.657097,-0.894143,1.94162
H,3.982843,-2.970767,-1.552259
C,-5.808468,-0.923271,-0.197411

C,-3.253566,-0.225513,-0.908373
C,-3.380366,-0.518477,1.548416
C,-4.012754,-0.464228,0.27454
C,2.546646,-1.613837,-1.128583
C,3.224089,-0.367949,0.812378
C,4.277399,-1.270222,0.953341
N,4.491366,-2.306758,0.12276
C,3.634017,-2.45895,-0.899675
H,0.529404,0.033809,1.619371
H,0.736023,0.239859,-1.453132
H,-1.536341,-0.373704,2.602552
H,-1.327614,0.133876,-1.713121
H,-3.736648,-0.180579,-1.872728
H,-3.99946,-0.699902,2.416018
H,1.891953,-1.786268,-1.974368
H,3.126295,0.469931,1.490949
H,4.987633,-1.158055,1.763598
H,3.829143,-3.291676,-1.564712
O,-5.314772,-0.645481,0.295464
C,-6.077792,-0.608412,-0.940976
H,-7.100087,-0.783662,-0.631639
H,-5.981747,0.370296,-1.404353
H,-5.739847,-1.398475,-1.60687
Br,1.517859,2.249732,-0.181937

Stilbene 24

C,-0.1040413823,-0.5628104719,1.8111952482
C,0.4480774988,0.6514616838,1.1804297724
C,-0.2420356325,1.6742894059,0.5636744957
C,0.4165713245,-1.7156538427,1.0089156453
C,-0.4438860804,-2.3544045286,0.1031298538
C,1.7645650484,-2.1060995212,1.0610224431
C,2.2321264552,-3.1241515899,0.243858626
C,0.0226800661,-3.371794553,-0.7175043929
C,1.3694214553,-3.7785631978,-0.6577777415
C,0.5118592488,2.7310940341,-0.0527333364
C,-1.6755681197,1.7494555884,0.5195404224
C,-2.3011711394,2.8024077774,-0.0841645476
C,-1.5330845357,3.8478499096,-0.6878997138
C,-0.1068845381,3.7867870165,-0.6582725187
H,-1.1893975903,-0.5767599055,1.8653531372
H,1.5340731125,0.6981339506,1.1779547358
H,-1.4884983114,-2.0672088341,0.0515573558
H,2.4308309822,-1.6489061878,1.7828017375
H,3.2690862935,-3.4318679708,0.3069811743
H,-0.6549735195,-3.8677897747,-1.402083287
H,1.5937227393,2.6814527971,-0.0270771813
H,-2.274183076,0.9725145712,0.9747488566
H,-3.3820607208,2.8600027564,-0.110219976
H,0.4693890575,4.5802456416,-1.1167553596
N,1.8526381117,-4.7427450115,-1.5181240412

H,-6.358797,-0.77775,0.728969
H,-6.226247,-0.277095,-0.967397
H,-5.956377,-1.957084,-0.519482
Br,0.947176,2.203911,-0.104989

H,1.1745612956,-5.37985541,-1.9057153514
H,2.7074377699,-5.200990682,-1.2436958109
N,-2.1495738975,4.8732329159,-1.2729216463
H,-3.1558022513,4.9361650337,-1.3002681461
H,-1.6294740346,5.6237623674,-1.7013884233
Br,0.5192899393,-0.5458021171,3.6848232122

Table S3: Cartesian coordinates for the optimised geometries of the cationic intermediates of the electrophilic bromination of substituted stilbenes and stilbazoles calculated at the M06-2X/6-31G(d,p) level of theory.

Stilbene 1

C,1.3990148403,-0.5344617215,1.5918862449
C,0.2819184326,0.4284151222,1.4934237892
C,0.2549889494,1.6296519625,0.8157117265
C,0.9289564518,-1.7646458199,0.8560794399
C,1.288721078,-1.9068609529,-0.4935808852
C,0.0816920413,-2.7092826923,1.4380552659
C,-0.385277294,-3.7925197205,0.7054888051
C,0.8300846053,-2.9770224993,-1.2326956366
C,-0.0126262526,-3.9318671875,-0.6381943009
C,-0.9706829468,2.3723066052,0.8004470336
C,1.3942621918,2.1877204154,0.1401337304
C,1.3050990478,3.3890341419,-0.4906770267
C,0.0725020112,4.1058749677,-0.4846449844
C,-1.0721091333,3.5816887751,0.1711969181
H,2.3366930944,-0.162688154,1.1840439377
H,-0.6318474851,0.0977724876,1.9868666067
H,1.9448299159,-1.1772259057,-0.9617976801
H,-0.1829765167,-2.619899595,2.487459537
H,-1.0213532912,-4.5247581945,1.1862245597
H,1.1107232345,-3.1150708743,-2.2704354794
H,-1.8359983011,1.9560306734,1.3080819686
H,2.3378875364,1.6538171735,0.1347939576
H,2.1462871369,3.8389746943,-1.0047167325
H,-2.006943454,4.1267777173,0.1754835878
O,-0.4008859609,-4.9375362094,-1.434076281
C,-1.233441666,-5.9497568581,-0.8882596006
H,-1.4127145115,-6.6556021486,-1.6965131669
H,-0.7345699812,-6.4607352076,-0.0584403061
H,-2.1865329013,-5.5318898967,-0.5477591434
O,0.0944794959,5.2511380684,-1.1159725114
C,-1.0805219553,6.0731302135,-1.1778846246
H,-0.7862121769,6.9505493884,-1.747387561
H,-1.8839337564,5.5422103613,-1.6935063169
H,-1.3887814086,6.3642467814,-0.1712121832
Br,1.7073048727,-0.7991642551,3.5017548845

Stilbene 3

C,-0.6595299348,-0.4951248954,0.557585698

Stilbene 2

C,-0.7476203566,-0.0266272813,0.7801560065
C,0.3253384238,-0.8280747034,1.4109064848
C,0.4095219694,-2.2153232062,0.8433253922
C,-0.7014640228,1.2931997078,0.3898610974
C,-1.8636293417,1.8727532544,-0.2279398255
C,0.448358643,2.1274823252,0.5876430586
C,0.4477962231,3.435665039,0.1986772618
C,-1.8730608006,3.1727314712,-0.6278161101
C,-0.7164357013,3.9753694946,-0.4202127557
C,1.5141336795,-2.5510649405,0.0615209764
C,-0.6196969843,-3.1457183222,1.0184603749
C,-0.5370251261,-4.389866521,0.413354663
C,0.5666597553,-4.7401975904,-0.3760226264
C,1.5873301733,-3.8023692605,-0.5413834747
H,-1.6755388799,-0.5749482185,0.6162948748
H,1.2970590431,-0.3385472865,1.4084035731
H,-2.7410742553,1.2504071378,-0.3760395592
H,1.331652835,1.723419647,1.0702129413
H,1.3200590897,4.0550682073,0.3623476324
H,-2.7331516894,3.6329979778,-1.0993171053
H,2.3217046072,-1.837459373,-0.0788071728
H,-1.4652777182,-2.9061093184,1.6582205717
H,-1.3352115907,-5.1112850845,0.5616297158
H,2.4535399913,-4.0556906869,-1.1449229884
O,-0.8136588768,5.2118988439,-0.8303340145
C,0.2819279365,6.1275031377,-0.6757515982
H,-0.0694099174,7.0658992978,-1.0961055441
H,0.5182921681,6.2550279309,0.3829160364
H,1.1518624686,5.7693248938,-1.2305712519
C,0.6572862794,-6.1072804502,-0.9976048771
H,-0.3136794205,-6.4322355491,-1.3783089277
H,1.3746551997,-6.1239924035,-1.8198529576
H,0.9820794145,-6.8425524609,-0.2547726585
Br,-0.2892754722,-0.7860384085,3.2912180287

Stilbene 4

C,-1.0638800399,0.1857928824,0.5816555386

C,0.4303716556,-1.3189638702,1.1308671188
C,0.5028897764,-2.6929051495,0.5261587209
C,-0.6390864644,0.8521765026,0.2773106792
C,-1.8045270168,1.4558887404,-0.3111866714
C,0.4878408142,1.6919750424,0.5664200022
C,0.4642687585,3.0269964536,0.2861039729
C,-1.8352982724,2.7830651886,-0.6062252464
C,-0.7004389746,3.5902826649,-0.3119534915
C,1.6006057596,-3.0096328036,-0.2741294927
C,-0.5291739019,-3.6197392947,0.6979167147
C,-0.461106065,-4.8534971054,0.0647672128
C,0.6345394157,-5.1679518233,-0.7395173945
C,1.6650058504,-4.2482774136,-0.9063772455
H,-1.5753485787,-1.047532745,0.34573143
H,1.401335539,-0.8278722256,1.1161403024
H,-2.66532956,0.8294491058,-0.5251189453
H,1.3680323247,1.2689420071,1.0386204625
H,1.3175211354,3.6502423203,0.5202052599
H,-2.6969012592,3.2622311621,-1.0556206992
H,2.4073941467,-2.2931960672,-0.4024863684
H,-1.3624286892,-3.3882484465,1.3563552214
H,-1.2565815402,-5.5765771494,0.2073854054
H,0.6870994526,-6.134924406,-1.2278349734
H,2.5225393087,-4.4944747795,-1.5227076607
O,-0.8179760996,4.8530324075,-0.6228111247
C,0.2526450515,5.7775230823,-0.3722792205
H,-0.1120240807,6.7380876891,-0.7258219667
H,0.4633642011,5.8261104263,0.6982681111
H,1.1419657556,5.4830411635,-0.9336788679
Br,-0.1336835253,-1.3344627536,3.0272930566

Stilbene 5

C,-0.4131466117,-0.0643729415,1.2127964584
C,0.710181995,0.7348191592,0.6614426771
C,0.7060099176,2.069023032,0.336284834
C,-0.4381534811,-1.4767449022,0.6899126256
C,-1.4658921323,-1.8431331121,-0.1799871843
C,0.572181485,-2.3881152784,1.0124199372
C,0.5629577987,-3.6601750352,0.4591126646
C,-1.4883950567,-3.1163004911,-0.7392845771
C,-0.4686671077,-3.9934437838,-0.4086804402
C,1.901362972,2.6528824061,-0.2165298479
C,-0.4331423396,2.9206710661,0.5433531347
C,-0.3936966056,4.2435119765,0.2179484923
C,0.8006148055,4.7853376693,-0.3453258045
C,1.9482805516,3.9675403803,-0.5565170467
H,-1.3830648881,0.4140755643,1.0914364659
H,1.6353340657,0.1758395787,0.5181399513

C,-0.1958477285,0.7984223659,-0.4535214111
C,1.2415470014,0.367905391,-0.3374065889
C,-2.3585481256,-0.2534430736,0.4392713593
C,-3.0179458804,-0.8477748069,1.5727148847
C,-3.095940785,-0.128631818,-0.7868741425
C,-4.3832416563,-0.5674029719,-0.88432863
C,-4.2968202879,-1.2995824585,1.4841293453
C,-5.0008213905,-1.1669345606,0.253135968
C,1.7685835057,-0.4596026016,-1.3281868822
C,2.0235717852,0.7306623598,0.7630006503
C,3.3222276983,0.2565615556,0.8737808589
C,3.8388485107,-0.5783116953,-0.1160681748
C,3.0717950629,-0.934362719,-1.2186872364
H,-0.5968134245,0.0916742571,1.5623863142
H,-0.5665110671,0.6606194494,-1.4673506622
H,-2.47110739,-0.9377764639,2.5065783744
H,-2.6349109712,0.3443963812,-1.6473958442
H,-4.9305864907,-0.4569777636,-1.8114876475
H,-4.8146090959,-1.7571711363,2.3186961588
H,1.1678607308,-0.7318832088,-2.1911272606
H,1.6288867874,1.4142410053,1.5095802883
H,3.944213743,0.5450366321,1.7140143636
H,3.4945231601,-1.5679930074,-1.990176669
O,-6.2230788969,-1.6218694919,0.2580644161
C,-7.0472093602,-1.544672039,-0.9171804639
H,-7.9947899177,-1.9918325578,-0.6296393708
H,-7.1946710957,-0.5010325891,-1.2029507528
H,-6.5934126998,-2.114443775,-1.7308051174
C,5.2330512681,-1.1317743159,0.0396516656
F,6.0345055635,-0.2550738043,0.6523894631
F,5.219479854,-2.2484302092,0.777608267
F,5.7712921574,-1.4361242552,-1.1448713675
Br,-0.4604905244,2.7106740431,-0.0389006944

Stilbene 6

C,0.0419081351,0.5190631519,0.8003374795
C,0.2034639611,-0.8749995955,1.2811292981
C,1.3946943061,-1.5646055902,0.6711994834
C,-1.1310252935,1.1686659972,0.5001012207
C,-2.4320433762,0.5679659997,0.644850499
C,-3.553372258,1.266743947,0.3327782057
C,3.445881849,2.6083786761,-0.147940936
C,-2.1770733189,3.2334616531,-0.2959312498
C,-1.0573748624,2.5239458591,0.029219021
C,1.1680081882,-2.582489036,-0.2556890978
C,2.2380077208,-3.196200919,-0.8951754852
C,3.5408994835,-2.7853975367,-0.603819045
C,3.7732120832,-1.7693029796,0.3314077551
C,2.7006383445,1.1629608703,0.9662784365
H,0.9768967843,1.0688377644,0.689893774
H,-0.6965332137,-1.477042305,1.1734618112

H,-2.2557778325,-1.1389435159,-0.4232980566
H,1.346117799,-2.1147479668,1.723853888
H,1.3244867299,-4.3944740068,0.690911444
H,-2.2728618444,-3.4359097612,-1.4140161318
H,2.7703042225,2.0191485886,-0.3667888861
H,-1.3343573858,2.5157175222,0.9914773006
H,-1.25491422,4.8760336216,0.3902395012
H,2.8308756367,4.4310629106,-0.9810284984
N,-0.48203996,-5.3474054224,-1.0021574577
O,-1.3997586011,-5.6113884923,-1.7517897105
O,0.4279991249,-6.0910189507,-0.6977839772
O,0.9343049827,6.0336483618,-0.6942348332
C,-0.1437330477,6.9711823371,-0.5291539654
H,-1.0055593175,6.6581065217,-1.1221502213
H,-0.4039961313,7.0587406967,0.5277543523
H,0.2430974661,7.9164670327,-0.8996523395
Br,-0.0054769897,0.0256757348,3.1406804933

Stilbene 7

C,-0.3055024398,0.6287881348,1.1827461066
C,0.3003907689,-0.6246383138,0.701062672
C,-0.3482416515,-1.8134492723,0.3745506902
C,0.3537060209,1.8844305955,0.7140456522
C,-0.395426935,2.786141457,-0.040077749
C,1.7062089788,2.1446778364,0.9605700995
C,2.2934822101,3.2883571037,0.4455528785
C,0.2051270317,3.9310845469,-0.5539290284
C,1.5542986936,4.2006247776,-0.3212221409
C,0.4391892483,-2.8906730483,-0.1231668434
C,-1.7572276283,-1.9935535,0.5088889423
C,-2.3308642296,-3.1853938496,0.1500192789
C,-1.543362073,-4.246123498,-0.3589915759
C,-0.1530580039,-4.0774031109,-0.4900196924
H,-1.3890133754,0.6680624196,1.0949163152
H,1.383261244,-0.585292137,0.5802117947
H,-1.4482476965,2.5975613514,-0.2316596403
H,2.2866882045,1.4725464177,1.5880807445
H,3.3411652041,3.4903052024,0.6480306757
H,-0.386368138,4.6275769421,-1.1399180219
H,1.5133557869,-2.7600999009,-0.2182668477
H,-2.3746588021,-1.1983780234,0.9129415908
H,-3.4013786266,-3.3293772494,0.2555638185
H,0.448456399,-4.8921906646,-0.8779373054
C,2.2030564131,5.4512218749,-0.8483032046
H,1.5842410329,5.9316240776,-1.60770769
H,2.360399124,6.1695854116,-0.0379074736
H,3.179918043,5.2318306662,-1.285943968
C,-2.2002260991,-5.5344036401,-0.735193066
H,-2.6246805537,-6.0065582221,0.1577838925
H,-3.0310511413,-5.351640916,-1.4233045443
H,-1.5013044226,-6.2307811668,-1.1976616217

H,-2.5239868235,-0.4434806039,1.0249173294
H,-4.547759659,0.8487159337,0.4368693176
H,-2.0993265745,4.251509029,-0.6546129826
H,-0.0792557326,2.9851402585,-0.0731942343
H,2.8784086265,-0.4009711069,1.7197752039
H,4.7904693396,-1.4720222436,0.5591519834
H,2.0714841929,-3.9914209179,-1.6126903978
H,0.1551533672,-2.9034847625,-0.4803498949
C,4.6540949901,-3.413966259,-1.265514366
N,5.5483501407,-3.9144682808,-1.8011183236
O,-4.5805537127,3.1874287072,-0.4239124761
C,-4.6198367789,4.5404009607,-0.9095315048
H,-5.6740269905,4.7602921711,-1.0537955196
H,-4.1915717366,5.2161035706,-0.1662110758
H,-4.0858574598,4.6119793979,-1.8594190583
Br,0.4089347878,-0.5557432639,3.2169198291.

Stilbene 8

C,-0.3229124018,0.4366778535,0.5867535845
C,-0.5518156573,-0.9396653632,1.0638169252
C,-1.75959566,-1.6157098513,0.4917856879
C,0.8964417063,1.0587777153,0.3393887889
C,0.8779269722,2.3916193352,-0.1654398045
C,2.155277574,0.4216066148,0.5585867162
C,3.3172893524,1.0886426455,0.2724293782
C,2.0530711538,3.0438480713,-0.4582719673
C,3.2894849437,2.4066260206,-0.245436582
C,-1.5681353695,-2.7628265483,-0.278614103
C,-3.0440662016,-1.0913106229,0.6643102766
C,-4.1277422337,-1.7106111024,0.0569647032
C,-3.9352615968,-2.8530982799,-0.7205428912
C,-2.6582741451,-3.3798103896,-0.8856274536
H,-1.2335146882,1.0082413047,0.4047820968
H,0.3301758304,-1.5756945819,1.035921874
H,-0.0777900603,2.8829874405,-0.3237956582
H,2.1968444749,-0.5809950329,0.9706115146
H,4.2769582415,0.6116094457,0.4436129961
H,2.0351390023,4.0550242522,-0.8498114541
H,-0.5714585472,-3.1762788531,-0.4052240394
H,-3.1987565424,-0.2264674937,1.3046646132
H,-5.1257095637,-1.3111232256,0.1992242857
H,-4.7853540488,-3.3371904448,-1.1887279684
H,-2.5084561219,-4.2737143084,-1.4806924144
C,4.5751582397,3.0995390341,-0.5588619776
H,4.4187341827,4.1292821975,-0.8787045525
H,5.2321581506,3.0930936726,0.3163903379
H,5.1013459554,2.5608786517,-1.3546751041
Br,-0.776119923,-0.3949215782,2.9645674334

Br,0.0752766914,0.1979933971,3.0956305035

Stilbene 9

C,0.5173091575,-1.6647922708,0.6751524411
C,-0.4197114947,-0.7021829453,1.2893317348
C,-0.2722441814,0.7071169515,0.7933257471
C,0.2761392849,-2.9924254757,0.3502164844
C,1.3239331131,-3.7293419805,-0.2794121989
C,-0.9675001461,-3.6471224799,0.6111814917
C,-1.1396805161,-4.9557006195,0.2464501354
C,1.130975543,-5.0387109694,-0.6501000604
C,-0.0993326947,-5.6742444396,-0.3936945913
C,-1.3283545259,1.2657124337,0.0748654129
C,0.9086276557,1.4309352872,0.9868598728
C,1.0322658201,2.7031626536,0.4502080389
C,-0.0237355852,3.2510378342,-0.2778445144
C,-1.2040470684,2.5428284548,-0.4640830146
H,1.5062727941,-1.2579990329,0.4609988916
H,-1.4572378346,-1.0294554663,1.2881366012
H,2.2732408524,-3.2374530342,-0.4713826095
H,-1.7689704358,-3.1180361746,1.1156953251
H,-2.0796957053,-5.4595791307,0.4470190037
H,1.9251512571,-5.5928089371,-1.1383472479
H,-2.2514862412,0.7107874186,-0.0643981601
H,1.7115083799,1.0160575665,1.5901431715
H,1.9357518867,3.2822406794,0.6078302974
H,-2.0225308354,2.9906188195,-1.0159598693
C,-0.3164565627,-7.1028732389,-0.7684362526
H,0.4909813559,-7.4917254457,-1.3881928635
H,-0.3799582507,-7.7117840745,0.1411535541
H,-1.2669375409,-7.2217274151,-1.2964266695
C,0.1472073329,4.6167317592,-0.8956903735
F,0.8209331002,5.4312613516,-0.0779537809
F,0.8379489865,4.5336990399,-2.0386814819
F,-1.0323417264,5.1789699213,-1.171451812
Br,0.235991924,-0.9526681289,3.1428725383

Stilbene 11

C,0.5153641731,0.1755407043,1.158649712
C,-0.5642326503,-0.705499095,0.6660508139
C,-0.4812044282,-2.0565647899,0.3643897326
C,0.4551773213,1.5795115162,0.6280231665
C,1.4768368379,2.0074723051,-0.2203341561
C,-0.6191448593,2.4259003968,0.9179341833
C,-0.677190788,3.6898788093,0.3526672502
C,1.4255241168,3.2737253299,-0.7899563681
C,0.3453971122,4.1126339939,-0.5059234248
C,-1.6507539611,-2.7056052305,-0.1359657252
C,0.7154523132,-2.8223039101,0.5296916607
C,0.7266649306,-4.1507010447,0.1996461626
C,-0.4348339214,-4.7819941988,-0.3126332478

Stilbene 10

C,-0.5312877949,0.0756856318,1.2184368535
C,0.0578776888,1.3222639442,0.6843418394
C,-0.5996750148,2.5022854962,0.3737678915
C,0.1129439998,-1.1794201319,0.6987351227
C,-0.6459069834,-2.0171539097,-0.1198742566
C,1.4518207398,-1.4781028512,0.9705930398
C,2.0370685937,-2.606588223,0.4153704877
C,-0.0708119755,-3.1524931463,-0.6807316922
C,1.2600378713,-3.4166038579,-0.4021887375
C,0.1701012113,3.5756061675,-0.1705511783
C,-2.0043176874,2.6903314575,0.5692804243
C,-2.5878049295,3.8797594851,0.2254168833
C,-1.8182865378,4.9324922337,-0.3315314946
C,-0.4333104332,4.7588073214,-0.5221771508
H,-1.6161454169,0.0336803511,1.1480769662
H,1.1365261889,1.2818622801,0.5281147571
H,-1.6882346187,-1.7904773501,-0.3225413823
H,2.0266683277,-0.8499120332,1.6450922734
H,3.0685003012,-2.874647435,0.6082795245
H,-0.6296275478,-3.8273279188,-1.3173032679
H,1.2387452797,3.4400604959,-0.3106887987
H,-2.6054297962,1.9027732398,1.011217202
H,-3.6512472849,4.031632619,0.3795880298
H,0.1520835773,5.5690348806,-0.9427908706
N,1.8805529406,-4.619949375,-0.9975721133
O,1.1740238911,-5.3123751791,-1.7006827607
O,3.0497127036,-4.8199245347,-0.7400613698
C,-2.4903379676,6.2090806201,-0.7129763145
H,-3.0991309645,6.5825215921,0.1159265823
H,-1.7765665907,6.9770500797,-1.0092159878
H,-3.1739952793,6.0259216032,-1.5502490145
Br,-0.1138513417,0.4333364469,3.1182837545

Stilbene 12

C,-0.5729605184,-0.4534779897,0.6172525408
C,0.5731559407,0.4534747903,0.6172555578
C,0.5048897299,1.8702049131,0.2990749804
C,-0.5046896695,-1.8702092027,0.2990740073
C,-1.6724703839,-2.4771704666,-0.1849274203
C,0.6792674445,-2.6176279969,0.4207032841
C,0.6919400861,-3.946697853,0.0371187582
C,-1.6491288643,-3.8088476431,-0.5796518429
C,-0.46967542,-4.5398935483,-0.4691906421
C,1.672678275,2.4771662153,-0.184908186
C,-0.6790696164,2.6176237469,0.4206846012
C,-0.6917362199,3.9466932609,0.0370990098
C,0.4698874797,4.5398887345,-0.4691920553

C,-1.6193455731,-4.0372875717,-0.473965656
H,1.5118048269,-0.251130964,1.0655565496
H,-1.527185414,-0.210652173,0.5344996201
H,2.3176475604,1.3560339552,-0.4392410158
H,-1.3907681986,2.1110253401,1.6149653424
H,-1.5005295211,4.3584213311,0.5766342842
H,2.2161314869,3.6166258068,-1.4473913619
H,-2.5641513833,-2.1295083821,-0.2536018987
H,1.6085397935,-2.3607064747,0.9372627377
H,1.6293277081,-4.7388358693,0.3304662513
H,-2.5067486499,-4.5255936229,-0.8614128727
C,0.2848857937,5.4247448027,-1.0947989031
N,0.2333048039,6.4768414978,-1.5716110618
C,-0.3831277128,-6.2294929913,-0.6727154779
H,-0.0373341137,-6.8187349679,0.1826839342
H,-1.3517968156,-6.6075981388,-0.9976066907
H,0.3441158984,-6.384581967,-1.4775253336
Br,0.0356707626,0.0441873982,3.0749467928

Stilbene 13

C,-1.2786092253,-0.2361187745,0.9288436567
C,-1.4733754442,-1.640782583,0.5575858329
C,-2.6963981513,-2.2746340702,0.2081429524
C,-0.0057322128,0.4514701292,0.5985694407
C,-0.0855167232,1.7206970798,0.0269810556
C,1.2401670633,-0.1571250018,0.7999627485
C,2.3937898322,0.4981684109,0.4070328435
C,1.0760336003,2.3765591006,-0.3735003184
C,2.3047022377,1.7606544173,-0.1846919308
C,-2.6197526433,-3.5867750051,-0.3110554591
C,-3.9533183533,-1.6344494368,0.321284606
C,-5.0928776062,-2.2906629328,-0.0950339599
C,-4.9984156424,-3.5844407043,-0.6281776137
C,-3.7673954609,-4.2324029029,-0.7376805509
H,-2.1605931983,0.3966302833,0.8658063128
H,-0.5557111897,-2.2075307909,0.4032927842
H,-1.0498534656,2.1992627831,-0.1150863662
H,1.3115423844,-1.1194773271,1.3001021828
H,3.3665498701,0.0450996419,0.5670686344
H,1.0269277528,3.3619038943,-0.8217878583
H,-1.6540318503,-4.0783424633,-0.3851465002
H,-4.0328696845,-0.6418406462,0.7531743456
H,-6.0605807122,-1.8104115362,-0.0087357662
H,-5.9004340199,-4.0911296923,-0.9559726397
H,-3.710819564,-5.2337130821,-1.1480769722
C,3.5839645405,2.4358034961,-0.6176932562
F,3.3630164557,3.6795878629,-1.0462451117
F,4.4541635842,2.4871050401,0.3949586719
F,4.1614209308,1.7486209853,-1.6084809126
Br,-1.2940593325,-1.0587930203,2.7839443901

C,1.649342926,3.8088430086,-0.5796338823
H,-1.5473390251,0.0162163261,0.5005911767
H,1.5475355236,-0.0162206387,0.5006073112
H,-2.5901497421,-1.9014661678,-0.2642000406
H,1.5746690049,-2.1742113902,0.847518504
H,1.6003583357,-4.5298718151,0.1354067885
H,-2.5483337804,-4.275157259,-0.9653441883
H,-0.4517417796,-5.5821232986,-0.769483568
H,2.590358941,1.9014619082,-0.2641656007
H,-1.5744781828,2.1742072712,0.8474851681
H,-1.6001561273,4.5298672017,0.1353717796
H,0.4519584812,5.5821182738,-0.769486029
H,2.5485538825,4.2751525705,-0.9653121917
Br,0.0000852791,-0.0000009513,2.6292521793

Stilbene 14

C,0.733802762,-0.5303229112,1.0229483518
C,0.1430331823,-1.7794700584,0.5183365378
C,0.8098556767,-2.9681771315,0.1822207345
C,0.0705246892,0.7495103334,0.6225607048
C,0.8416399874,1.699706682,-0.0486466407
C,-1.2899044366,0.975924595,0.8574632287
C,-1.8848819431,2.1441371409,0.4057348553
C,0.2551723673,2.8749375756,-0.5065963865
C,-1.0960840902,3.0654015747,-0.2713103886
C,0.0324452994,-4.0197886803,-0.3730884352
C,2.2119183674,-3.1393854884,0.3458041238
C,2.8048168459,-4.3169491697,-0.0505638262
C,2.0207609665,-5.3366931523,-0.6152518082
C,0.639862907,-5.1920241653,-0.7780997883
H,1.819281978,-0.4819747338,0.9787318169
H,-0.9336180336,-1.7382782944,0.3511344219
H,1.9000255984,1.5285735773,-0.2196611536
H,-1.8776696175,0.2604419906,1.4259729036
H,-2.9329789323,2.3596123083,0.5734294244
H,0.821273921,3.6349541662,-1.0309830277
H,-1.0396705908,-3.8869535562,-0.4855238175
H,2.8135604673,-2.3585108167,0.7991316472
H,3.8716665315,-4.461648098,0.0729007831
H,2.499304555,-6.2598073219,-0.9274637919
H,0.0539749767,-5.9933369241,-1.2124739183
N,-1.7285440935,4.3126366992,-0.755387286
O,-1.0130071442,5.1008508185,-1.3373542935
O,-2.9142278727,4.4473308056,-0.5347563366
Br,0.2630213065,-1.1217574831,2.870176607

Stilbene 15

C,-0.4924025221,-0.3356346169,0.9245924558
C,0.5974758854,-1.228154007,0.5115490952
C,0.5087084482,-2.6019185056,0.1928205057
C,-0.4293906109,1.1020660375,0.5412353364
C,-1.5443891568,1.6569959512,-0.0883788888
C,0.7196989373,1.8725900136,0.7501290003
C,0.7601774156,3.1854001108,0.3116051702
C,-1.5085457104,2.9727568432,-0.5338598024
C,-0.354572732,3.7340638294,-0.3368261739
C,1.672042718,-3.2266084005,-0.3202223188
C,-0.6889913521,-3.3486872444,0.3305758047
C,-0.7149378492,-4.6720696824,-0.0531515664
C,0.4415866514,-5.269247325,-0.5782103497
C,1.6320696903,-4.5517281883,-0.7132819296
H,-1.4917641725,-0.761301554,0.875014196
H,1.5555738604,-0.7352358855,0.3474834668
H,-2.4419763182,1.0649652945,-0.2392421327
H,1.5688517604,1.462671354,1.2905720686
H,1.6409601901,3.7959509916,0.4737680793
H,-2.3677448393,3.412610305,-1.026846977
H,2.5896995042,-2.6530233781,-0.4132160925
H,-1.5785090063,-2.8942790212,0.754771661
H,-1.623577249,-5.2533514005,0.0513980699
H,2.5162144252,-5.0305591603,-1.1171936004
C,-0.3110572042,5.0982366117,-0.7937980847
N,-0.2735020099,6.1931160115,-1.1633364908
H,0.4096308523,-6.3113365152,-0.8802303417
Br,0.1959168509,-0.6996471072,2.7816648393

Stilbene 17

C,-0.6005059392,0.9326806683,0.6477753804
C,0.5305398996,0.0254582466,0.8487507723
C,0.4581364901,-1.407508597,0.5039129405
C,-0.5164373248,2.3394394774,0.3423517724
C,-1.6713031605,2.9547291684,-0.1724103078
C,0.6689546248,3.0843562084,0.5021310913
C,0.7010549856,4.4126084248,0.1305510495
C,-1.6394101947,4.2848844528,-0.5582883281
C,-0.4530005177,5.0105059705,-0.4063354828
C,1.6008718769,-1.9916943732,-0.050374219
C,-0.7151463222,-2.1560956708,0.6726692741
C,-0.7535195581,-3.478483243,0.2639382713
C,0.3914679721,-4.0248503531,-0.3055628947
C,1.5696468265,-3.3170556125,-0.4708155404
H,-1.5614794463,0.4506735193,0.4744606634
H,1.5199209366,0.4713261465,0.7764072347

Stilbene 16

C,-0.5298784667,-0.9277025243,0.9141988957
C,0.5575820297,0.0241904294,0.6803560917
C,0.412460935,1.4304320477,0.4099417215
C,-0.4164795824,-2.3505359368,0.5321745972
C,-1.5496874685,-2.9606566253,-0.0127899127
C,0.7846431804,-3.0616247716,0.6588998437
C,0.8595845475,-4.3722753789,0.218001768
C,-1.482316172,-4.2742926407,-0.4649161785
C,-0.2776426166,-4.9448482877,-0.340655571
C,1.5241374748,2.0949997776,-0.1359870457
C,-0.7938874368,2.1288509929,0.6264246622
C,-0.8818073328,3.4608349274,0.2791296043
C,0.2283420457,4.1030210804,-0.2847498695
C,1.4272811268,3.4322689624,-0.4959931403
H,-1.5369978135,-0.5184614234,0.8821481766
H,1.5291333905,-0.4196391913,0.4675841037
H,-2.4831708754,-2.4127262272,-0.0961639831
H,1.6503273499,-2.6115698852,1.1372567862
H,1.765828525,-4.959258918,0.3030234968
H,-2.3363513476,-4.7792347506,-0.8995366624
H,2.4550876497,1.5579343726,-0.2915178991
H,-1.646516602,1.6405394094,1.088354092
H,-1.800629089,4.0153580663,0.4367981209
H,2.2705912073,3.9528810866,-0.9341532949
N,-0.1976240655,-6.3461444147,-0.8153408406
O,-1.2075088184,-6.8209311041,-1.2896218963
O,0.8727239415,-6.9035808929,-0.6925304725
C,0.1013306384,5.5732299068,-0.625175077
F,-1.0341553275,5.7966582552,-1.2893738975
F,0.0722158263,6.299007003,0.4938134986
F,1.1221808721,5.9887487445,-1.3725585137
Br,0.1974657744,-0.5242360899,2.7923440377

Stilbene 18

C,-0.4979301834,0.4756357574,0.5440555162
C,0.4954899745,0.4747967733,-0.5288198722
C,1.9053745779,0.1514683746,-0.3456158749
C,-1.9099343939,0.1623332695,0.3587005428
C,-2.5995312094,-0.3572090412,1.4602702021
C,-2.5644904373,0.3234326288,-0.8752161754
C,-3.8857752742,-0.0582685857,-1.0016778365
C,-3.9262125715,-0.7526715732,1.3264415856
C,-4.55700038,-0.6026643287,0.0989812722
C,2.5912833952,-0.3667489149,-1.4501717288
C,2.5605724918,0.2993743621,0.8896526218
C,3.8790239984,-0.0925403949,1.0139166803
C,4.5476669933,-0.6314470565,-0.0909999982
C,3.9156298442,-0.770872859,-1.3190476502
H,-0.1074811028,0.346134209,1.5514314378
H,0.1039427647,0.3541034105,-1.5368823556

H,-2.5883092358,2.3837113753,-0.282451293
H,1.5548984572,2.6372088091,0.9424858129
H,1.6024101056,5.0022438118,0.2508554532
H,-2.5191052111,4.766820352,-0.9684737552
H,2.5129622535,-1.4143845319,-0.1661300723
H,-1.5861714246,-1.724836345,1.1586307767
H,-1.6368701688,-4.0941528266,0.3813738158
H,2.4314436878,-3.8027814933,-0.9119796859
C,-0.4115420003,6.3936054449,-0.7961874651
N,-0.3756175683,7.5061388023,-1.1094518703
N,0.3501083545,-5.4391707662,-0.7461862501
O,-0.6984072644,-6.0285185234,-0.5896426995
O,1.366595773,-5.8907576119,-1.2286666418
Br,-0.1535834691,0.4501788293,2.7460471976

Stilbene 19

C,0.6796111211,1.3787781829,0.7481198156
C,-0.4650432969,0.4688348916,0.7758017151
C,-0.4058232508,-0.9532033312,0.4907839097
C,0.5817013454,2.7966479164,0.3950795371
C,1.6937932114,3.3831783031,-0.2202839561
C,-0.5830028984,3.5484760414,0.6147720987
C,-0.6411432571,4.8650444361,0.1983895126
C,1.6365976707,4.7019408343,-0.6497539966
C,0.4685416393,5.4395968367,-0.4416378016
C,-1.5935494622,-1.5731250597,0.0781977526
C,0.7876116126,-1.6942284538,0.574076977
C,0.7880800917,-3.0292463873,0.2214721651
C,-0.3980201477,-3.6287769207,-0.2174226246
C,-1.5867051473,-2.913436824,-0.288846281
H,1.6499383796,0.9162729217,0.5808492308
H,-1.4439625096,0.9375706476,0.6938918195
H,2.600424206,2.8065179197,-0.3766583722
H,-1.4306738751,3.122288206,1.1440988289
H,-1.5306083303,5.4611084807,0.366522682
H,2.487534664,5.1631472982,-1.1372946345
H,-2.5174577409,-1.0043833012,0.0316143396
H,1.7011713334,-1.2410625382,0.9479072973
H,1.694911621,-3.6201105143,0.2921074411
H,-2.4958710504,-3.4029176989,-0.6177650262
C,0.4025496638,6.8090741897,-0.8772782663
N,0.3469459493,7.9094489953,-1.2278162179
C,-0.3511344982,-5.0804039783,-0.642298782
F,0.3576236458,-5.7989380781,0.2311328312
F,-1.574515723,-5.6013924527,-0.7290809844
F,0.2381257581,-5.1892654169,-1.8350362783
Br,0.2102027643,0.9818459212,2.7557402677

H,-2.0976734511,-0.4654739681,2.4171597313
H,-2.0574768318,0.7805620532,-1.7203115625
H,-4.4103451334,0.0696092304,-1.9426181344
H,-4.4689700048,-1.1652782767,2.1686295566
H,2.087878874,-0.4684041499,-2.4069808769
H,2.0555758052,0.7512136813,1.7387712067
H,4.4013666911,0.0165566064,1.9584626402
H,4.4540700759,-1.1869130855,-2.162327314
C,-5.9940725383,-1.0349898347,-0.0884789495
F,-6.5591119523,-1.3698733926,1.0710403586
F,-6.7072077986,-0.0502064191,-0.6401634668
F,-6.0547436683,-2.0883033924,-0.9069996699
C,5.997267926,-1.0269786202,0.0806501228
F,6.1392056881,-1.8167859227,1.1480264514
F,6.4577671861,-1.6736152672,-0.9897320438
F,6.7508907828,0.0578034134,0.2749636642
Br,0.0054558618,2.4709183135,0.0136459187

Stilbene 20

C,0.0950491493,0.7252349243,0.766998945
C,-0.0950788904,-0.7252718336,0.7669999189
C,-1.3579096012,-1.3889535222,0.4473152743
C,1.3578802154,1.3889163312,0.4473155099
C,1.2809941113,2.6776368553,-0.0967602786
C,2.6027519456,0.7629578802,0.6253305828
C,3.760921902,1.4123976749,0.2373370012
C,2.438818507,3.3327733367,-0.4993977143
C,3.6478750704,2.6812126197,-0.3232750941
C,-1.2810227665,-2.6776743132,-0.0967597221
C,-2.602781553,-0.7629950242,0.625328479
C,-3.7609510127,-1.4124350851,0.2373338086
C,-3.6479034386,-2.6812503281,-0.3232774748
C,-2.4388466323,-3.3328110632,-0.4993982479
H,-0.8057605689,1.3218164146,0.6365913918
H,0.8057309353,-1.3218535558,0.6365942327
H,0.3184247713,3.1646686113,-0.2191533789
H,2.6760752098,-0.2116611264,1.0994478068
H,4.7416079696,0.9696698705,0.3615476025
H,2.4203734942,4.3247843397,-0.9339962373
H,-0.3184532639,-3.1647060992,-0.2191513759
H,-2.6761054271,0.2116242226,1.0994451322
H,-4.7416372643,-0.9697072497,0.3615429793
H,-2.4204010288,-4.3248222789,-0.9339962218
N,4.8900187608,3.3750626369,-0.7429879117
O,4.7606500481,4.4809386844,-1.2218389983
O,5.9309280122,2.7768285208,-0.5727980426
N,-4.8900465692,-3.3751006267,-0.7429914552
O,-5.9309560272,-2.7768663978,-0.5728030599
O,-4.7606773421,-4.4809768719,-1.2218418928
Br,-0.0000163488,-0.0000174379,2.7506836831

Stilbene 21

C,0.5703482253,0.4575419764,0.7065529967
C,-0.5704123631,-0.4575773364,0.7065529967
C,-0.4867677601,-1.8782806094,0.3888210699
C,0.4867036224,1.8782452493,0.3888210699
C,1.6385855168,2.4902105562,-0.1236218761
C,-0.6982443308,2.6177055657,0.5408526668
C,-0.7347377398,3.9448451005,0.1593872373
C,1.6033798009,3.8197354405,-0.5189634077
C,0.4164074369,4.5437731555,-0.3783391097
C,-1.6386496546,-2.4902459163,-0.1236218761
C,0.698180193,-2.6177409257,0.5408526668
C,0.734673602,-3.9448804606,0.1593872373
C,-0.4164715746,-4.5438085156,-0.3783391097
C,-1.6034439386,-3.8197708006,-0.5189634077
H,1.5481494962,-0.0031040371,0.5810107504
H,-1.5482136339,0.0030686771,0.5810107504
H,2.5588259104,1.923201188,-0.2268577201
H,-1.58110737,2.1720703417,0.9902786652
H,-1.6387485852,4.5312314501,0.2759716656
H,2.4845175132,4.3002679597,-0.9278271306
H,-2.5588900482,-1.9232365481,-0.2268577201
H,1.5810432322,-2.1721057017,0.9902786652
H,1.6386844474,-4.5312668102,0.2759716656
H,-2.484581651,-4.3003033197,-0.9278271306
C,0.372348311,5.9246374051,-0.7784210715
N,0.3342740925,7.0344897109,-1.1003589706
C,-0.3724124488,-5.9246727652,-0.7784210715
N,-0.3343382303,-7.0345250709,-1.1003589706
Br,-0.0000320689,-0.00001768,2.7024134688

Stilbazole 23

C,-0.2184848909,-0.1245711452,0.5182755511
C,0.8183159492,0.228920583,-0.4741052644
C,2.1372819543,-0.4564839861,-0.2457693583
C,-1.5789282373,-0.281374863,0.3001525956
C,-2.3964308208,-0.6626904421,1.4074311472
C,-2.1934451242,-0.0856492052,-0.9762277076
C,-3.5415281558,-0.2757283884,-1.1210584338
C,-3.746165038,-0.860505937,1.2425829112
C,-4.3415833285,-0.6721130035,-0.0201188717
C,2.555785405,-1.4207039623,-1.1574158017
C,2.9213703937,-0.2093429566,0.8798786701
C,4.0878325025,-0.9506552738,1.0413860155
N,4.4969499048,-1.8830667159,0.1786732028
C,3.7441315928,-2.1035872947,-0.8962190577
H,0.1587174386,-0.2715936831,1.5310444407
H,0.4915330513,0.1470142872,-1.5085959974
H,-1.9345019063,-0.8019341919,2.3806723212
H,-1.5998512069,0.2349629833,-1.8257033291

Stilbazole 22

C,-0.6365806721,-0.473769912,0.4777851957
C,0.4598108045,-1.2976599518,1.0457742641
C,0.5241163697,-2.6728954892,0.4336883978
C,-0.6269863311,0.8783481503,0.2355121809
C,-1.7921421824,1.4872159118,-0.3525266844
C,0.4888751385,1.722238423,0.5629951307
C,0.4566142553,3.062432853,0.3160573648
C,-1.8308929199,2.8200805206,-0.6148382441
C,-0.7060708546,3.6300958761,-0.2856131758
C,1.5642521091,-2.9747596552,-0.4395439802
C,-0.4623395323,-3.6316975722,0.6578918606
C,-0.3611256583,-4.8472227856,-0.011601315
N,0.6281468042,-5.1470153812,-0.8559847778
C,1.5682047783,-4.2263623986,-1.0557798055
H,-1.5447716317,-1.0307311838,0.2452367815
H,1.4316916801,-0.8087286675,1.0138228673
H,-2.6440062555,0.8584898729,-0.5937923188
H,1.3646776174,1.295590112,1.0403355337
H,1.2996026252,3.6882715588,0.5788774275
H,-2.690444053,3.303164306,-1.0640665961
H,2.3603004605,-2.264777101,-0.6414871581
H,-1.2707393735,-3.4552733385,1.3608052632
H,-1.1093530568,-5.6194594871,0.1442177794
H,2.3693145294,-4.4949608286,-1.7390803398
O,-0.8301590669,4.8968409781,-0.5673627842
C,0.2285374912,5.8274432883,-0.2836551637
H,-0.1425119328,6.7911623464,-0.6214107899
H,0.4246399981,5.8546133843,0.7902827603
H,1.1269004398,5.5532569851,-0.8406480975
Br,-0.069376588,-1.3347446162,2.9434936658

H,-4.0147637294,-0.1206959565,-2.0852479607
H,-4.3634603589,-1.1571197254,2.0834598143
H,1.9838904654,-1.6432335906,-2.0528122781
H,2.6566360249,0.5627082293,1.5959916707
H,4.7267807031,-0.7808679472,1.9035167503
H,4.1018510537,-2.8598321184,-1.5895794698
C,-5.8041932132,-0.8946412433,-0.2172823345
H,-6.3310786543,-1.0208076232,0.7281394607
H,-6.24908731,-0.0638284662,-0.7721359585
H,-5.9553610592,-1.7973920568,-0.8212326885
Br,0.8644015943,2.1587346934,-0.0541470397

Table S4: Cartesian coordinates for the geometries of the charge transfer complexes between bromine and substituted stilbenes and stilbazoles optimised at the MP2/6-31G(d,p) level of theory with the inclusion of BSSE through the CP correction.

Stilbene 1

C,0.0183427586,-0.6797026846,0.2022638574
C,-0.0183536774,0.6797055015,0.2022638602
C,-2.175788429,-3.700441926,0.6607302375
C,-1.0753577721,-2.8570082721,0.6705001319
C,-1.1535012914,-1.5503260932,0.1517382042
C,-2.3720924363,-1.1361287232,-0.4054303256
C,-3.4904080596,-1.9704066418,-0.4140856895
C,-3.3934947531,-3.2599121428,0.1228810988
C,1.1534903719,1.5503289103,0.151738194
C,1.0753468597,2.8570110873,0.6705001276
C,2.1757775165,3.7004447412,0.6607302211
C,3.3934838332,3.25991496,0.1228810639
C,3.4903971322,1.970409461,-0.4140857305
C,2.3720815091,1.1361315424,-0.4054303542
O,4.4149095587,4.1701634836,0.1627702931
C,5.6679006395,3.7470065806,-0.3632506492
O,-4.4149204781,-4.1701606665,0.1627703387
C,-5.6679115662,-3.7470037616,-0.3632505847
H,-0.9859650239,1.1728846934,0.2477508785
H,0.9859541057,-1.1728818767,0.2477508605
H,0.1421600163,3.2031934092,1.1000207622
H,2.4463452012,0.1558575994,-0.8606744141
H,4.4091273782,1.6161902948,-0.8584753979
H,2.1244029539,4.7028984618,1.0647064272
H,-0.1421709227,-3.2031905956,1.1000207523
H,-2.4463561347,-0.1558547786,-0.8606743809
H,-4.4091383117,-1.616187474,-0.8584753429
H,-2.1244138608,-4.7028956481,1.0647064392
H,6.3398923259,4.5882448752,-0.226580624
H,6.0520214416,2.8795141103,0.1764929632
H,5.5928338201,3.507908422,-1.4257223241
H,-6.3399032507,-4.5882420567,-0.2265805533
H,-6.0520323608,-2.8795112933,0.1764930362
H,-5.5928447614,-3.5079055991,-1.4257222598

Stilbene 2

C,-0.31686,-1.438353,0.596839
C,0.570239,-1.545576,-0.427569
C,2.011926,-1.731617,-0.271665
C,-1.766494,-1.341872,0.445216
C,-2.533825,-0.726096,1.452457
C,-2.438876,-1.849879,-0.675824
C,-3.820623,-1.719019,-0.817667
C,-3.908694,-0.596089,1.329002
C,-4.560988,-1.087429,0.189159
C,2.878593,-1.32879,-1.301214
C,2.573157,-2.316946,0.876312
C,3.953167,-2.449212,1.00212
C,4.819272,-2.033567,-0.018256
C,4.25715,-1.471581,-1.171712
H,0.065224,-1.412815,1.6141
H,0.197956,-1.482647,-1.446789
H,-2.037923,-0.332376,2.332355
H,-1.881309,-2.376323,-1.441114
H,-4.302121,-2.129786,-1.693128
H,-4.503243,-0.117188,2.095743
H,2.464397,-0.885191,-2.199766
H,1.924895,-2.689124,1.660487
H,4.364858,-2.909809,1.893382
H,4.906072,-1.150347,-1.978832
O,-5.917595,-0.908084,0.167708
C,-6.606694,-1.385144,-0.982736
H,-7.65086,-1.138137,-0.819625
H,-6.251129,-0.89365,-1.89015
H,-6.49922,-2.466062,-1.090783
C,6.311366,-2.151391,0.138069
H,6.573877,-3.00427,0.762925
H,6.798189,-2.276848,-0.828328
H,6.728287,-1.257666,0.605443
Br,0.427803,1.475646,0.012048

Br,-0.0000054389,0.000001403,3.1746013458
Br,-0.0000054227,0.0000013986,5.5171277757

Stilbene 3

C,-0.5983171813,-0.5147136726,0.0946150606
C,0.5399693819,-1.2564631786,0.1156367792
C,0.5894754193,-2.716512559,0.0310973004
C,-0.6492650925,0.9452589797,0.0910268125
C,-1.7898384339,1.6044638833,0.5878985721
C,0.4034815397,1.7311990066,-0.3996245448
C,0.3494832567,3.1248492786,-0.3645646383
C,-1.8608187001,2.9887385572,0.6218455779
C,-0.7880315038,3.7587256681,0.1502549803
C,1.6852080765,-3.4029573291,0.5811755047
C,-0.4272436115,-3.4618345092,-0.5909428181
C,-0.3649288248,-4.8532228611,-0.6261500651
C,0.7225884474,-5.5246327735,-0.0618238743
C,1.7505521764,-4.7938329941,0.5381268267
H,-1.5546161172,-1.031446802,0.0904472848
H,1.4940039937,-0.7443870293,0.2093049529
H,-2.6200837279,1.0185742421,0.9654870097
H,1.2706593902,1.2514655295,-0.8373055877
H,1.1783260746,3.6947747689,-0.7585090943
H,-2.7310966866,3.5016921637,1.009410682
H,2.4785999503,-2.8381260576,1.0573750636
H,-1.252691004,-2.947074942,-1.0673124981
H,-1.1545586208,-5.4135242331,-1.1110170415
H,0.7724703077,-6.6054390218,-0.0977855789
H,2.5992931323,-5.3067533708,0.9727127596
O,-0.9608585109,5.1139560468,0.2286307516
C,0.1163171429,5.922935202,-0.2311685868
H,-0.2019238708,6.948380545,-0.0728789877
H,1.0278365623,5.7300373108,0.3374154612
H,0.3106696129,5.7601252773,-1.2929097818
Br,-0.1072312279,-0.967259035,3.0971248992
Br,-0.1698907373,-1.0194674285,5.4354068187

Stilbene 5

C,0.311316,-1.309531,0.603557
C,-0.634232,-1.403916,-0.366761
C,-2.076769,-1.442604,-0.154902
C,1.75368,-1.316516,0.363552
C,2.616854,-1.743761,1.387752
C,2.318864,-0.905151,-0.85789
C,3.691638,-0.962314,-1.070706
C,3.994805,-1.797172,1.202172
C,4.507299,-1.407031,-0.031929
C,-2.902075,-1.926078,-1.179961

Br,0.655394,3.80499,-0.04327

Stilbene 4

C,-0.866787,-1.374678,0.566663
C,0.01513,-1.31048,-0.464156
C,1.469469,-1.257473,-0.312928
C,-2.314539,-1.504029,0.427816
C,-3.155883,-1.047644,1.46044
C,-2.911663,-2.076039,-0.704977
C,-4.298142,-2.160247,-0.831946
C,-4.53535,-1.130916,1.350488
C,-5.116316,-1.683448,0.199935
C,2.248031,-0.65697,-1.31711
C,2.121819,-1.789623,0.813228
C,3.503378,-1.696491,0.946568
C,4.256505,-1.080767,-0.057063
C,3.631134,-0.568913,-1.196813
H,-0.484008,-1.308028,1.581981
H,-0.367202,-1.284697,-1.480785
H,-2.717198,-0.609292,2.349563
H,-2.28814,-2.48455,-1.491171
H,-4.720025,-2.614438,-1.716611
H,-5.188382,-0.775369,2.136466
H,1.758553,-0.245403,-2.191995
H,1.544888,-2.29925,1.574729
H,3.997804,-2.104577,1.817861
H,4.220551,-0.094174,-1.969432
O,-6.483299,-1.718535,0.19388
C,-7.104635,-2.26446,-0.965236
H,-8.172152,-2.189431,-0.785098
H,-6.842784,-1.696479,-1.859661
H,-6.830159,-3.311319,-1.107011
C,5.748146,-1.056168,0.048279
F,6.160964,-0.980394,1.335584
F,6.304061,-2.175528,-0.477323
F,6.284091,-0.003239,-0.612287
Br,-0.600838,1.679364,0.010026
Br,-0.739996,4.010573,-0.021534

Stilbene 6

C,-0.426688,-1.447754,-0.378197
C,0.529472,-1.42292,0.586402
C,1.966231,-1.530244,0.338638
C,-1.866943,-1.387082,-0.15638
C,-2.440664,-0.922666,1.044789
C,-3.81468,-0.917502,1.219867
C,-4.663491,-1.361982,0.193486
C,-4.116965,-1.808349,-1.014488
C,-2.730966,-1.812114,-1.175438
C,2.803006,-2.012711,1.360164

C,-2.689541,-1.019057,1.042045
C,-4.061916,-1.108225,1.207084
C,-4.870807,-1.609949,0.174877
C,-4.286161,-2.017559,-1.028902
H,0.000107,-1.307993,1.643976
H,-0.305573,-1.51673,-1.396846
H,2.198115,-2.048574,2.339705
H,1.680808,-0.519462,-1.642717
H,4.135902,-0.647421,-2.003246
H,4.663818,-2.129349,1.981978
H,-2.453257,-2.246586,-2.1136
H,-2.090937,-0.594294,1.838376
H,-4.541983,-0.778072,2.118894
H,-4.883813,-2.399583,-1.843494
N,5.95909,-1.459115,-0.244852
O,6.666438,-1.848917,0.699578
O,6.391466,-1.112001,-1.356945
O,-6.209171,-1.645707,0.449073
C,-7.060658,-2.134523,-0.582841
H,-8.066298,-2.082588,-0.178453
H,-6.992915,-1.51466,-1.478525
H,-6.820752,-3.168304,-0.837564
Br,-0.214127,1.700284,0.047599
Br,-0.26303,4.032308,-0.027344

Stilbene 7

C,0.465139,-1.575883,-0.49519
C,-0.465171,-1.575873,0.495191
C,-1.911738,-1.615354,0.286884
C,1.911706,-1.615378,-0.286883
C,2.768718,-1.109838,-1.278413
C,2.488047,-2.158054,0.874449
C,3.868863,-2.150719,1.050126
C,4.149072,-1.112536,-1.098777
C,4.723903,-1.632371,0.06806
C,-2.768745,-1.109798,1.27841
C,-2.488085,-2.158031,-0.874444
C,-3.868901,-2.150685,-1.050121
C,-4.723936,-1.632321,-0.068059
C,-4.149099,-1.112483,1.098775
H,0.12664,-1.532386,-1.527074
H,-0.126672,-1.532374,1.527075
H,2.343773,-0.697389,-2.186722
H,1.853607,-2.606627,1.6294
H,4.293347,-2.580873,1.950536
H,4.790263,-0.713935,-1.877034
H,-2.343795,-0.697347,2.186716
H,-1.85365,-2.606617,-1.629392
H,-4.293389,-2.580841,-1.950528
H,-4.790286,-0.713869,1.877028
C,6.213564,-1.599529,0.278915

C,4.171248,-2.162466,1.163517
C,4.732254,-1.818256,-0.075339
C,3.915677,-1.318648,-1.103029
C,2.551748,-1.165211,-0.887909
H,-0.113566,-1.580651,-1.410676
H,0.225007,-1.40287,1.628689
H,-1.808422,-0.540196,1.836539
H,-4.264398,-0.555325,2.134982
H,-4.745326,-2.147988,-1.824729
H,-2.311969,-2.162385,-2.112248
H,1.937994,-0.73871,-1.671153
H,4.359158,-1.033324,-2.04823
H,4.805676,-2.540024,1.954885
H,2.369161,-2.2834,2.315789
C,6.142427,-1.968502,-0.290936
N,7.305905,-2.094844,-0.469308
O,-5.999216,-1.305792,0.47728
C,-6.889544,-1.734267,-0.548587
H,-7.886371,-1.613476,-0.137131
H,-6.785632,-1.120091,-1.44474
H,-6.723186,-2.781971,-0.805128
Br,0.210787,1.6112,0.030436
Br,0.321257,3.941791,-0.047845

Stilbene 8

C,0.594613,-1.544797,-0.415292
C,-0.329181,-1.762399,0.555113
C,-1.725295,-2.135388,0.320086
C,2.005539,-1.230526,-0.191869
C,2.93096,-1.484836,-1.216863
C,2.483221,-0.676511,1.008838
C,3.83962,-0.420598,1.180039
C,4.287411,-1.222663,-1.039528
C,4.766827,-0.691649,0.163439
C,-2.688009,-1.841106,1.300126
C,-2.137456,-2.798667,-0.848729
C,-3.478626,-3.119838,-1.044849
C,-4.429251,-2.805841,-0.07012
C,-4.028339,-2.167775,1.105464
H,0.29408,-1.6623,-1.453122
H,-0.031869,-1.657079,1.594761
H,2.581453,-1.902522,-2.154642
H,1.790252,-0.425522,1.80267
H,4.186098,0.007396,2.114271
H,4.98299,-1.43682,-1.843238
H,-2.38026,-1.337531,2.209535
H,-1.403662,-3.080817,-1.593711
H,-3.780377,-3.632868,-1.949427
H,-5.469719,-3.062839,-0.222555
H,-4.757704,-1.926196,1.86831

H,6.745255,-1.657309,-0.670078
H,6.518993,-0.676222,0.774105
H,6.539777,-2.431978,0.901297
C,-6.213597,-1.599464,-0.278913
H,-6.539816,-2.431904,-0.901304
H,-6.745288,-1.65725,0.67008
H,-6.519018,-0.676149,-0.774093
Br,0.000008,1.419336,-0.000001
Br,0.000044,3.759035,-0.000001

Stilbene 9

C,-1.028627,-1.572238,0.452949
C,-0.129364,-1.415044,-0.551779
C,1.311837,-1.248695,-0.360566
C,-2.460134,-1.803912,0.269877
C,-3.35409,-1.448484,1.293322
C,-2.982853,-2.385575,-0.89791
C,-4.355344,-2.562034,-1.046777
C,-4.725038,-1.633586,1.138829
C,-5.250249,-2.193075,-0.033007
C,2.063352,-0.562989,-1.33005
C,1.976842,-1.754419,0.770271
C,3.342651,-1.554149,0.942079
C,4.067795,-0.854924,-0.026914
C,3.431366,-0.366689,-1.170847
H,-0.678654,-1.502964,1.479756
H,-0.48686,-1.394448,-1.577478
H,-2.968353,-1.009389,2.206605
H,-2.31109,-2.721423,-1.678731
H,-4.738046,-3.019801,-1.952185
H,-5.396529,-1.348766,1.940996
H,1.563851,-0.171073,-2.208278
H,1.424367,-2.327176,1.504555
H,3.847013,-1.942708,1.816589
H,3.999291,0.172876,-1.916521
C,-6.734841,-2.357976,-0.215007
H,-7.232569,-2.51032,0.741819
H,-7.172841,-1.472853,-0.679355
H,-6.958994,-3.211613,-0.853499
C,5.549541,-0.712794,0.118882
F,5.922314,-0.634606,1.418182
F,6.207139,-1.770979,-0.415683
F,6.014496,0.395288,-0.504055
Br,-0.994041,1.516439,-0.007183
Br,-1.306622,3.829613,0.023458

Stilbene 11

C,0.3215582484,-1.383421624,0.5303931878
C,-0.6013601451,-1.6967786071,-0.413524724
C,-2.0480544669,-1.7238673613,-0.205879457
C,1.7703615794,-1.4072254053,0.3296678873

C,6.224884,-0.365281,0.342905
H,6.847932,-0.995753,-0.290127
H,6.429927,0.674109,0.081052
H,6.534668,-0.512228,1.377017
Br,-0.636802,1.250497,-0.082891
Br,-1.241064,3.508309,-0.158062

Stilbene 10

C,0.111398,-1.468206,0.563162
C,-0.795513,-1.596408,-0.438599
C,-2.23571,-1.758827,-0.252124
C,1.557198,-1.364861,0.366617
C,2.341356,-0.702854,1.327682
C,2.198433,-1.916136,-0.757352
C,3.570164,-1.778198,-0.942575
C,3.716395,-0.5639,1.169962
C,4.305518,-1.102739,0.028876
C,-3.111938,-1.37857,-1.282049
C,-2.784679,-2.295957,0.925012
C,-4.163852,-2.405782,1.075407
C,-5.040736,-2.011756,0.055246
C,-4.489981,-1.496705,-1.125189
H,-0.242362,-1.418648,1.589035
H,-0.444521,-1.554156,-1.466651
H,1.862051,-0.280983,2.203136
H,1.620383,-2.475215,-1.482234
H,4.074158,-2.198742,-1.800055
H,4.326157,-0.051515,1.899106
H,-2.70618,-0.97331,-2.202264
H,-2.129631,-2.650325,1.71185
H,-4.567458,-2.830271,1.987897
H,-5.147461,-1.193893,-1.932321
N,5.756555,-0.964845,-0.151673
O,6.39328,-0.370148,0.734237
O,6.258068,-1.450664,-1.179569
C,-6.531325,-2.104228,0.23897
H,-6.795101,-2.93713,0.889567
H,-6.927062,-1.192917,0.690413
H,-7.035876,-2.246738,-0.715767
Br,-0.609975,1.509063,-0.010403
Br,-0.797858,3.833651,-0.060044

Stilbene 12

C,0.479873,-1.741664,0.480236
C,-0.479746,-1.741708,-0.480223
C,-1.920421,-1.779391,-0.225277
C,1.920549,-1.77927,0.225288

C,2.6118535427,-1.5650831319,1.4443648755
C,2.3616219504,-1.2577211909,-0.9382658059
C,3.7409796225,-1.3108870086,-1.0945556974
C,3.9945684032,-1.6133864696,1.3051012857
C,4.5642312818,-1.4881899297,0.029507226
C,-2.9018240767,-1.5994825853,-1.3142293656
C,-2.6273271915,-1.8942723811,1.0634192709
C,-4.0104245485,-1.8925870598,1.2151869698
C,-4.863977604,-1.750153909,0.1122007866
C,-4.2846870116,-1.6023186499,-1.1541667981
H,-0.0156584249,-1.1510686701,1.5365410146
H,-0.2603613799,-1.9447226198,-1.4151788276
H,2.1717351429,-1.6644866966,2.4298045041
H,1.7391494062,-1.0817720094,-1.8063503983
H,4.1889014731,-1.1927153241,-2.072729263
H,4.6333439035,-1.742209433,2.1691828084
H,-2.4737150372,-1.4810387903,-2.3033955878
H,-1.9959001384,-2.0479764582,1.9301245527
H,-4.4373260828,-2.0325972534,2.2020424115
H,-4.9234559599,-1.500014223,-2.0241795708
C,5.9893277023,-1.5355044468,-0.1274486943
N,7.1653268582,-1.5764304497,-0.2569160753
C,-6.3576547167,-1.7165685852,0.2905448473
H,-6.6657903866,-2.3349282933,1.1327501793
H,-6.7060900163,-0.7000952331,0.480957102
H,-6.8671012208,-2.0797116586,-0.6010598171
Br,-0.3164903064,1.430385349,-0.604744511
Br,-0.4441454002,3.6914561091,-1.1676143166

Stilbene 13

C,-0.257314,-1.551138,-0.569506
C,-1.143249,-1.795821,0.428851
C,-2.544739,-2.167698,0.233676
C,1.158999,-1.241959,-0.368753
C,1.844363,-0.483738,-1.333156
C,1.863525,-1.679935,0.766343
C,3.201395,-1.344577,0.947104
C,3.184822,-0.151822,-1.164689
C,3.859326,-0.575359,-0.016814
C,-3.480185,-1.876407,1.240733
C,-2.988533,-2.813828,-0.933185
C,-4.336065,-3.125365,-1.099248
C,-5.259851,-2.815878,-0.097648
C,-4.826452,-2.194099,1.075399
H,-0.608599,-1.565037,-1.597497
H,-0.809839,-1.69294,1.458252
H,1.313997,-0.142932,-2.214594
H,1.36616,-2.305629,1.496822
H,3.73636,-1.681711,1.824751
H,3.70092,0.442514,-1.90637
H,-3.146814,-1.385288,2.147861

C,2.80373,-1.247796,1.180067
C,2.454989,-2.337976,-0.948643
C,3.829789,-2.329812,-1.173967
C,4.178836,-1.2467,0.956766
C,4.696606,-1.783884,-0.223877
C,-2.803631,-1.248011,-1.180081
C,-2.454831,-2.338084,0.948674
C,-3.829633,-2.329996,1.173992
C,-4.69648,-1.78416,0.223876
C,-4.178738,-1.24699,-0.956786
H,0.174245,-1.697527,1.522249
H,-0.17412,-1.697582,-1.522236
H,2.402856,-0.821036,2.092436
H,1.793095,-2.799834,-1.671039
H,4.227311,-2.766393,-2.081638
H,4.844786,-0.827158,1.700234
H,5.765029,-1.785889,-0.398125
H,-2.402778,-0.821262,-2.092465
H,-1.792912,-2.799871,1.671092
H,-4.227131,-2.766565,2.081678
H,-5.764903,-1.786225,0.39812
H,-4.84471,-0.82752,-1.700274
Br,-0.000032,1.274446,-0.000003
Br,-0.000143,3.611541,-0.000005

Stilbene 14

C,0.006614,-1.574687,0.581264
C,-0.887678,-1.80577,-0.41272
C,-2.299121,-2.132756,-0.211757
C,1.429212,-1.304499,0.37292
C,2.138788,-0.55509,1.32768
C,2.120676,-1.778708,-0.756361
C,3.465617,-1.482839,-0.952657
C,3.487025,-0.257475,1.158534
C,4.125375,-0.725517,0.012703
C,-3.225126,-1.829226,-1.224048
C,-2.762034,-2.746112,0.965444
C,-4.118317,-3.014101,1.135453
C,-5.032389,-2.692594,0.128663
C,-4.580356,-2.103138,-1.05399
H,-0.342389,-1.565327,1.609951
H,-0.553559,-1.723898,-1.443897
H,1.62091,-0.191035,2.2071
H,1.605477,-2.401667,-1.476548
H,4.008082,-1.842826,-1.814212
H,4.039162,0.322911,1.882614
H,-2.87699,-1.363383,-2.138922

H,-2.272631,-3.093655,-1.6964
H,-4.663678,-3.626224,-2.001549
H,-6.305166,-3.065848,-0.226567
H,-5.535737,-1.956965,1.858198
C,5.318541,-0.285956,0.138915
F,5.674356,0.863622,-0.480607
F,5.672849,-0.172148,1.440698
F,6.081924,-1.272664,-0.391561
Br,-1.408239,1.291798,-0.016926
Br,-1.940465,3.563228,0.024131

Stilbene 15

C,-0.323578,-1.568856,0.538876
C,0.588671,-1.783142,-0.442897
C,2.00013,-2.101759,-0.231377
C,-1.742959,-1.294792,0.319327
C,-2.661063,-1.585115,1.343558
C,-2.231613,-0.748507,-0.881968
C,-3.591927,-0.538397,-1.070104
C,-4.024482,-1.372236,1.173367
C,-4.495103,-0.850048,-0.040608
C,2.706254,-2.762571,-1.250688
C,2.679027,-1.777147,0.956817
C,4.013585,-2.135054,1.127469
C,4.700862,-2.806658,0.112239
C,4.043382,-3.115778,-1.079761
H,-0.012473,-1.675105,1.574123
H,0.249807,-1.78715,-1.475519
H,-2.297945,-1.992654,2.279892
H,-1.540199,-0.466166,-1.665688
H,-3.960458,-0.115135,-1.995558
H,-4.723733,-1.603931,1.966225
H,2.196211,-3.00647,-2.175809
H,2.170085,-1.221369,1.734676
H,4.524709,-1.874363,2.045644
H,4.570676,-3.628471,-1.874223
C,-5.899377,-0.625412,-0.22848
N,-7.058584,-0.442183,-0.383875
H,5.740701,-3.075946,0.246183
Br,0.747525,1.340468,0.018534
Br,1.193099,3.6291,-0.019889

Stilbene 17

C,-0.673216,-1.481388,0.498148
C,0.239735,-1.422215,-0.503847
C,1.687243,-1.343792,-0.315182
C,-2.118445,-1.593167,0.311336

H,-2.055217,-3.035614,1.733525
H,-4.461014,-3.490309,2.04544
H,-6.084773,-2.908659,0.261102
H,-5.282161,-1.857187,-1.840766
N,5.549151,-0.420212,-0.179785
O,6.119551,0.245395,0.700831
O,6.095177,-0.845686,-1.211723
Br,-1.053823,1.310622,0.000088
Br,-1.500152,3.598403,-0.060274

Stilbene 16

C,-0.6832,-1.311392,-0.477622
C,0.221404,-1.251326,0.53145
C,1.672277,-1.196554,0.35578
C,-2.131751,-1.404168,-0.301001
C,-2.911564,-1.955266,-1.332891
C,-2.781017,-0.959612,0.865792
C,-4.155877,-1.09747,1.018825
C,-4.290133,-2.093654,-1.205543
C,-4.887221,-1.66338,-0.023914
C,2.502164,-1.631556,1.403104
C,2.272814,-0.71639,-0.82231
C,3.655704,-0.715171,-0.964544
C,4.462842,-1.166568,0.08447
C,3.887367,-1.626966,1.270671
H,-0.322698,-1.361532,-1.501102
H,-0.133436,-1.314095,1.556419
H,-2.426918,-2.288237,-2.243177
H,-2.209839,-0.483142,1.65227
H,-4.665913,-0.757731,1.907965
H,-4.896564,-2.520431,-1.990458
H,2.052894,-1.986351,2.323356
H,1.656892,-0.321602,-1.620386
H,4.111326,-0.3358,-1.869219
H,4.517609,-1.963453,2.082508
N,-6.341825,-1.80261,0.126451
O,-6.973058,-2.30012,-0.821088
O,-6.84974,-1.415854,1.19241
C,5.947438,-1.220986,-0.095056
F,6.336499,-2.391704,-0.655619
F,6.392491,-0.230163,-0.902608
F,6.602505,-1.110188,1.083871
Br,-0.404168,1.828552,-0.011703
Br,-0.549522,4.152296,-0.037667

Stilbene 18

C,-0.468428,-1.19594,0.519118
C,0.43632,-1.212203,-0.491406
C,1.888463,-1.247814,-0.31848
C,-1.920919,-1.201859,0.345464

C,-2.900388,-2.131703,1.34841
C,-2.762384,-1.180413,-0.870115
C,-4.133701,-1.336625,-1.026478
C,-4.274681,-2.287302,1.208352
C,-4.896314,-1.89227,0.014182
C,2.535173,-1.786944,-1.345521
C,2.269479,-0.837055,0.861727
C,3.649671,-0.811413,1.02565
C,4.451427,-1.27519,-0.015821
C,3.919267,-1.761235,-1.206882
H,-0.320991,-1.514084,1.525367
H,-0.104191,-1.50314,-1.531098
H,-2.419555,-2.440391,2.269324
H,-2.190399,-0.713192,-1.661731
H,-4.623963,-1.014049,-1.935832
H,-4.868059,-2.707839,2.009728
H,2.100897,-2.165723,-2.263288
H,1.639431,-0.440083,1.647426
H,4.108676,-0.422451,1.922401
H,4.578539,-2.104276,-1.990261
C,-6.313799,-2.046599,-0.141731
N,-7.483573,-2.175942,-0.27102
N,5.911113,-1.241413,0.146333
O,6.360586,-0.807926,1.22051
O,6.604387,-1.650182,-0.800253
Br,-0.421294,1.663292,-0.016133
Br,-0.569774,3.986292,-0.027715

Stilbene 19

C,-0.901564,-1.453796,-0.472855
C,0.000223,-1.336963,0.534018
C,1.444302,-1.191325,0.354215
C,-2.340714,-1.638298,-0.293971
C,-3.086398,-2.229761,-1.32864
C,-3.01374,-1.245504,0.877839
C,-4.376129,-1.471517,1.027885
C,-4.451799,-2.455374,-1.195594
C,-5.101342,-2.078832,-0.010494
C,2.303164,-1.575768,1.397867
C,2.009933,-0.672182,-0.824567
C,3.389599,-0.584497,-0.971297
C,4.226669,-0.98676,0.074227
C,3.685003,-1.484546,1.261216
H,-0.540787,-1.480547,-1.497187
H,-0.346883,-1.422856,1.559914
H,-2.583701,-2.524205,-2.242534
H,-2.472202,-0.739596,1.667045
H,-4.888782,-1.164019,1.930093

C,-2.730215,-1.680757,1.389528
C,-2.54332,-0.738503,-0.827843
C,-3.925191,-0.795959,-0.969213
C,-4.114625,-1.734806,1.258687
C,-4.710816,-1.290021,0.07684
C,2.685071,-1.765393,-1.353811
C,2.521401,-0.792212,0.852258
C,3.90164,-0.879451,0.99347
C,4.673877,-1.414153,-0.042577
C,4.068014,-1.849312,-1.223041
H,-0.109605,-1.251231,1.543016
H,0.076071,-1.269517,-1.514729
H,-2.264937,-2.023377,2.306451
H,-1.945737,-0.311298,-1.623118
H,-4.397757,-0.429302,-1.870433
H,-4.728698,-2.104723,2.068375
H,2.211032,-2.111581,-2.264895
H,1.933976,-0.344802,1.644009
H,4.381424,-0.5298,1.897721
H,4.671446,-2.258871,-2.021576
C,-6.19167,-1.407187,-0.101803
F,-6.849946,-1.333766,1.078424
F,-6.68059,-0.430584,-0.901445
F,-6.530952,-2.589411,-0.670888
C,6.164714,-1.432389,0.082422
F,6.558003,-1.620557,1.364165
F,6.721162,-2.416515,-0.661762
F,6.713738,-0.264862,-0.331001
Br,0.020273,1.897572,0.001718
Br,0.047846,4.2271,-0.007431

Stilbene 20

C,0.451282,-1.423102,-0.506407
C,-0.451256,-1.423103,0.506416
C,-1.902326,-1.444715,0.327592
C,1.902352,-1.444704,-0.327584
C,2.728758,-0.899527,-1.326213
C,2.505218,-2.000491,0.815556
C,3.885951,-1.97976,0.980271
C,4.112402,-0.877714,-1.186773
C,4.665704,-1.416356,-0.027694
C,-2.728737,-0.899538,1.326217
C,-2.505188,-2.000514,-0.815545
C,-3.88592,-1.979792,-0.980263
C,-4.665678,-1.416386,0.027696
C,-4.112382,-0.877733,1.186773
H,0.091176,-1.375172,-1.530412
H,-0.091151,-1.375165,1.530421
H,2.277597,-0.476834,-2.216096
H,1.889586,-2.472292,1.570988
H,4.362096,-2.405312,1.851095

H,-5.016747,-2.916203,-1.995366
H,1.879935,-1.959782,2.318746
H,1.367851,-0.314942,-1.619701
H,3.817712,-0.175561,-1.876521
H,4.337647,-1.782687,2.070331
C,-6.509969,-2.305292,0.138415
N,-7.67216,-2.494159,0.26186
C,5.711142,-0.948191,-0.110083
F,6.091043,0.069968,-0.91692
F,6.361982,-0.799065,1.066979
F,6.170592,-2.091322,-0.674353
Br,-0.818904,1.691213,0.004886
Br,-1.106575,4.002356,-0.009979

Stilbene 21

C,0.5413598399,0.4089360165,0.0674233167
C,-0.5414239362,-0.4089713728,0.0674233167
C,-0.4896784253,-1.8695170092,0.0501769532
C,0.489614329,1.8694816529,0.0501769533
C,1.5960435039,2.5854899398,-0.4395912017
C,-0.6283593186,2.5918140329,0.5073699839
C,-0.657004594,3.9789868051,0.4407063804
C,1.5842088772,3.9740977734,-0.5054491954
C,0.45140748,4.6764082275,-0.0674171347
C,-1.5961076002,-2.5855252961,-0.4395912018
C,0.6282952223,-2.5918493892,0.5073699839
C,0.6569404977,-3.9790221614,0.4407063803
C,-0.4514715763,-4.6764435838,-0.0674171348
C,-1.5842729735,-3.9741331297,-0.5054491955
H,1.5316908948,-0.0340126639,0.0102565825
H,-1.5317549911,0.0339773076,0.0102565825
H,2.4695178627,2.0426366071,-0.7815666083
H,-1.4707501253,2.0662394097,0.9389431595
H,-1.5180899625,4.5292778757,0.7971332218
H,2.4382729347,4.5168518877,-0.889033544
H,-2.469581959,-2.0426719634,-0.7815666084
H,1.470686029,-2.066274766,0.9389431595
H,1.5180258662,-4.529313232,0.7971332217
H,-2.438337031,-4.516887244,-0.8890335441
C,0.4276617812,6.1093024656,-0.1291560686
N,0.4074722019,7.2918682362,-0.1820989122
C,-0.4277258775,-6.1093378219,-0.1291560687
N,-0.4075362982,-7.2919035925,-0.1820989124
Br,-0.0000320482,-0.0000176782,3.1831385277
Br,-0.0000320482,-0.0000176782,5.5114676271

Stilbazole 23

C,-0.339114,-1.646418,0.577402
C,0.605324,-1.743043,-0.390918
C,2.034621,-1.943156,-0.145811

H,4.756308,-0.455652,-1.943911
H,-2.277581,-0.476836,2.216098
H,-1.889551,-2.472314,-1.570974
H,-4.362061,-2.405355,-1.851083
H,-4.756291,-0.455666,1.943906
N,6.125977,-1.401608,0.133291
O,6.800567,-0.905158,-0.784413
O,6.594368,-1.885623,1.177464
N,-6.125951,-1.401647,-0.133291
O,-6.594341,-1.885727,-1.177434
O,-6.800541,-0.905137,0.78438
Br,-0.000012,1.681077,-0.000004
Br,-0.00004,4.008842,-0.000003

Stilbazole 22

C,-0.177441,-1.557495,0.663662
C,0.711111,-1.744407,-0.344315
C,2.12417,-2.078871,-0.160017
C,-1.603126,-1.286266,0.498287
C,-2.31029,-0.653262,1.538109
C,-2.312733,-1.647772,-0.656103
C,-3.668859,-1.354989,-0.797211
C,-3.659583,-0.359807,1.413232
C,-4.34797,-0.706352,0.242035
C,2.825021,-2.737613,-1.179709
C,2.846293,-1.763556,1.001104
C,4.182573,-2.141493,1.096657
N,4.856787,-2.787736,0.126422
C,4.165551,-3.068202,-0.99226
H,0.182147,-1.603769,1.688241
H,0.358205,-1.711917,-1.371165
H,-1.785647,-0.373675,2.444628
H,-1.809616,-2.182304,-1.45275
H,-4.181749,-1.655452,-1.699183
H,-4.206921,0.134675,2.20475
H,2.327507,-2.996847,-2.106577
H,2.385736,-1.21459,1.812229
H,4.751311,-1.905469,1.989085
H,4.715422,-3.581944,-1.772927
O,-5.674228,-0.374367,0.222322
C,-6.39921,-0.702733,-0.958543
H,-7.410888,-0.350279,-0.785546
H,-5.980463,-0.201036,-1.832661
H,-6.411556,-1.780597,-1.129947
Br,0.848613,1.321371,-0.066503
Br,1.271667,3.61432,-0.186105

C,-1.775663,-1.500921,0.346899
C,-2.579859,-0.94819,1.356942
C,-2.395605,-1.915141,-0.844456
C,-3.763278,-1.736831,-1.028611
C,-3.94811,-0.776349,1.166086
C,-4.564608,-1.168434,-0.02861
C,2.837566,-2.528339,-1.13456
C,2.672221,-1.567213,1.046248
C,4.032751,-1.818458,1.199871
N,4.806054,-2.393909,0.259511
C,4.193766,-2.732719,-0.888657
H,-0.023086,-1.669169,1.616962
H,0.296024,-1.734343,-1.432136
H,-2.121736,-0.635427,2.288622
H,-1.810681,-2.395122,-1.61967
H,-4.223504,-2.069713,-1.952264
H,-4.547904,-0.34296,1.958466
H,2.407307,-2.828449,-2.082492
H,2.127002,-1.067674,1.83655
H,4.537567,-1.534486,2.116434
H,4.82305,-3.188862,-1.644699
C,-6.036785,-0.949458,-0.249789
H,-6.582593,-0.973809,0.692499
H,-6.22528,0.019671,-0.715813
H,-6.453208,-1.715549,-0.90274
Br,0.437876,1.335331,-0.074482
Br,0.656768,3.657276,-0.150332

Table S5: Cartesian coordinates for the intermediates of the electrophilic bromination of selected stilbenes calculated using different DFT methods within the 6-31G(d,p) basis.

Stilbene 2

M06/6-31G(d,p)

C,-0.6950893592,-0.0185926775,0.6508010768
C,0.398885243,-0.819486177,1.2212197018
C,0.4494878261,-2.225711526,0.7309580071
C,-0.6786378773,1.320617524,0.3163753212
C,-1.8502681338,1.9037735481,-0.2657481799
C,0.4520920509,2.1639944497,0.5448566635
C,0.4248350197,3.4881360737,0.2132010735
C,-1.8833361427,3.2199115251,-0.6110780269
C,-0.7459989935,4.0331924835,-0.3764548017
C,1.5712417047,-2.6516712131,0.0205322007
C,-0.6186270294,-3.1092839133,0.9180639209
C,-0.5594156465,-4.388391378,0.3947596435
C,0.5603096952,-4.8259493003,-0.3246110099
C,1.6207189083,-3.9370812407,-0.5024322489
H,-1.6223202433,-0.5711492187,0.4801294391
H,1.3768182433,-0.3364731123,1.1567078433
H,-2.719501756,1.2722577524,-0.4358229911
H,1.3436464349,1.7555884921,1.0138952922

M06-L/6-31G(d,p)

C,-0.7590196667,-0.0323410612,0.8508985066
C,0.3248061141,-0.8337345813,1.432461981
C,0.4104048973,-2.2015948667,0.8461225784
C,-0.7142783988,1.2893471416,0.4360932298
C,-1.8893663217,1.876179062,-0.136213041
C,0.4506333494,2.1075081759,0.5649899461
C,0.4487064813,3.4129316474,0.1555667713
C,-1.8996140559,3.174431023,-0.5541998336
C,-0.729601992,3.96328502,-0.4135308407
C,1.5458033701,-2.5543305337,0.111261875
C,-0.6458175624,-3.1160705698,0.9566325757
C,-0.5589140808,-4.3546795142,0.3452975379
C,0.5759812134,-4.7209442477,-0.3960731448
C,1.6228945301,-3.7985982828,-0.500665524
H,-1.7017123102,-0.56734888,0.7265588544
H,1.2931718249,-0.3323454417,1.4338221751
H,-2.782187134,1.2655145345,-0.2358072089
H,1.3524002996,1.6958471544,1.0074102589

H,1.2883064628,4.1162122693,0.4045735728
H,-2.7566073909,3.6834371142,-1.0594270388
H,2.4114748061,-1.9748998221,-0.1280588785
H,-1.4819461272,-2.8042643404,1.5089690369
H,-1.390113136,-5.0739372715,0.5517846483
H,2.5008335768,-4.2594737282,-1.0549887808
O,-0.8705802467,5.2870200638,-0.7344075665
C,0.2038062817,6.2154900467,-0.5452093329
H,-0.1625246909,7.1671149818,-0.9266616774
H,0.4439951331,6.3113088866,0.5183592609
H,1.0847901936,5.9031716474,-1.1147318322
C,0.6208178081,-6.2222092586,-0.8580309105
H,-0.3404140477,-6.5305798918,-1.282324498
H,1.387145754,-6.3278924892,-1.6312184781
H,0.8602246739,-6.9334422196,-0.0579735988
Br,-0.1300012487,-0.6773707785,3.1433783908

M06-HF/6-31G(d,p)

C,-0.1801069247,-0.0479036268,0.5814967325
C,0.7594918468,0.4657694889,-0.4573014342
C,2.1427722345,-0.1200721554,-0.3168340426
C,-1.5220352267,-0.2926415252,0.4398984834
C,-2.2510713372,-0.8457656725,1.5549998184
C,-2.242123771,0.0098922671,-0.7683028806
C,-3.5772453071,-0.2338406694,-0.8730505875
C,-3.5786820062,-1.1083314188,1.4604629209
C,-4.2622789482,-0.8082574145,0.2430200645
C,2.5420326725,-1.0893470829,-1.2332094163
C,2.9867682643,0.2287672051,0.7402437088
C,4.216173706,-0.3993894083,0.8726972237
C,4.6314582002,-1.3785398189,-0.038493064
C,3.7791139498,-1.7125159185,-1.0898779826
H,0.2853741287,-0.2358244951,1.5451773184
H,0.3865471501,0.3644391882,-1.469515419
H,-1.7160292959,-1.0613890628,2.4716499621
H,-1.7241833936,0.4718900666,-1.5984649586
H,-4.111766436,0.0110119345,-1.7786498522
H,-4.1559167078,-1.5319910448,2.2700234712
H,1.8962894597,-1.3624116681,-2.0596365271
H,2.6964596051,1.0106442984,1.4325623434
H,4.8725493803,-0.1195953749,1.6876250021
H,4.0838809037,-2.4621433909,-1.8091280785
O,-5.5294200799,-1.0844963481,0.2339569058
C,-6.3554328812,-0.8361512436,-0.9178450586
H,-7.3442099664,-1.1717197354,-0.6281931678
H,-6.3629543888,0.2306096332,-1.1366580823
H,-5.986589877,-1.4167881892,-1.7620462713
C,5.9945732176,-2.0278901378,0.1050226204
H,6.1897496049,-2.2740580902,1.1485668988
H,6.0527846872,-2.9383415601,-0.4890034602
H,6.7681938219,-1.3383977492,-0.2370951566

H,1.3384720694,4.0208334915,0.2676587701
H,-2.7783554645,3.6341144923,-0.9916137069
H,2.3723642927,-1.8533500918,0.0197841942
H,-1.5156427744,-2.8645444141,1.5604560551
H,-1.3772891556,-5.0623974868,0.4480903546
H,2.5127455889,-4.0644322788,-1.0647220871
O,-0.8334222161,5.2051384561,-0.8403122492
C,0.2922216632,6.0950312753,-0.7399970883
H,-0.0526498945,7.038889884,-1.1534969916
H,0.5807835486,6.2283546011,0.3053517821
H,1.1323058558,5.7150850941,-1.3262820736
C,0.6691914133,-6.0719283925,-1.0272321584
H,-0.2777520811,-6.3693289327,-1.4852844073
H,1.4482056572,-6.1123270616,-1.7908756791
H,0.9078605487,-6.8349399996,-0.2781253721
Br,-0.2692818625,-0.8238871154,3.3453592025

B3LYP/6-31G(d,p)

C,-0.7811252802,-0.0202413779,0.8750275602
C,0.2975723599,-0.8513342867,1.4449210795
C,0.3869681568,-2.2220293527,0.8504306179
C,-0.7221675211,1.3023716803,0.4618809614
C,-1.9090762757,1.9091720989,-0.0811017588
C,0.4618436592,2.1088538497,0.5499171569
C,0.4668248701,3.4142028903,0.1338257853
C,-1.9128439223,3.2081123208,-0.5022964574
C,-0.7243807505,3.9847164476,-0.4004798736
C,1.5576708624,-2.5848705106,0.1711018307
C,-0.6820523476,-3.1321002583,0.9015855387
C,-0.5755992737,-4.3689214752,0.2806824432
C,0.5924092319,-4.741491504,-0.4081695552
C,1.6536122952,-3.8272603029,-0.4504308755
H,-1.7311367012,-0.5365212043,0.755517238
H,1.2672211411,-0.3609374365,1.4755299753
H,-2.8144930942,1.3143896005,-0.1530471418
H,1.3730067466,1.6873906733,0.9589678877
H,1.3701002219,4.0053944547,0.2130660351
H,-2.7980593162,3.6791428421,-0.9138226495
H,2.3974486496,-1.896475242,0.1254999919
H,-1.5790611978,-2.8870804371,1.4633468804
H,-1.4061468989,-5.0666158145,0.3374293139
H,2.5687914087,-4.0932282302,-0.970923098
O,-0.8251192419,5.2266271939,-0.8273802081
C,0.3001860368,6.1329410121,-0.779360462
H,-0.0747626911,7.068892224,-1.1877591998
H,0.626520028,6.2789323421,0.2533493108
H,1.1185871406,5.7557245998,-1.3976483782
C,0.7055597051,-6.0994020621,-1.0510308252
H,-0.2315687806,-6.3916340751,-1.5336988095
H,1.5011828638,-6.1255401799,-1.799308228
H,0.9337540439,-6.8644157499,-0.2991205914

Br,0.6829987144,2.3907917191,-0.0364580347

Br,-0.3176183821,-0.8533974295,3.3828837469

B97-D/6-31G(d,p)

C,-0.7178447429,-0.0154831938,0.7328850144
C,0.4106965724,-0.8347381456,1.2072207164
C,0.4560261044,-2.2358616512,0.7156657546
C,-0.6998311529,1.3378651008,0.3840584071
C,-1.9144823797,1.9413162368,-0.1066192195
C,0.47149037,2.1652809438,0.4970459997
C,0.4401260887,3.4974355914,0.1429926648
C,-1.9548847491,3.2668624032,-0.4702333367
C,-0.7769157853,4.0670524366,-0.3502362064
C,1.6514157566,-2.7118702545,0.1388405982
C,-0.6736439867,-3.084755155,0.7680466609
C,-0.6043996331,-4.3724322192,0.2408036542
C,0.5862941547,-4.8554640831,-0.3523614471
C,1.7088750276,-4.0038616851,-0.3934119325
H,-1.6614185423,-0.552812654,0.617774392
H,1.3853425547,-0.3427694459,1.1685744937
H,-2.8100865618,1.3252878495,-0.1899526948
H,1.3973016916,1.7448380992,0.8851503071
H,1.332874959,4.1095893086,0.2425234366
H,-2.862788004,3.735054327,-0.8459428424
H,2.5307495358,-2.0666394934,0.1014337667
H,-1.5848408379,-2.7447206705,1.2620750036
H,-1.4763718791,-5.0253572765,0.2937026766
H,2.6356792915,-4.3622619869,-0.8422081348
O,-0.9150738659,5.3343763523,-0.7200877609
C,0.2137932671,6.2506272833,-0.6365183696
H,-0.1741190754,7.2071429636,-0.9966959681
H,0.5485573434,6.3374144078,0.4064110504
H,1.030878264,5.8976274729,-1.2807959314
C,0.6541221677,-6.2626755022,-0.894621411
H,-0.2645562117,-6.521551851,-1.4407103646
H,1.5140793176,-6.3949541892,-1.5642565849
H,0.7553522484,-6.9856734956,-0.0686045293
Br,-0.1383495607,-0.6905205229,3.2274373791

Stilbene 7

M06/6-31G(d,p)

C,-0.5412365679,-0.0943016191,0.5036981651
C,0.4512543674,0.3788650241,-0.4662267332
C,1.8332863016,-0.1319738981,-0.2746748636
C,-1.8837188777,-0.3799337114,0.28000235
C,-2.6545509875,-0.8808820718,1.3663248919
C,-2.5188247755,-0.1964029123,-0.9822619836
C,-3.8429538531,-0.5088098453,-1.1347709087
C,-3.979008685,-1.2012230831,1.1954324131
C,-4.598113015,-1.0196168853,-0.0540346275
C,2.4395745518,-0.8308857189,-1.3181967987
C,2.5186272055,0.0248623584,0.9353694848

M06-L/6-31G(d,p)

C,-0.3276258002,0.6286148353,0.7681841004
C,0.274152039,-0.622024993,1.2341966959
C,-0.3562346711,-1.8673136641,0.7349522405
C,0.3243717477,1.81030237,0.4118928835
C,-0.4610864904,2.9013902532,-0.0585016407
C,1.7376682868,1.9748653236,0.493135241
C,2.3165329477,3.1608122063,0.1182219282
C,0.1337939006,4.0817545521,-0.4382548392
C,1.5318589154,4.2377434841,-0.3590409757
C,0.4351849141,-2.8007356782,0.0597138875
C,-1.7307636181,-2.1059982632,0.8745532355

C,3.7795954216,-0.5204433883,1.0918262185
C,4.3956511352,-1.2319015674,0.0531604283
C,3.7053214268,-1.3763727867,-1.1504215122
H,-0.1555450595,-0.2443467021,1.5153264644
H,0.1263599804,0.3136237689,-1.5069434206
H,-2.1756116766,-1.0159386637,2.3339694009
H,-1.9595838939,0.210501578,-1.8208687129
H,-4.3323728482,-0.364689039,-2.0951461159
H,-4.560790487,-1.5936386031,2.0253316515
H,1.9191743173,-0.9537844917,-2.2668152217
H,2.0787461928,0.6101139633,1.7426220722
H,4.311641757,-0.3876566749,2.0319773241
H,4.1692328076,-1.9204773511,-1.9703327874
C,-6.0363485168,-1.3354364017,-0.2475131877
H,-6.4552721591,-1.8987458773,0.5892213176
H,-6.6105922188,-0.4044908563,-0.3499659208
H,-6.1951865039,-1.8983845019,-1.1740615067
C,5.7700561984,-1.7933679563,0.2333431289
H,6.521314587,-0.9944367413,0.2161807813
H,5.8692481011,-2.3029850109,1.1977405149
H,6.0252967996,-2.5039114955,-0.5576853233
Br,0.2388729746,2.3116831622,0.0377320173

M06-HF/6-31G(d,p)

C,-0.514751,0.079478,0.520744
C,0.514751,0.079478,-0.520743
C,1.920083,-0.231098,-0.28885
C,-1.920083,-0.231098,0.28885
C,-2.650043,-0.731225,1.372004
C,-2.537101,-0.087317,-0.966831
C,-3.854033,-0.466978,-1.12384
C,-3.972684,-1.120661,1.196519
C,-4.590312,-0.99645,-0.047677
C,2.650042,-0.731227,-1.372003
C,2.537101,-0.087314,0.96683
C,3.854034,-0.466975,1.12384
C,4.590312,-0.99645,0.047678
C,3.972684,-1.120663,-1.196517
H,-0.156363,-0.037067,1.537337
H,0.156363,-0.037068,-1.537337
H,-2.183882,-0.828383,2.34516
H,-2.006304,0.354926,-1.801769
H,-4.335525,-0.349616,-2.086659
H,-4.528836,-1.517925,2.035309
H,2.183881,-0.828386,-2.345159
H,2.006305,0.354931,1.801767
H,4.335526,-0.349611,2.086658
H,4.528836,-1.517929,-2.035307
C,-6.031719,-1.410164,-0.257131
H,-6.476355,-1.756367,0.673371
H,-6.608234,-0.564028,-0.633247

C,-2.2940394941,-3.2513851585,0.3413057409
C,-1.5110945389,-4.1931491713,-0.3470563406
C,-0.1404166923,-3.9455153451,-0.4760800616
H,-1.4141382565,0.6040586828,0.6695032556
H,1.3623627898,-0.6489935201,1.177184262
H,-1.540113291,2.7859430713,-0.1155128501
H,2.3594739006,1.1677767754,0.8680023548
H,3.392977823,3.2855165279,0.1885298916
H,-0.4722247786,4.9073066236,-0.7981734477
H,1.5033466355,-2.6289034393,-0.0500209087
H,-2.3464625212,-1.4102663657,1.4419739641
H,-3.358135049,-3.4340410994,0.4651201711
H,0.4839985118,-4.6644951588,-0.9991006647
C,2.1836090309,5.5025714592,-0.7808993336
H,1.4720896574,6.3215730239,-0.889971981
H,2.9698770282,5.8005728215,-0.081962795
H,2.6780995489,5.3625702727,-1.7502690485
C,-2.1289945831,-5.436722148,-0.8977944512
H,-3.067600478,-5.2234464823,-1.4164249405
H,-1.462146199,-5.9501517839,-1.5926579165
H,-2.3698236309,-6.1404322247,-0.0936148752
Br,-0.140888306,-0.2273420878,3.1782524599

B3LYP/6-31G(d,p)

C,-0.3804131241,0.6713697463,0.7655517355
C,0.1715027151,-0.5922836705,1.2753326128
C,-0.4332704798,-1.8496134901,0.7616565145
C,0.3108662608,1.8350538295,0.4120969002
C,-0.4449202394,2.9393794193,-0.089779932
C,1.7305848401,1.9741753052,0.5119284045
C,2.3398185753,3.1452898,0.1279904353
C,0.1811635248,4.1053905677,-0.4747596304
C,1.5831438955,4.2341734996,-0.3750455578
C,0.4150619505,-2.8217768477,0.213366096
C,-1.8208767019,-2.0760583873,0.7625058757
C,-2.3369349399,-3.2412047109,0.2147068378
C,-1.4953877731,-4.2182908605,-0.3485449761
C,-0.1136753532,-3.9857251366,-0.3380315897
H,-1.4578800232,0.6709280823,0.617187407
H,1.2567340135,-0.6330646193,1.3091776293
H,-1.524551407,2.849379709,-0.1652151812
H,2.3339094401,1.1610050284,0.8993917731
H,3.4173929105,3.2458580159,0.2106016151
H,-0.4041367508,4.9361579528,-0.8546908009
H,1.4908285673,-2.667971431,0.2111613011
H,-2.4926728524,-1.3612796907,1.2297873488
H,-3.4101035394,-3.4076230091,0.2303554609
H,0.5573293131,-4.7268953676,-0.7614329332
C,2.2737436628,5.4899302376,-0.8068560578
H,1.5755256732,6.317802827,-0.9405055444
H,3.0448118558,5.78360731,-0.0878006968

H,-6.079809,-2.213729,-0.993676
C,6.031719,-1.410164,0.257132
H,6.608232,-0.564034,0.633263
H,6.079806,-2.213741,0.993666
H,6.476359,-1.756355,-0.673372
Br,-0.000000164,2.097067,-0.000001

H,2.7844303311,5.3212850609,-1.7645406615
C,-2.0697318154,-5.4900148709,-0.9155868782
H,-2.35695069,-6.1760183507,-0.1097324594
H,-2.9696738064,-5.2919676856,-1.5053587163
H,-1.3488594643,-6.0094644837,-1.5508952494
Br,-0.3691992903,-0.1490780799,3.2153641594

B97-D/6-31G(d,p)

C,-0.3355921251,0.6735103389,0.7821030979
C,0.2786261766,-0.6527178103,0.8258601742
C,-0.3761012396,-1.882186218,0.4795910907
C,0.3459166247,1.8930989514,0.4529949727
C,-0.4475658453,3.0354329345,0.1504267957
C,1.7648294612,2.0089321316,0.3984209286
C,2.3512804687,3.2136197937,0.0367691237
C,0.1523752064,4.2356529959,-0.2176026004
C,1.5602191343,4.3485689944,-0.2831354654
C,0.4375205966,-3.0319495994,0.2742803174
C,-1.7863735195,-2.001207003,0.3162648321
C,-2.3437480301,-3.2166210697,-0.0553417789
C,-1.531158702,-4.3595119089,-0.2783345844
C,-0.1327915503,-4.2430998479,-0.1048796217
H,-1.4230253868,0.7014903562,0.7022019016
H,1.368938792,-0.6817600044,0.833149147
H,-1.5345432318,2.9605799672,0.2050816086
H,2.3995521062,1.1633954591,0.6600055083
H,3.4375976612,3.2979303028,0.0021994771
H,-0.4643050777,5.1027934989,-0.4530823315
H,1.5168455915,-2.9542736124,0.4126058865
H,-2.4388330662,-1.1491271738,0.5019745826
H,-3.4240158978,-3.3031632961,-0.1733252782
H,0.499590638,-5.1160327956,-0.2653749187
C,2.2167603442,5.6379238571,-0.6972324898
H,1.5255487451,6.4870226144,-0.6228404498
H,3.1078079911,5.8417875395,-0.0862024854
H,2.5544550778,5.5666866651,-1.7450612816
C,-2.1543495173,-5.6611698409,-0.7052754727
H,-3.0912094317,-5.8481329715,-0.1610124458
H,-2.4079480938,-5.62095598,-1.7781819023
H,-1.4721807564,-6.5069328436,-0.5516295837
Br,-0.1165138654,0.042871274,3.0239684875

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M06/6-31G(d,p)

C,-0.5178558148,-0.445009119,0.929650307
C,0.5566737787,0.4398211712,0.4767034098
C,0.4794308296,1.806960692,0.1883314127
C,-0.4783466834,-1.8533166579,0.4596177182
C,-1.6014574136,-2.3585005953,-0.196831075
C,0.6585161007,-2.6529843164,0.6151776958

M06-L/6-31G(d,p)

C,-0.535358002,-0.4491988116,0.8735435598
C,0.5622837665,0.4438688832,0.5030581754
C,0.4902508687,1.8187800859,0.2102574335
C,-0.4945447231,-1.8557028715,0.4278062058
C,-1.6480142635,-2.404244155,-0.1425129843
C,0.6721055435,-2.6263056174,0.5234881746

C,0.6705371305,-3.9405674328,0.103043735
C,-1.5831847247,-3.6492203746,-0.7110610524
C,-0.4481515725,-4.4378383738,-0.5639723026
C,1.6493926163,2.4453156808,-0.3025131909
C,-0.7137997455,2.5621396441,0.3463792091
C,-0.7271758737,3.8961104618,0.0126890891
C,0.4359993751,4.5011333532,-0.4849436668
C,1.6220029049,3.7805471656,-0.6438052266
H,-1.5180992311,-0.0104800799,0.8758313959
H,1.5211018497,-0.052100396,0.3259574089
H,-2.4909814417,-1.7409375585,-0.3091873739
H,1.5180929917,-2.2838566583,1.1738805695
H,1.5495464323,-4.5653735437,0.2328359907
H,-2.4587162009,-4.0397313522,-1.2215391019
H,-0.4352825527,-5.4490518383,-0.9610029123
H,2.5625510638,1.8643397066,-0.4132904415
H,-1.609715225,2.0949968906,0.7471073184
H,-1.6323352168,4.4827750487,0.1342457111
H,0.4136517779,5.5556164399,-0.7489369155
H,2.5114953409,4.2699287115,-1.0274522325
Br,0.0688615043,-0.2207746692,2.8420845206

M06-HF/6-31G(d,p)

C,-0.5771130315,-0.4504459597,0.6149824518
C,0.5773128314,0.4504417381,0.6149811216
C,0.5049492519,1.8785816267,0.3032313352
C,-0.5047474912,-1.8785864114,0.3032321856
C,-1.6503219951,-2.4634277873,-0.2473437996
C,0.6629064227,-2.6354333373,0.4915957753
C,0.6810462509,-3.9628893795,0.1026812981
C,-1.6196961527,-3.7954794829,-0.6462473578
C,-0.4572312898,-4.5395651926,-0.4727266025
C,1.6505284531,2.4634242455,-0.2473341021
C,-0.6627066875,2.6354280337,0.4915855495
C,-0.6808435816,3.9628844549,0.1026725382
C,0.4574389363,4.5395613357,-0.4727246166
C,1.6199056874,3.7954763499,-0.6462362055
H,-1.5445640024,0.0236499544,0.4911724129
H,1.5447636056,-0.0236553997,0.4911737484
H,-2.5536454517,-1.8795474685,-0.3756475986
H,1.5330365129,-2.2065213832,0.9748435263
H,1.5722079381,-4.5566394055,0.2515706743
H,-2.4989690397,-4.2483117347,-1.0826365569
H,-0.4341018874,-5.5778728754,-0.7755634799
H,2.5538531548,1.8795442702,-0.3756306951
H,-1.5328411385,2.2065152267,0.9748245882
H,-1.5720068051,4.5566340141,0.2515545218
H,0.4343117544,5.5778693732,-0.7755604797
H,2.499182157,4.2483095662,-1.0826171894
Br,0.0000975978,-0.000023714,2.6191669566

C,0.6846886859,-3.9241110976,0.0363773241
C,-1.6278384646,-3.7044265386,-0.6356083843
C,-0.4635518647,-4.4620983903,-0.548567576
C,1.6763581818,2.4656566656,-0.2272228431
C,-0.7146371762,2.5645690431,0.3036141198
C,-0.7244363183,3.8988981068,-0.0413908431
C,0.4551345606,4.5152099425,-0.4853399906
C,1.6530392038,3.800817146,-0.5798337856
H,-1.5293781096,-0.0049953314,0.8293545442
H,1.5293182973,-0.0443944328,0.3742082437
H,-2.5566936027,-1.8106778305,-0.2060167795
H,1.5529554129,-2.2237601801,1.0202990444
H,1.5846436785,-4.5241177607,0.1205285799
H,-2.5229135791,-4.1259935356,-1.0804795841
H,-0.4503142153,-5.4793103446,-0.9264494441
H,2.5981555109,1.8937387451,-0.2895000559
H,-1.6248090027,2.0925103213,0.6607419322
H,-1.6405123811,4.4744594996,0.0308159228
H,0.436637456,5.5665947293,-0.756455595
H,2.5560609752,4.293010558,-0.9228927138
Br,0.0841215614,-0.1888348287,2.807177319

B3LYP/6-31G(d,p)

C,-0.5602307169,-0.4677617306,0.6361818854
C,0.5604419804,0.4677594014,0.6361459285
C,0.4937115536,1.865764923,0.2895273611
C,-0.4935045962,-1.8657722172,0.2895472427
C,-1.7172509035,-2.5355344695,0.0597724421
C,0.7215172106,-2.5740730991,0.1391212214
C,0.7032060711,-3.9065708917,-0.240901297
C,-1.7271257113,-3.8693428346,-0.3255270922
C,-0.5180898773,-4.5547706104,-0.4746413445
C,1.7174582119,2.5355373027,0.0597675892
C,-0.7213145222,2.5740623794,0.1390970867
C,-0.7030065371,3.9065628593,-0.2409123096
C,0.5182894259,4.55477055,-0.4746352459
C,1.7273290505,3.8693483632,-0.3255184505
H,-1.550177545,-0.0243929878,0.5990122616
H,1.5503882916,0.024388956,0.5989806498
H,-2.6537754603,-1.9988064492,0.1814703792
H,1.6747574413,-2.091524855,0.3275510056
H,1.6352956607,-4.4490094115,-0.3563890458
H,-2.66884523,-4.3756366907,-0.5070748008
H,-0.5231374985,-5.5986024423,-0.7721527716
H,2.653983905,1.9988120251,0.1814681408
H,-1.6745535034,2.0915054946,0.3275097794
H,-1.6350972322,4.4489984322,-0.3564044337
H,0.5233340191,5.5986053325,-0.7721366621
H,2.669046647,4.3756499783,-0.5070541346
Br,0.0001018654,-0.0000253081,2.7671946148

B97-D/6-31G(d,p)

C,-0.5676907998,-0.4626128636,0.6269249937
C,0.5678907344,0.4626086261,0.6269139947
C,0.5002780813,1.862124054,0.287893995
C,-0.5000764599,-1.8621295934,0.2879005349
C,-1.7237013592,-2.5228920417,-0.012012706
C,0.7225750523,-2.5861892601,0.2157635148
C,0.7140726129,-3.9246967251,-0.1671536775
C,-1.7224025163,-3.8622467665,-0.4026903864
C,-0.5051241962,-4.5628504619,-0.4802424349
C,1.723905841,2.5228879102,-0.0120086874
C,-0.7223732846,2.5861850366,0.2157501887
C,-0.7138674108,3.9246935235,-0.1671622352
C,0.5053322777,4.5628478358,-0.4802396093
C,1.722610227,3.8622436616,-0.4026814263
H,-1.5588853246,-0.0099863524,0.5715750015
H,1.5590846225,0.0099800844,0.5715681205
H,-2.6617201153,-1.9703563868,0.0564573834
H,1.6653792016,-2.1091761872,0.4800727779
H,1.6486271762,-4.4813969041,-0.2206108584
H,-2.6596582665,-4.3626548031,-0.641627629
H,-0.5025982859,-5.6110268355,-0.7791521346
H,2.6619237439,1.9703514696,0.0564662894
H,-1.6651798629,2.1091713481,0.4800490567
H,-1.6484212126,4.4813944088,-0.2206250101
H,0.5028088241,5.6110252679,-0.7791456891
H,2.6598676113,4.362652584,-0.641610302
Br,0.0000950885,-0.0000086291,2.8086269352

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M06/6-31G(d,p)

C,-0.5164252789,-0.9220059314,1.1007409222
C,0.5121862515,0.0164671558,0.6452150509
C,0.3667234679,1.3826885145,0.3688947433
C,-0.4046618093,-2.3321867763,0.6338104796
C,-1.4891163877,-2.8818257427,-0.051754789
C,0.7619479385,-3.0796548931,0.8251141776
C,0.8512088007,-4.3649581055,0.3179113314
C,-1.4086886117,-4.1694982836,-0.564939669
C,-0.2371089571,-4.8813623386,-0.3724048558
C,1.4999156334,2.0798487843,-0.1289967282
C,-0.8590326886,2.0764078558,0.5421591326
C,-0.9454604179,3.410940746,0.2161926545
C,0.1814245789,4.069696429,-0.2882430496
C,1.4023928794,3.4115525755,-0.4628121558
H,-1.5382383243,-0.5409415577,1.0483187022
H,1.498181272,-0.4266399122,0.4818821231
H,-2.4010477431,-2.3047608457,-0.1900092299
H,1.5890355939,-2.6741222796,1.4057516365
H,1.7363854952,-4.9784422475,0.4515080492
H,-2.2314167494,-4.6286100091,-1.1033580825

M06-L/6-31G(d,p)

C,-0.5235160801,-0.9282691646,1.0771245898
C,0.5223907603,0.0194853733,0.6844828031
C,0.3772104624,1.3897853967,0.3974969865
C,-0.4144302187,-2.3331582045,0.6158681602
C,-1.5304616077,-2.917401305,0.0078930093
C,0.7814129012,-3.0541432148,0.7365423431
C,0.8684578342,-4.3429195731,0.2369086609
C,-1.4513934497,-4.2084338785,-0.4997679655
C,-0.2514363593,-4.8932530931,-0.3782600358
C,1.5254616362,2.0987612891,-0.0485523638
C,-0.8633482266,2.0719908753,0.4996260093
C,-0.949081451,3.4037169322,0.15445116
C,0.1935916912,4.077964403,-0.2973965516
C,1.4298531857,3.4280625079,-0.3999381276
H,-1.5401495324,-0.5378945042,1.0401876675
H,1.5113149206,-0.4191078301,0.5423267052
H,-2.4611889873,-2.3628467405,-0.074481729
H,1.631510552,-2.6218417882,1.259893282
H,1.7729068648,-4.934153259,0.3182022008
H,-2.2946663651,-4.6917038738,-0.9789623464

H,2.4410194679,1.5485569582,-0.2525151131
H,-1.7285869801,1.5672326484,0.9495067671
H,-1.8737122498,3.9578959852,0.346379995
H,2.2578061666,3.955927879,-0.853410552
N,-0.1429642493,-6.2537024018,-0.9178230613
O,-1.1161739741,-6.677694795,-1.5111904391
O,0.901928
7663,-6.8482854584,-0.7323355277
C,0.1201955195,5.5345694792,-0.6656336833
F,-1.0809434254,6.0496895142,-0.4424133631
F,1.0187970932,6.2121947014,0.0416348739
F,0.4149830233,5.6697993821,-1.9549068748
Br,0.0757093985,-0.6675410301,2.997111777

M06-HF/6-31G(d,p)

C,-0.8599560487,0.395461518,-0.5704110747
C,0.1299276084,0.4056827236,0.5095811852
C,1.5549881924,0.1276030541,0.3345672551
C,-2.2802851168,0.0456717844,-0.3543648164
C,-2.9142763625,-0.6616936147,-1.378547453
C,-2.9531569691,0.3543009497,0.8366174806
C,-4.2584016416,-0.0714702609,1.0135104146
C,-4.2237795527,-1.1015064255,-1.2065619558
C,-4.8515937133,-0.7946739949,-0.0143506189
C,2.2358858408,-0.3737525669,1.4480642426
C,2.2128080042,0.2961040484,-0.8967778015
C,3.54182851,-0.0623406625,-1.0075457142
C,4.2064771812,-0.5852387492,0.1070807416
C,3.5725405263,-0.7450068463,1.3295949799
H,-0.4733706358,0.2354856446,-1.5707645998
H,-0.2687175901,0.3011771312,1.513489841
H,-2.3941955836,-0.8824296055,-2.3020865764
H,-2.4835410251,0.9572526021,1.6047517959
H,-4.8238720993,0.1458151426,1.9087932721
H,-4.7531190244,-1.6596613335,-1.9661998673
H,1.7272231192,-0.4887397217,2.3972603798
H,1.7064964735,0.736366135,-1.7474654881
H,4.0718676998,0.0584900911,-1.9432639704
H,4.1125862224,-1.1500467838,2.1741675584
N,-6.2429503272,-1.2513624645,0.1759913567
O,-6.7399671796,-1.8703912874,-0.7295747052
O,-6.7676663863,-0.9689285628,1.2231178558
C,5.6749568929,-0.9349312507,-0.038355671
F,5.8820792879,-1.6087728099,-1.1729470802
F,6.4118719794,0.1774611654,-0.0815696262
F,6.096546347,-1.6804724336,0.984299257
Br,-0.4257686296,2.3846073843,-0.0997015973

B97-D/6-31G(d,p)

C,-0.5816610311,-0.9299951686,0.9860642015
C,0.508221696,0.0283531998,0.7433668648

H,2.4768161036,1.5792087841,-0.1195056301
H,-1.7473639991,1.5560625442,0.8612192132
H,-1.8897196065,3.937212491,0.227093932
H,2.2986006324,3.97435121,-0.752064384
N,-0.1604178403,-6.2700444186,-0.9161246505
O,-1.1680147104,-6.7250222107,-1.4440424757
O,0.9165726952,-6.8416054538,-0.7920018984
C,0.1269330925,5.5407133443,-0.6771908423
F,-1.119275179,6.016247163,-0.6018605719
F,0.9097873785,6.2544816857,0.1435311218
F,0.5758036962,5.7047109389,-1.9289291058
Br,0.1021027062,-0.6597204265,2.9856160756

B3LYP/6-31G(d,p)

C,-0.4546270752,-0.9340123646,1.132334406
C,0.5687796933,0.0260798351,0.6938499696
C,0.4020059903,1.3919143376,0.3869793258
C,-0.3698923848,-2.3417435503,0.6500643328
C,-1.5223122924,-2.9092705411,0.0864860107
C,0.8227882182,-3.0829110109,0.7043486236
C,0.8688004324,-4.3692048108,0.1828357999
C,-1.4846372923,-4.1974539601,-0.4419668832
C,-0.2871191343,-4.9005482519,-0.3870280929
C,1.5453329147,2.1076613204,-0.0733279481
C,-0.8488968309,2.0700069523,0.477819
C,-0.9417774,3.3982434645,0.1174525013
C,0.2016939414,4.0811793736,-0.3375743754
C,1.4422607702,3.4383315368,-0.4373594994
H,-1.4709140704,-0.5503775536,1.1474754925
H,1.5578448749,-0.3978027173,0.5351323677
H,-2.4511202813,-2.3477205225,0.0533860085
H,1.7047858573,-2.6761532077,1.1897274446
H,1.7701144698,-4.9683948621,0.215630467
H,-2.357613374,-4.6598272496,-0.8853978594
H,2.5015499358,1.5981260247,-0.1431820622
H,-1.7332219653,1.5536979756,0.8335077436
H,-1.8900462421,3.9202141072,0.1750603803
H,2.306074734,3.9832787068,-0.7991178548
N,-0.2384089327,-6.272593113,-0.9475918596
O,-1.2747488282,-6.7125225161,-1.4332625743
O,0.8359274676,-6.8608996128,-0.8849481677
C,0.0855911865,5.559816992,-0.6764190424
F,-1.0957665338,5.8186099058,-1.2584559499
F,0.1683463012,6.2830459785,0.4525024555
F,1.067110015,5.9461092935,-1.5035475032
Br,0.2283593352,-0.6836439603,3.053972585

C,0.3801177995,1.4092916378,0.4421754384
C,-0.4384291823,-2.3389958128,0.5601490205
C,-1.5621658532,-2.9703109076,-0.0168844564
C,0.7842989516,-3.0400503818,0.6788947257
C,0.8903262817,-4.346442882,0.2034973094
C,-1.4625494859,-4.2785967734,-0.5019944164
C,-0.2359066807,-4.9413364258,-0.3864324886
C,1.569496812,2.1246936396,0.0982419425
C,-0.8753194744,2.0956515509,0.4386905014
C,-0.9293643333,3.4354451713,0.0872842572
C,0.2581664075,4.1200235429,-0.2675808179
C,1.5053024631,3.4669703955,-0.2631608128
H,-1.5935604337,-0.5343225395,0.8771428909
H,1.5090594672,-0.4042607951,0.6800503758
H,-2.5093325434,-2.4357016034,-0.0952054583
H,1.6361435926,-2.5804265747,1.1802776144
H,1.8143632843,-4.9137697797,0.2858008981
H,-2.3092689198,-4.7871329896,-0.9569385505
H,2.5283735532,1.6058880257,0.111799049
H,-1.7885581057,1.5794564425,0.7288368595
H,-1.8762050751,3.9720828312,0.0887272624
H,2.4051657267,4.0149101773,-0.5333028577
N,-0.1213084788,-6.3477371881,-0.9038611278
O,-1.1366163386,-6.8470959402,-1.390401709
O,0.980517235,-6.8898165386,-0.8029749862
C,0.1428928657,5.5815670817,-0.7001640714
F,-0.6569607559,6.2604400485,0.1545566945
F,1.3455701105,6.1917673251,-0.7436850369
F,-0.4140145597,5.6304610522,-1.9342090218
Br,-0.110531495,-0.6197738204,3.0306251476

Stilbene 18

M06/6-31G(d,p)

C,0.5189522524,-0.4858521098,1.1180805155
C,-0.4921251645,0.4745494351,0.6750427057
C,-0.3164713689,1.8364757327,0.3813153304
C,0.3676771524,-1.8976398907,0.6813278858
C,1.4439468336,-2.5037025675,0.0357496981
C,-0.829915213,-2.6002856366,0.8581711238
C,-0.9478357833,-3.8889688221,0.3720004897
C,1.3229881621,-3.7990615018,-0.45484643
C,0.1281016376,-4.4833626541,-0.2892829531
C,-1.435664293,2.5527843887,-0.1169234828
C,0.9257576091,2.5019432793,0.5355313844
C,1.0417976419,3.8300013736,0.1904553139
C,-0.0721831171,4.5088939257,-0.3144969287
C,-1.3090820446,3.8774863266,-0.4705605135
H,1.5491713381,-0.1294555176,1.0582165161
H,-1.4896285407,0.0542259275,0.5229252839
H,2.380666417,-1.9645835104,-0.0915848852
H,-1.655934037,-2.1549564167,1.4110331999

M06-L/6-31G(d,p)

C,0.5232894519,-0.4922047512,1.0578644005
C,-0.506918323,0.4842425619,0.703549272
C,-0.3287199743,1.8516607987,0.4021224796
C,0.3699345936,-1.8987050084,0.6377470835
C,1.4791651429,-2.5501594068,0.0921013832
C,-0.8567564621,-2.5714546566,0.7373881728
C,-0.9702019616,-3.8705548726,0.2771392473
C,1.3620766651,-3.8548233394,-0.3752476563
C,0.1396398912,-4.5104215834,-0.2844026238
C,-1.4656966686,2.5899251626,-0.0184267667
C,0.9321447077,2.4965381657,0.4659819065
C,1.0480968692,3.8233867122,0.1083027741
C,-0.0849591595,4.5286500816,-0.3174669099
C,-1.3409773381,3.9142701836,-0.3822753173
H,1.5488551265,-0.127958511,1.0063655139
H,-1.5101060434,0.0742223812,0.5803101768
H,2.4346596455,-2.036626205,0.0258317798
H,-1.7089336787,-2.0928370896,1.2153777262

H,-1.8692408236,-4.4492778027,0.5095117978
H,2.1562736945,-4.2763694385,-0.9607895254
H,-2.3901769495,2.0427086094,-0.2261470059
H,1.7857891491,1.9774812039,0.9437455299
H,1.9841119011,4.3556748897,0.3064071061
H,-2.1545204644,4.4362451818,-0.8625901392
C,-0.0529304933,-5.8833794371,-0.8115023244
F,1.0515224222,-6.3435476979,-1.3926335006
F,-0.3837269116,-6.7119218061,0.1796427877
F,-1.0423186254,-5.9153613122,-1.7069635533
C,0.020187766,5.9664736189,-0.7107775081
F,1.2366825617,6.4549551398,-0.5098715129
F,-0.288514446,6.095411398,-1.9978243396
F,-0.8515005656,6.6759535481,-0.0003573051
Br,-0.0676463133,-0.1713592918,3.0173804811

M06-HF/6-31G(d,p)

C,-0.4932253706,0.4736468264,0.5433822845
C,0.4907967378,0.4673729964,-0.5412868161
C,1.9136549432,0.1527264493,-0.353756838
C,-1.9173402666,0.1640319984,0.3592195454
C,-2.5756683627,-0.4236371867,1.4409864872
C,-2.5870768561,0.3911675147,-0.8550411188
C,-3.906274125,0.002734061,-0.9819960071
C,-3.9031175042,-0.8255195037,1.3056915327
C,-4.5489798328,-0.609961599,0.0993429666
C,2.5683647992,-0.4529054341,-1.4281664689
C,2.5840218058,0.3892622557,0.8578572083
C,3.9007724692,-0.0069710597,0.9906591253
C,4.5403433347,-0.6344631905,-0.0833264935
C,3.8928830796,-0.8610735542,-1.2873581252
H,-0.0950149389,0.3460365521,1.5442473853
H,0.0923866383,0.3326020496,-1.5411359748
H,-2.0594005813,-0.5808450711,2.3798813683
H,-2.0991201918,0.9031728288,-1.6759606383
H,-4.4476570456,0.1764289058,-1.9029755076
H,-4.4271749278,-1.2916925472,2.1283393453
H,2.0506707307,-0.6202544334,-2.3645107568
H,2.098302808,0.9118060488,1.6734705772
H,4.4402971056,0.1663378798,1.9126239058
H,4.4128863527,-1.3452013326,-2.1023168077
C,-5.993276975,-1.0303392996,-0.0852993507
F,-6.4997984656,-1.5397636125,1.0388156999
F,-6.7370716911,0.017413481,-0.4507344637
F,-6.0871480964,-1.9516461598,-1.0484462932
C,5.9944576589,-1.0265167348,0.0865058654
F,6.1708846764,-1.6685819633,1.2450877616
F,6.4014274319,-1.8197961556,-0.9061231793
F,6.7687591313,0.061556411,0.1010920191
Br,0.0033815281,2.4597605792,-0.0078092385

H,-1.9120963595,-4.4032784689,0.3609179879
H,2.2180699182,-4.3656962411,-0.8010489348
H,-2.4336233209,2.0985463291,-0.0604340591
H,1.8102507962,1.9573374366,0.8075482951
H,2.0061690249,4.3282627715,0.1514188686
H,-2.2029725108,4.4825625575,-0.7156814428
C,-0.0269417414,-5.9213590251,-0.7840973794
F,1.1361227532,-6.4502034217,-1.1873567262
F,-0.5355824482,-6.7062504607,0.1805340964
F,-0.8841833203,-5.9528883066,-1.8199522599
C,0.0145331119,5.9874404014,-0.7025153606
F,1.28064214,6.4156496088,-0.7002141699
F,-0.499729311,6.1734751554,-1.9260343896
F,-0.6906316906,6.7307864678,0.1621344114
Br,-0.0804081418,-0.1493568627,2.9819036629

B3LYP/6-31G(d,p)

C,0.5528835782,-0.4975315985,1.0628004655
C,-0.4903340898,0.4982041764,0.7977799128
C,-0.3197530213,1.864798936,0.4648261628
C,0.3732308468,-1.9061190336,0.6472314054
C,1.4733983075,-2.562469158,0.0750804106
C,-0.8529961165,-2.5830971203,0.7704707449
C,-0.9775405295,-3.8842893892,0.3051122347
C,1.3446717426,-3.8661113427,-0.3973489505
C,0.1194116649,-4.5231285104,-0.2867103951
C,-1.4875767477,2.6152916373,0.156522695
C,0.9510920376,2.4998398405,0.3878086998
C,1.040114229,3.8234948186,0.0057436356
C,-0.1278615046,4.5410018264,-0.3084746034
C,-1.3900895829,3.9407292352,-0.2318076002
H,1.5743128265,-0.1416176193,0.9647569242
H,-1.5040672527,0.1078725727,0.7562803136
H,2.4301528021,-2.055247929,-0.0082383352
H,-1.6976512209,-2.114871165,1.26706039
H,-1.9164347234,-4.4154454503,0.4125006924
H,2.1940037491,-4.3741168758,-0.8389991206
H,-2.4617074009,2.1403606377,0.2228740277
H,1.8569386116,1.9585255632,0.636285315
H,2.0034438858,4.3175489062,-0.0474958751
H,-2.2777133546,4.5156246189,-0.4676608012
C,-0.0460511468,-5.9212593399,-0.8442761951
F,1.1286628379,-6.5740702,-0.8881808885
F,-0.9029984673,-6.641637467,-0.0973376437
F,-0.5381024095,-5.8711641361,-2.0978694653
C,-0.0009157519,5.9790765674,-0.7847726927
F,0.9932988084,6.6068623807,-0.1365943696
F,0.2787651667,5.9935863766,-2.0993569478
F,-1.1397920877,6.6588038525,-0.5858761575
Br,0.0814156971,-0.1472670461,3.0672512535

B97-D/6-31G(d,p)

C,0.525177187,-0.501473533,0.8440059328
C,-0.5439725788,0.5009054857,0.8086568057
C,-0.3655959801,1.8933084971,0.4699240077
C,0.3617024194,-1.8984736203,0.5115168596
C,1.5328977419,-2.6390107248,0.2008491428
C,-0.9062792876,-2.5394082425,0.4564458973
C,-0.9932267458,-3.8733100913,0.0759905104
C,1.4398532945,-3.9749549204,-0.1905841902
C,0.1783257091,-4.5902927506,-0.2526352191
C,-1.5218076575,2.6300416582,0.099334754
C,0.9045095954,2.5338796735,0.4624706391
C,1.007670103,3.863126794,0.0721120678
C,-0.148963718,4.5764543167,-0.3147628331
C,-1.4120658191,3.9625987023,-0.3003367077
H,1.5462822559,-0.1198462648,0.7929579104
H,-1.5617509561,0.1177827501,0.7178063621
H,2.5083466822,-2.1548463798,0.2579744057
H,-1.8122163043,-2.0044164938,0.7375315081
H,-1.9577351252,-4.3761620068,0.0402812423
H,2.3336907009,-4.5432597358,-0.4380129306
H,-2.4985187913,2.1453422423,0.1162782711
H,1.7978613884,2.0009272405,0.7845196704
H,1.974739515,4.3625451616,0.0610527762
H,-2.2934155649,4.5262936284,-0.5976261207
C,0.0399518403,-6.0337369095,-0.7267337446
F,1.2131329494,-6.7017811708,-0.6571385046
F,-0.875866761,-6.6965158226,0.0199642402
F,-0.3824184537,-6.0439074612,-2.0156846991
C,0.0094643655,6.0435592253,-0.7016848042
F,1.016481096,6.1850154389,-1.5982085865
F,-1.1197454681,6.5518364945,-1.2425233012
F,0.3238540419,6.7701238101,0.3989811256
Br,-0.0561502902,0.0098335741,2.9866627544

Table S6: Comparison of key bond distances (in Å) and angles (in °) from the optimised geometries of selected stilbenes obtained using MP2 and different DFT methods, all within the 6-31G(d,p) basis.

Compound	Functional	Intermediate Type	$r_{\text{CB}r1}/\text{Å}$	$r_{\text{CB}r2}/\text{Å}$	$r_{\text{CC}1}/\text{Å}$	$r_{\text{CC}2}/\text{Å}$	$r_{\text{CC}3}/\text{Å}$	$\theta/^\circ$
2	MP2	Carbocation	1.97751	2.73138	1.47510	1.50048	1.38181	103.622
	M06	Carbocation	1.99865	2.63937	1.47091	1.4901	1.38043	97.899
	M06-L	Carbocation	2.00305	2.66426	1.46803	1.49069	1.38597	99.014
	M06-2X	Carbocation	1.97866	2.66312	1.48034	1.50123	1.37710	99.687
	M06-HF	Carbocation	1.97197	2.65971	1.49191	1.50878	1.37139	99.386
	B3LYP	Carbocation	2.03326	2.68297	1.47917	1.49673	1.38689	98.479
	B97-D	Carbocation	2.09846	2.64845	1.47302	1.48554	1.39770	94.090
7	MP2	Carbocation	2.00510	2.60963	1.46924	1.49162	1.39331	96.343
	M06	Carbocation	2.00870	2.57186	1.46618	1.48582	1.39064	94.186
	M06-L	Carbocation	2.02667	2.56436	1.46404	1.48236	1.39586	93.141
	M06-2X	Carbocation	1.99742	2.54192	1.47316	1.49361	1.39306	92.936
	M06-HF	Bromonium Ion	2.14635	2.14635	1.46443	1.45780	1.45780	70.053
	B3LYP	Carbocation	2.06016	2.58357	1.47014	1.48677	1.39891	92.467
	B97-D	Bromonium Ion	2.33916	2.33916	1.46221	1.43533	1.43533	71.787
12	MP2	Carbocation	2.02486	2.46531	1.46390	1.48435	1.40521	88.402
	M06	Carbocation	2.01294	2.50387	1.4638	1.4852	1.39936	90.727
	M06-L	Carbocation	2.04707	2.43678	1.46275	1.47601	1.40759	86.245
	M06-2X	Bromonium Ion	2.1406	2.1406	1.46156	1.45363	1.45362	70.039
	M06-HF	Bromonium Ion	2.13374	2.13374	1.46434	1.46356	1.46356	69.932
	B3LYP	Carbocation	2.08803	2.47328	1.46672	1.47987	1.41103	86.312
	B97-D	Bromonium Ion	2.30135	2.30135	1.46478	1.44158	1.44158	71.444
16	MP2	Open Bromonium Ion	2.0433	2.34276	1.46169	1.47849	1.41812	82.080
	M06	Carbocation	2.0029	2.48793	1.46502	1.48967	1.40145	90.312
	M06L	Carbocation	2.02629	2.43581	1.46503	1.48269	1.40754	86.92
	M06-2X	Open Bromonium Ion	2.05408	2.21155	1.46402	1.47758	1.43934	75.837
	M06HF	Open Bromonium Ion	2.08968	2.14387	1.46505	1.47864	1.46245	71.755
	B3LYP	Carbocation	2.05471	2.48793	1.47017	1.49046	1.40978	88.165
	B97-D	Carbocation	2.12095	2.45652	1.47145	1.47892	1.41920	84.215
18	MP2	Bromonium Ion	2.14633	2.14633	1.45924	1.45068	1.45068	70.127
	M06	Carbocation	2.01255	2.46656	1.46319	1.48552	1.40427	88.956
	M06L	Carbocation	2.04546	2.40297	1.46298	1.47589	1.41154	84.727
	M06-2X	Bromonium Ion	2.12506	2.12577	1.46217	1.45804	1.45817	69.855
	M06HF	Bromonium Ion	2.11938	2.12016	1.46453	1.46925	1.46897	69.820
	B3LYP	Carbocation	2.08873	2.42776	1.46630	1.47956	1.41688	84.202

	B97-D	Bromonium Ion	2.27824	2.28535	1.46598	1.44530	1.44407	71.526
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Table S7: The type of intermediates observed for the electrophilic bromination of stilbenes 1 – 21 grouped according to the magnitude of the angle θ calculated at the M06-2X/6-31G(d,p) level of theory.

Group	Compound	X ₁	X ₂	Intermediate Observed	$\theta / ^\circ$
1	1	OCH ₃	OCH ₃	Carbocation	105.831
	2	OCH ₃	CH ₃		99.687
	3	OCH ₃	H		99.527
	4	OCH ₃	CF ₃		100.079
	5	OCH ₃	NO ₂		100.486
	6	OCH ₃	CN		100.212
2	7	CH ₃	CH ₃	Carbocation	92.936
	8	CH ₃	H		94.072
	9	CH ₃	CF ₃		95.545
	10	CH ₃	NO ₂		96.340
	11	CH ₃	CN		96.089
3	12	H	H	Bromonium Ion	70.039
	13	H	CF ₃	Carbocation	80.912
	14	H	NO ₂		88.345
	15	H	CN		84.019
4	16	CF ₃	NO ₂	Open Bromonium Ion	75.837
	17	CN	NO ₂		75.061
5	18	CF ₃	CF ₃	Bromonium Ion	69.855
	19	CF ₃	CN		71.899
	20	NO ₂	NO ₂		69.759
	21	CN	CN		69.879

Table S8: The Cartesian coordinates of the bromonium ion intermediates of stilbenes **1**, **7** and **12** with C_2 symmetry imposed during the MP2/6-31G(d,p) geometry optimisations.

Stilbene 1

C,-0.511084,0.517423,0.199089
C,0.511084,-0.517423,0.199089
C,0.297489,-1.887693,-0.149944
C,-0.297489,1.887693,-0.149944
C,-1.438582,2.686342,-0.402933
C,-1.303256,4.00758,-0.773537
C,-0.020736,4.585583,-0.861784
C,1.124669,3.807511,-0.590472
C,0.98121,2.47912,-0.22725
C,-0.98121,-2.47912,-0.22725
C,-1.124669,-3.807511,-0.590472
C,0.020736,-4.585583,-0.861784
C,1.303256,-4.00758,-0.773537
C,1.438582,-2.686342,-0.402933
H,1.537184,-0.170547,0.139609
H,-1.537184,0.170547,0.139609
H,-2.426832,2.247582,-0.329564
H,-2.161763,4.630044,-0.984997
H,2.113232,4.238103,-0.644745
H,1.872623,1.908361,0.000773
H,2.426832,-2.247582,-0.329564
H,2.161763,-4.630044,-0.984997
H,-2.113232,-4.238103,-0.644745
H,-1.872623,-1.908361,0.000773
O,0,-5.878141,-1.217587
C,-1.274009,-6.536246,-1.325448
H,-1.789154,-6.534702,-0.365812
H,-1.04002,-7.552527,-1.619004
H,-1.888341,-6.059886,-2.088353
O,0,5.878141,-1.217587
C,1.274009,6.536246,-1.325448
H,1.04002,7.552527,-1.619004
H,1.789154,6.534702,-0.365812
H,1.888341,6.059886,-2.088353
Br,0,0,2.310084

Stilbene 7

C,-0.5767365674,0.4449831946,0.8381641857
C,0.5767365674,-0.4449831946,0.8381641857
C,0.5271944624,-1.8470857078,0.5051898423
C,-0.5271944624,1.8470857078,0.5051898423
C,-1.7198793469,2.445871343,0.0568385155
C,-1.7189070021,3.7747211675,-0.3503417174
C,-0.5502859329,4.5466689664,-0.2850750132
C,0.6293724075,3.9438276907,0.1922386983
C,0.6515897778,2.6155730078,0.5878933462
C,1.7198793469,-2.445871343,0.0568385155
C,1.7189070021,-3.7747211675,-0.3503417174
C,0.5502859329,-4.5466689664,-0.2850750132
C,-0.6293724075,-3.9438276907,0.1922386983
C,-0.6515897778,-2.6155730078,0.5878933462
H,-1.5432704688,-0.037902495,0.7323671284
H,1.5432704688,0.037902495,0.7323671284
H,2.6322056119,-1.8625034004,0.0091307765
H,2.6373853401,-4.2251278144,-0.7052701047
H,-1.5334600918,-4.535781941,0.2656559594
H,-1.5641976653,-2.1947356175,0.9925871419
H,-2.6322056119,1.8625034004,0.0091307765
H,-2.6373853401,4.2251278144,-0.7052701047
H,1.5334600918,4.535781941,0.2656559594
H,1.5641976653,2.1947356175,0.9925871419
C,0.5412790004,-5.9761812523,-0.7432770034
H,1.5388206223,-6.4084552609,-0.7027705399
H,0.1881422197,-6.0411811309,-1.773605249
H,-0.1225499795,-6.5795253589,-0.126579806
C,-0.5412790004,5.9761812523,-0.7432770034
H,-1.5388206223,6.4084552609,-0.7027705399
H,0.1225499795,6.5795253589,-0.126579806
H,-0.1881422197,6.0411811309,-1.773605249
Br,0,0,2.8927076763

Stilbene 12

C,-0.5304210002,-0.073038,0.5000609998
C,0.5304209993,-0.0730380067,-0.5000609998
C,1.912167,-0.404543,-0.225593
C,-1.9121670051,-0.4045429758,0.225593
C,2.485608,-0.280717,1.055391
C,3.79738,-0.68908,1.25653
C,4.542862,-1.219903,0.194774
C,3.980798,-1.330505,-1.078821
C,2.671608,-0.910276,-1.297308
C,-2.6716080115,-0.9102759662,1.297308

C,-3.9807980168,-1.3305049497,1.078821
C,-4.5428620154,-1.2199029426,-0.194774
C,-3.7973800087,-0.689079952,-1.25653
C,-2.4856080035,-0.2807169686,-1.055391
H,-0.204527,-0.188417,1.529397
H,0.2045269976,-0.1884170026,-1.529397
H,1.932241,0.167778,1.871667
H,4.247003,-0.590487,2.235302
H,5.563658,-1.537222,0.362412
H,4.562114,-1.732115,-1.897539
H,2.2297,-0.988814,-2.283688
H,-1.9322409979,0.1677780244,-1.871667
H,-4.2470030075,-0.5904869463,-2.235302
H,-5.5636580194,-1.5372219297,-0.362412
H,-4.5621140219,-1.7321149424,1.897539
H,-2.2297000125,-0.9888139718,2.283688
Br,0.000000124,1.961008,0.

Table S9: Cartesian coordinates for the optimised geometries of the cationic intermediates of the electrophilic bromination of stilbazoles **22** and **23** using the PCM method for the inclusion of solvent effects (all in tetrahydrofuran).

Stilbazole 22

MP2/6-31G(d,p)

C,-0.7896076665,-0.4974889287,0.800570782
C,0.2943346339,-1.3448744482,1.3517653009
C,0.4582780611,-2.5863755936,0.5189106009
C,-0.7148257943,0.8328558041,0.4646233631
C,-1.8850434553,1.4523345076,-0.1053687284
C,0.4734970974,1.6248535261,0.6364471958
C,0.4963048282,2.9408111198,0.2646125219
C,-1.8637398647,2.7620518763,-0.4835042814
C,-0.6718708573,3.5234631951,-0.3109970663
C,1.5526927701,-2.6833227889,-0.3441661932
C,-0.4833501521,-3.6197321351,0.5182342316
C,-0.2845143378,-4.6995802106,-0.339550713
N,0.7652950419,-4.8109273566,-1.176297857
C,1.661757788,-3.8081127325,-1.162211871
H,-1.73306916,-1.0111215513,0.6357738312
H,1.2408724387,-0.8248228618,1.4628515308
H,-2.7820428638,0.8592911029,-0.2311345295
H,1.3599267136,1.1908484374,1.0773027784
H,1.3931504899,3.5244225622,0.4024040408
H,-2.7230400536,3.252207826,-0.9179575349
H,2.3082361916,-1.908673485,-0.3806157104
H,-1.3337612577,-3.6039435864,1.1868818075
H,-0.9959256348,-5.5165389405,-0.3565821326
H,2.5056132824,-3.9114024408,-1.8339358069
O,-0.7506402472,4.7704454299,-0.7131917102
C,0.402974761,5.6479250966,-0.5855544531
H,0.0679711098,6.5921940662,-0.9937158482
H,0.6668578112,5.7552101726,0.4625676615
H,1.2312950794,5.2512980172,-1.1654101738
Br,-0.2894417607,-1.764109482,3.1966342055

Stilbazole 23

MP2/6-31G(d,p)

C,-0.3669262522,0.5165396814,0.7679359498
C,-0.6211394037,-0.8446597122,1.2854574748
C,-1.7151733861,-1.5185682138,0.5067202314
C,0.8570022856,1.0684010014,0.4333117159
C,0.8547496001,2.4120743965,-0.0622712586
C,2.0961723558,0.3600833866,0.5476358633
C,3.264450252,0.9885892291,0.1863325732
C,2.0389627639,3.0158970908,-0.4228023638
C,3.2588832563,2.3180621895,-0.3045167024
C,-1.374925259,-2.5329896666,-0.3919122973
C,-3.0531003794,-1.1224196626,0.5922031814
C,-3.9868087964,-1.7608688749,-0.2215657081
N,-3.67819558,-2.7413269638,-1.0919755596

M06-2X/6-31G(d,p)

C,-0.6909779159,-0.4730672726,0.5598355252
C,0.3998536073,-1.3037164977,1.136548447
C,0.5010495121,-2.6482656565,0.4603215285
C,-0.6513959299,0.8654375082,0.2811036061
C,-1.8270567967,1.4837536165,-0.2839995355
C,0.4977409965,1.6940483466,0.5411836211
C,0.480778684,3.0266019433,0.2659718601
C,-1.8504537469,2.809852205,-0.5694288908
C,-0.6981588523,3.6039643383,-0.2952477626
C,1.5669747038,-2.8956751203,-0.3993269651
C,-0.4730210238,-3.6333938057,0.6147308889
C,-0.3347932216,-4.81617681,-0.1026217041
N,0.6823374039,-5.0670193175,-0.9330273788
C,1.6095222037,-4.118181564,-1.0675804483
H,-1.6154326534,-1.0115578756,0.3535531565
H,1.3647855329,-0.8031292627,1.1534013179
H,-2.6964786053,0.8644403267,-0.4798362008
H,1.390699729,1.2604375299,0.9764790944
H,1.3483315521,3.638816996,0.4729857745
H,-2.7171147725,3.3001122325,-0.9953449535
H,2.3519146128,-2.1622562975,-0.5522994238
H,-1.307099041,-3.498146292,1.2955842879
H,-1.0781172858,-5.6019404542,0.0007472454
H,2.4337793942,-4.3381249704,-1.7407494283
O,-0.8111875751,4.8673443359,-0.5900286956
C,0.2751226244,5.7803615656,-0.3496144745
H,-0.0909253611,6.7484922275,-0.6786643246
H,0.5095078222,5.8060755379,0.7156642212
H,1.1464172486,5.4853556552,-0.9362264271
Br,-0.1384178536,-1.4752569706,3.0252712806

M06-2X/6-31G(d,p)

C,-0.355072762,0.5080718414,0.6760373589
C,-0.6106962106,-0.8499170539,1.2146060032
C,-1.737025733,-1.539424319,0.4856401712
C,0.8682903617,1.0723565229,0.3828928826
C,0.8774808686,2.4098018803,-0.1302626987
C,2.1168022092,0.3891658043,0.5597550545
C,3.2869169178,1.0185038472,0.2375338276
C,2.0614334091,3.0230041166,-0.4522631433
C,3.2821364834,2.3413611415,-0.2735484597
C,-1.4212625945,-2.5254781969,-0.4449979617
C,-3.0726750787,-1.1809018973,0.6534538512
C,-4.0296949923,-1.8285011955,-0.120816942
N,-3.7425461329,-2.7768092062,-1.0173655356

C,-2.3864967356,-3.1103371212,-1.1599032937	C,-2.4598818047,-3.1112984942,-1.1657817655
H,-1.2543081865,1.1319658252,0.6415754516	H,-1.2505481718,1.1056608052,0.5049841847
H,0.2663907246,-1.4663725235,1.3435136193	H,0.2745112981,-1.4785926794,1.2627286891
H,-0.0869016823,2.9397076535,-0.1477616284	H,-0.0674651161,2.9273204785,-0.2622379805
H,2.1227025697,-0.6530120647,0.9235160012	H,2.1399311383,-0.6205759909,0.9534666556
H,4.2075728096,0.4653305754,0.2724630673	H,4.2359782793,0.5105931092,0.3706779749
H,2.0398290494,4.0293586181,-0.7998364502	H,2.0674080857,4.0336439096,-0.8438271265
H,-0.3524161083,-2.8743078096,-0.4927403806	H,-0.395498607,-2.8373946875,-0.611893322
H,-3.370414623,-0.3615084471,1.292906313	H,-3.368712671,-0.4355762875,1.3839377249
H,-5.031498635,-1.4783318639,-0.1725814373	H,-5.0795878689,-1.572356351,-0.0086242629
H,-2.1517676695,-3.9046591609,-1.8582571362	H,-2.2424866869,-3.8874955432,-1.8944555917
C,4.5512641329,2.9667289075,-0.6742026046	C,4.5786237964,2.9966741644,-0.6085146017
H,4.3986804798,3.9540963188,-1.1004287535	H,4.4391988405,3.992027083,-1.0279352311
H,5.1801559369,3.0577237457,0.2130629588	H,5.193426713,3.070941787,0.294994291
H,5.0911681763,2.3458650807,-1.3894889594	H,5.1364060207,2.377961245,-1.3184691264
Br,-1.1370730889,-0.4848114564,3.1629953748	Br,-1.0645513844,-0.4165156742,3.0796703219