

## **SUPPLEMENTARY INFORMATION FILE**

# New trans-stilbene derivatives with large two-photon absorption cross-section and non-linear optical susceptibility values - A theoretical investigation

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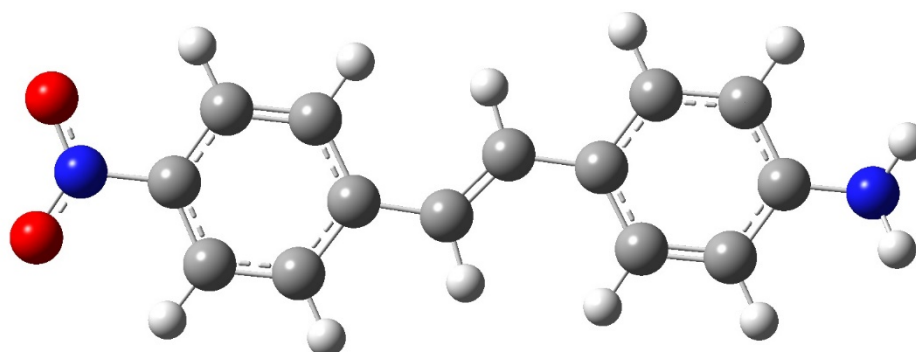
Optimized geometry and corresponding Cartesian co-ordinates of the systems studied.

Comparison of previously reported geometries with optimized geometries in present study.

Representation of (a) TSB and (b) TSBD-2 geometries.

Scatter diagram of spatial overlap and TPA values.

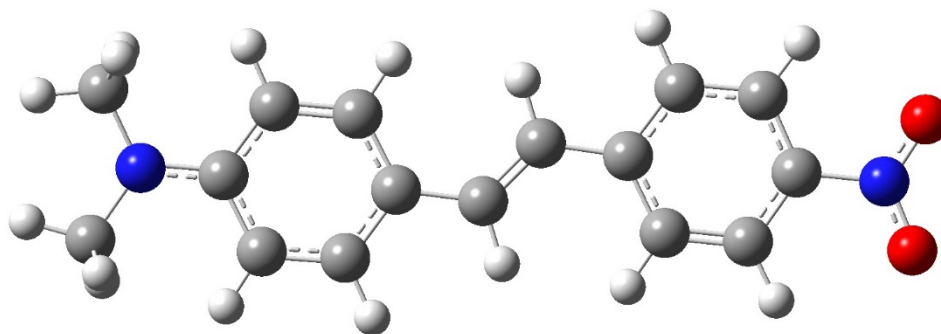
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C	-2.035209000	-1.422948000	-0.008865000
C	-3.416244000	-1.285568000	-0.007824000
C	-3.963561000	-0.003006000	0.000826000
C	2.673841000	0.225543000	-0.004840000
C	3.521048000	1.351226000	-0.013742000
C	3.295674000	-1.040912000	0.005157000
C	4.903440000	1.232649000	-0.012169000
C	0.266036000	-0.525061000	-0.003006000
C	1.230464000	0.424090000	-0.004126000
C	4.674267000	-1.172632000	0.006293000
C	5.508948000	-0.036399000	-0.002344000
H	-3.609780000	2.114193000	0.015189000
H	-1.150944000	1.868011000	0.013989000
H	-1.601483000	-2.419446000	-0.015772000

H	-4.073810000	-2.146148000	-0.013569000
H	0.559426000	-1.573418000	-0.004358000
H	0.927353000	1.470489000	-0.006015000
H	3.078024000	2.344649000	-0.019511000
H	2.689414000	-1.941925000	0.015157000
H	5.525710000	2.124559000	-0.023030000
H	5.122803000	-2.163590000	0.009654000
N	-5.416763000	0.156338000	0.002473000
N	6.890336000	-0.171425000	-0.056831000
O	-6.108259000	-0.864991000	-0.003839000
O	-5.870186000	1.303448000	0.010357000
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H	7.264985000	-1.048383000	0.281171000

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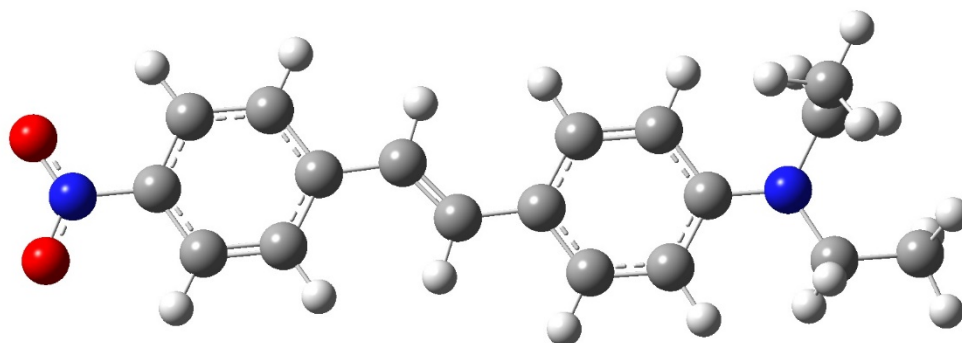


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C	2.896779000	1.418875000	-0.014490000

C	4.278615000	1.293121000	-0.009130000
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C	-1.797140000	-0.269457000	-0.017142000
C	-2.639295000	-1.397892000	-0.024238000
C	-2.433703000	0.988672000	-0.010664000
C	-4.021956000	-1.294523000	-0.027552000
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C	-3.812187000	1.113399000	-0.014160000
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H	4.500633000	-2.104743000	0.024529000
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H	4.928912000	2.159272000	-0.015485000
H	0.300627000	1.547551000	-0.017710000
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H	-6.701083000	-1.650296000	0.977023000
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H	-6.342876000	2.057146000	-0.769542000
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H	-6.390401000	1.911796000	1.002236000
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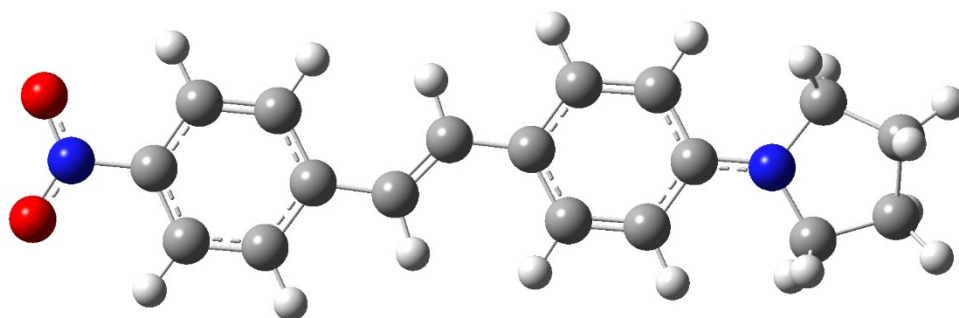


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C	-3.666685000	1.368550000	-0.318831000
C	-5.048833000	1.254400000	-0.272963000
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C	1.664211000	0.917171000	-0.268435000
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C	-1.376296000	0.459178000	-0.146974000
C	-0.423689000	-0.489425000	0.013899000
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C	3.887434000	-0.106335000	-0.182123000
C	6.068779000	-1.218250000	-0.063554000
C	5.916417000	1.298032000	-0.137219000
H	-5.281301000	-2.054826000	0.495677000
H	-2.820189000	-1.849602000	0.416826000
H	-3.221256000	2.333124000	-0.547823000
H	-5.696208000	2.102485000	-0.459197000
H	-1.069196000	1.482302000	-0.356633000
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H	1.409042000	-2.408374000	0.298057000
H	1.074805000	1.821391000	-0.391617000
H	3.817304000	-2.246292000	0.216994000
H	3.465426000	2.009295000	-0.490683000
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H	5.987795000	-1.548998000	0.986006000
H	5.404603000	2.022472000	-0.776829000
H	6.926371000	1.224149000	-0.543311000
N	-7.065375000	-0.122291000	0.072545000
N	5.270774000	-0.007121000	-0.293941000
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H	4.96686000	1.90567600	1.73239600
H	6.54265600	1.12590000	1.94756400
H	6.45610900	2.79226500	1.34873400
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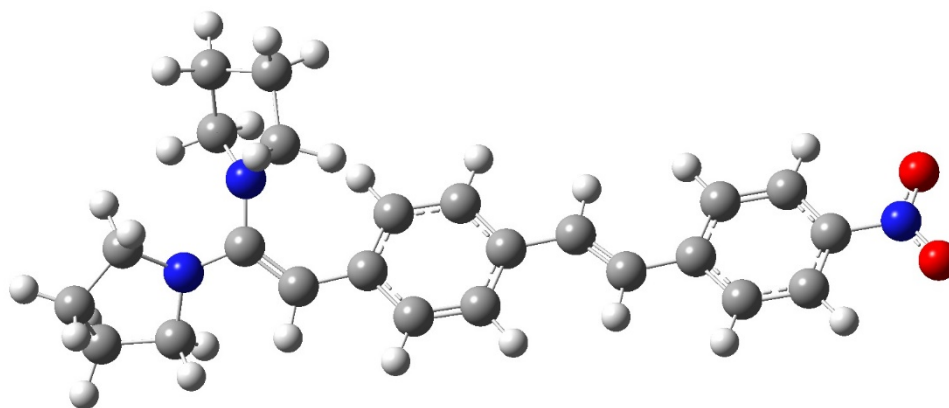
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C	-2.80797800	-0.29033800	0.00765100
C	-3.65109500	-1.42336200	0.04518200
C	-5.03362600	-1.30704000	0.04406400
C	-5.60161600	-0.03346900	0.00475400
C	1.03055800	0.30065400	-0.01908100
C	1.86129400	1.43774300	-0.06877900
C	1.67858800	-0.95166700	0.03470500
C	3.24431600	1.34815500	-0.06684400
C	-1.36390000	-0.49099100	0.01096000

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C	6.154410000	1.131929000	0.061978000
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H	1.089582000	-1.863311000	0.079843000
H	3.833804000	2.256687000	-0.119893000
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H	5.578222000	-1.935155000	-0.851445000
H	5.870392000	-1.842971000	0.894236000
N	-7.055781000	0.103697000	0.003042000
N	5.253270000	-0.018514000	-0.004708000
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O	-7.527493000	1.243327000	-0.031843000
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H	7.660813000	0.394413000	1.437091000
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TSBD-5

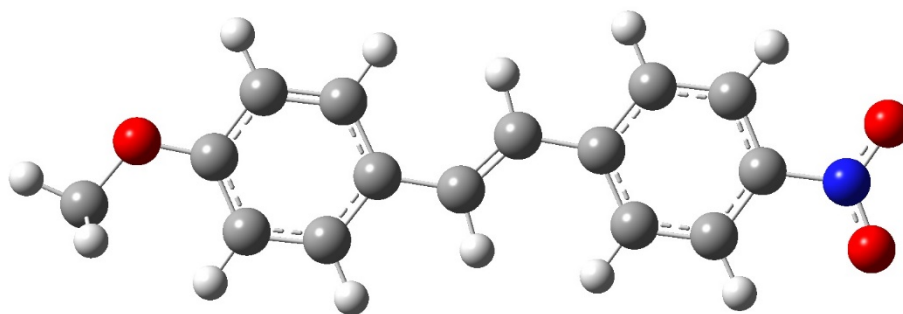


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C	7.565065000	0.012956000	-0.069954000
C	0.933391000	-0.302449000	-0.061195000
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C	0.407877000	-1.472223000	0.531200000
C	-1.366955000	0.411297000	-0.495815000
C	3.389026000	-0.767331000	0.268069000
C	2.353994000	-0.016631000	-0.180197000
C	-0.956046000	-1.686997000	0.607856000

C	-1.899078000	-0.752625000	0.107644000
H	7.051430000	1.764723000	-1.199226000
H	4.619794000	1.356659000	-1.037616000
H	5.392918000	-2.213452000	1.252491000
H	7.836173000	-1.783449000	1.072664000
H	3.175235000	-1.696016000	0.794082000
H	2.577014000	0.918677000	-0.692624000
H	0.370539000	1.526353000	-1.056257000
H	1.080287000	-2.224862000	0.933412000
H	-2.041793000	1.135795000	-0.939675000
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N	8.999780000	0.263753000	-0.176435000
O	9.767531000	-0.538915000	0.361001000
O	9.365805000	1.264943000	-0.798153000
C	-3.310027000	-1.074688000	0.183941000
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H	-3.521693000	-2.124373000	0.367206000
C	-6.896988000	-0.293566000	0.352084000
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H	-7.278481000	0.592486000	-0.173127000
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H	-5.925543000	1.700908000	-1.191247000
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H	-3.945655000	3.940735000	1.801647000
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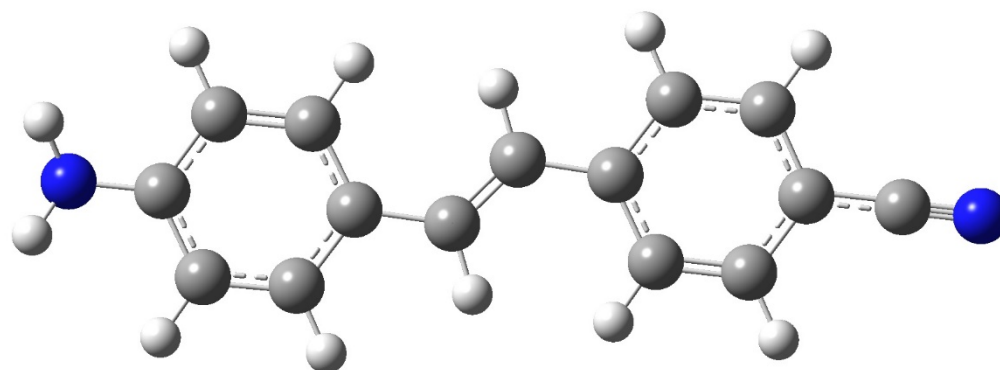
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C	3.905080000	1.256992000	0.000631000
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C	-2.216656000	-0.120254000	-0.000440000
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C	-4.471876000	-1.078643000	0.000228000
C	0.207028000	0.574267000	0.000162000
C	-0.775904000	-0.353706000	-0.000406000
C	-4.178849000	1.326667000	-0.000893000
C	-5.028649000	0.205561000	-0.000230000
C	-7.273249000	-0.612501000	0.001236000
H	4.026704000	-2.146285000	-0.000798000
H	1.573018000	-1.847779000	-0.000783000
H	2.114243000	2.429094000	0.001065000
H	4.580904000	2.103308000	0.001020000
H	-0.063983000	1.628507000	0.000729000
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H	-2.176993000	2.049868000	-0.001603000
H	-5.099924000	-1.961931000	0.000646000
H	-4.628647000	2.314560000	-0.001334000

H	-7.153030000	-1.235747000	0.896748000
H	-8.269483000	-0.167343000	0.001662000
H	-7.154386000	-1.236999000	-0.893591000
N	5.875264000	-0.227090000	0.000075000
O	6.587401000	0.779339000	0.000435000
O	6.303514000	-1.383352000	-0.000307000
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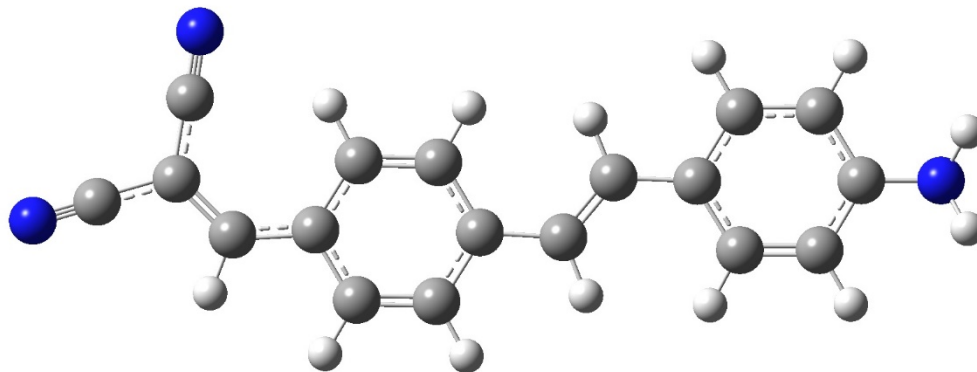
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C	2.516851000	1.395681000	-0.009687000
C	3.897253000	1.251729000	-0.008256000
C	4.468519000	-0.031733000	0.001913000
C	-2.200970000	-0.231742000	-0.004668000
C	-3.053476000	-1.352942000	-0.012705000
C	-2.816947000	1.037167000	0.003910000
C	-4.435718000	-1.227733000	-0.011660000

C	0.210629000	0.507307000	-0.003280000
C	-0.757218000	-0.436971000	-0.003337000
C	-4.195328000	1.175461000	0.004436000
C	-5.035397000	0.043684000	-0.003358000
H	4.060658000	-2.151998000	0.018678000
H	1.622246000	-1.888488000	0.016718000
H	2.087343000	2.394210000	-0.017793000
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H	-0.459315000	-1.484977000	-0.003764000
H	-2.615413000	-2.348595000	-0.017309000
H	-2.206569000	1.935443000	0.013278000
H	-5.061985000	-2.116916000	-0.021790000
H	-4.638915000	2.168697000	0.006615000
N	-6.417337000	0.185276000	-0.059028000
H	-6.955941000	-0.608597000	0.262787000
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N	7.047216000	-0.326176000	0.005663000

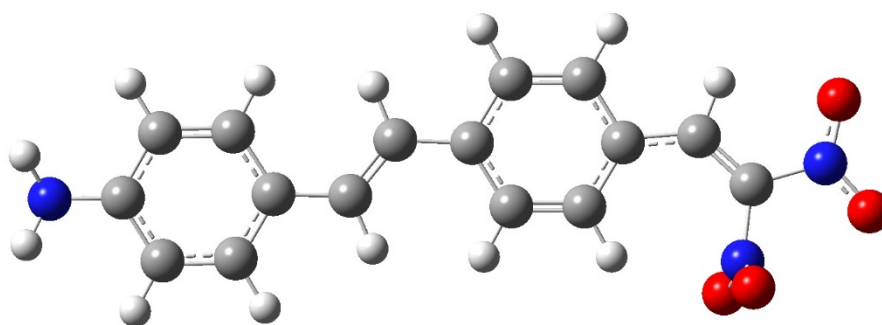
TSBD-8



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<b>C</b>	<b>-3.066741000</b>	<b>-0.647635000</b>	<b>-0.001672000</b>
<b>C</b>	<b>3.565153000</b>	<b>0.200010000</b>	<b>-0.004641000</b>
<b>C</b>	<b>4.300867000</b>	<b>1.402431000</b>	<b>-0.012040000</b>
<b>C</b>	<b>4.305424000</b>	<b>-1.001828000</b>	<b>0.004081000</b>
<b>C</b>	<b>5.687595000</b>	<b>1.416702000</b>	<b>-0.010236000</b>
<b>C</b>	<b>1.241102000</b>	<b>-0.778523000</b>	<b>-0.003175000</b>
<b>C</b>	<b>2.111575000</b>	<b>0.260056000</b>	<b>-0.004434000</b>
<b>C</b>	<b>5.689746000</b>	<b>-1.000934000</b>	<b>0.005531000</b>
<b>C</b>	<b>6.411889000</b>	<b>0.210736000</b>	<b>-0.001685000</b>
<b>H</b>	<b>-2.815937000</b>	<b>1.512430000</b>	<b>0.000458000</b>
<b>H</b>	<b>-0.397531000</b>	<b>1.469168000</b>	<b>-0.000331000</b>
<b>H</b>	<b>-0.443922000</b>	<b>-2.840984000</b>	<b>-0.005267000</b>
<b>H</b>	<b>-2.898628000</b>	<b>-2.803647000</b>	<b>-0.004392000</b>
<b>H</b>	<b>1.633413000</b>	<b>-1.793892000</b>	<b>-0.003098000</b>

H	1.709635000	1.272312000	-0.006636000
H	3.764182000	2.348497000	-0.016852000
H	3.788273000	-1.956817000	0.012669000
H	6.221944000	2.363846000	-0.019775000
H	6.231560000	-1.944080000	0.008103000
N	7.797683000	0.208802000	-0.054580000
H	8.260124000	1.054562000	0.251951000
H	8.259040000	-0.629888000	0.272262000
C	-4.507549000	-0.732600000	-0.000922000
C	-5.480161000	0.235272000	0.002229000
H	-4.895649000	-1.749021000	-0.003086000
C	-5.244041000	1.645781000	0.005936000
N	-5.070726000	2.797306000	0.009144000
C	-6.857581000	-0.160636000	0.002275000
N	-7.974248000	-0.489716000	0.002397000

### TSBD-9



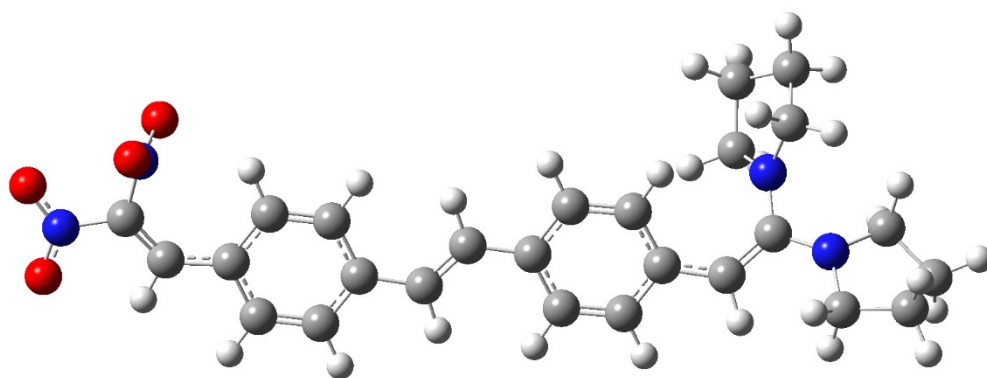
C	1.558611000	-0.426838000	-0.151491000
C	0.176942000	-0.425071000	-0.128119000
C	-0.565893000	0.776041000	-0.031308000



C	0.165914000	1.981821000	0.031784000
C	1.549357000	1.986836000	0.006142000
C	2.287645000	0.784856000	-0.076025000
C	-4.322934000	-0.192072000	-0.018487000
C	-5.035281000	-1.407022000	-0.081467000
C	-5.085838000	0.992235000	0.072222000
C	-6.421003000	-1.449473000	-0.055392000
C	-2.019054000	0.832383000	-0.000193000
C	-2.869186000	-0.222081000	-0.048446000
C	-6.469418000	0.963276000	0.098648000
C	-7.168099000	-0.260667000	0.035167000
H	2.072757000	-1.374157000	-0.253816000
H	-0.340815000	-1.376517000	-0.193684000
H	-0.372202000	2.923645000	0.101256000
H	2.083508000	2.932224000	0.059005000
H	-2.430572000	1.837594000	0.069993000
H	-2.447411000	-1.223791000	-0.118673000
H	-4.480700000	-2.340160000	-0.150323000
H	-4.586941000	1.955419000	0.125771000
H	-6.937216000	-2.405097000	-0.109753000
H	-7.029083000	1.893518000	0.164867000
N	-8.553780000	-0.284027000	0.007611000
H	-8.995183000	-1.155361000	0.270132000
H	-9.026521000	0.525627000	0.386961000
C	3.728165000	0.903498000	-0.071586000

C	4.719291000	-0.007815000	-0.014057000
H	4.116694000	1.919138000	-0.091431000
N	6.116352000	0.389354000	-0.022111000
O	6.372887000	1.594281000	-0.012631000
O	6.947276000	-0.518200000	-0.060270000
N	4.553243000	-1.464004000	0.098846000
O	4.197716000	-2.068735000	-0.910474000
O	4.755578000	-1.954945000	1.201491000

### TSBD-10



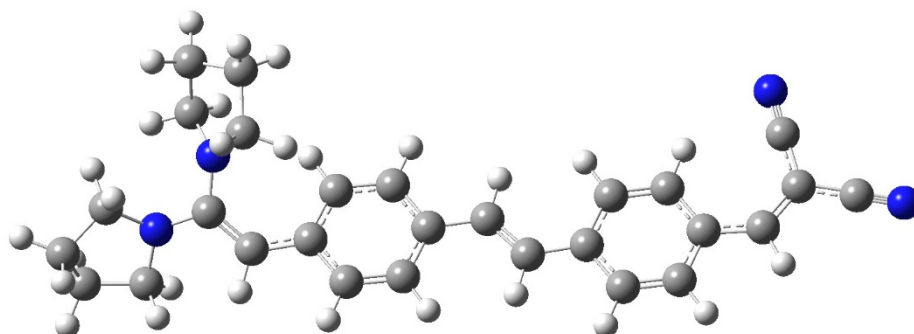
C	-5.101648000	0.285816000	0.069375000
C	-3.729575000	0.128394000	0.057210000
C	-3.119775000	-1.083542000	-0.351151000
C	-3.979231000	-2.129555000	-0.756376000
C	-5.353626000	-1.977040000	-0.748503000
C	-5.958755000	-0.770353000	-0.327688000
C	0.712735000	-0.600831000	-0.040407000
C	1.551529000	0.454566000	0.376441000
C	1.348711000	-1.796059000	-0.448017000

C	2.932800000	0.341314000	0.377465000
C	-1.684584000	-1.299903000	-0.381497000
C	-0.724768000	-0.410051000	-0.019688000
C	2.725500000	-1.912244000	-0.445467000
C	3.575641000	-0.847408000	-0.045802000
H	-5.509038000	1.243974000	0.366469000
H	-3.111885000	0.966149000	0.364133000
H	-3.546283000	-3.072202000	-1.081111000
H	-5.986869000	-2.802527000	-1.064056000
H	-1.381832000	-2.284286000	-0.733540000
H	-1.037978000	0.571961000	0.332725000
H	1.096122000	1.381966000	0.718517000
H	0.751983000	-2.644502000	-0.771063000
H	3.532390000	1.167910000	0.744006000
H	3.180089000	-2.847119000	-0.765566000
C	-7.401501000	-0.726089000	-0.338734000
C	-8.291856000	0.191109000	0.092489000
H	-7.896561000	-1.604065000	-0.747379000
N	-9.720569000	-0.016744000	-0.040097000
O	-10.107417000	-1.092429000	-0.501528000
O	-10.448777000	0.916421000	0.301622000
N	-7.971800000	1.459364000	0.762953000
O	-7.533556000	2.370031000	0.063055000
O	-8.140290000	1.498020000	1.974735000
C	5.005487000	-1.064362000	-0.037899000

C	6.032192000	-0.148832000	0.053363000
H	5.300361000	-2.108732000	-0.085385000
C	8.534599000	-0.025301000	-0.169985000
C	7.544704000	-1.826252000	1.121823000
H	8.842374000	0.922563000	0.292372000
H	8.387587000	0.164842000	-1.239159000
H	7.290295000	-2.684032000	0.477757000
H	6.935651000	-1.901848000	2.028592000
N	7.300081000	-0.546061000	0.450844000
C	9.582321000	-1.119289000	0.103462000
C	9.054832000	-1.803887000	1.374787000
H	10.591212000	-0.710218000	0.213299000
H	9.601543000	-1.838244000	-0.724304000
H	9.468687000	-2.804372000	1.531812000
H	9.282522000	-1.197997000	2.260056000
C	5.209794000	1.695781000	-1.453838000
C	6.399023000	2.294580000	0.589206000
H	4.188830000	1.309406000	-1.528738000
H	5.748948000	1.386400000	-2.360544000
H	7.375270000	2.071337000	1.026580000
H	5.703996000	2.479037000	1.425528000
N	5.916055000	1.199012000	-0.261172000
C	5.218787000	3.224817000	-1.278084000
C	6.428060000	3.491555000	-0.366781000
H	4.297745000	3.546961000	-0.776805000

H	5.27344000	3.75094000	-2.23570600
H	7.35647400	3.47939400	-0.95088800
H	6.37049100	4.45035400	0.15739500

TSBD-11

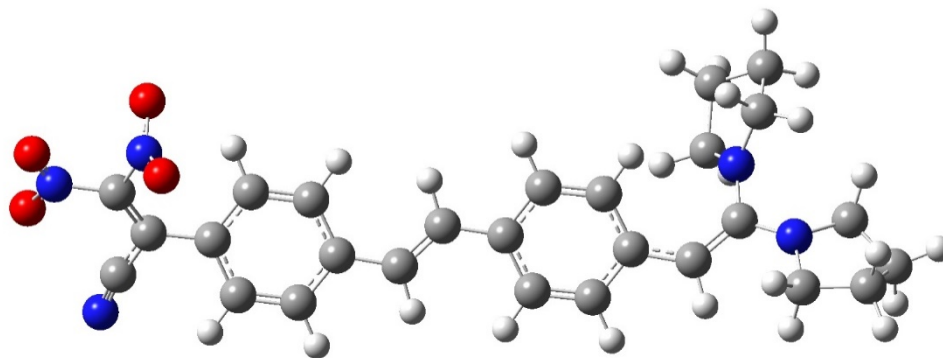


C	5.89545600	0.40177900	-0.25974000
C	4.52571000	0.22807000	-0.22118700
C	3.93763300	-0.96877500	0.25718700
C	4.81629400	-1.98467500	0.69632900
C	6.18843200	-1.81644600	0.65981400
C	6.77309200	-0.62013100	0.18207100
C	0.09358300	-0.54780900	-0.01114100
C	-0.76574200	0.47686100	-0.46078600
C	-0.51962800	-1.73086000	0.46081300
C	-2.14553700	0.34659200	-0.43277100
C	2.50543800	-1.20106200	0.31964400
C	1.52862000	-0.34013800	-0.06454500
C	-1.89488400	-1.86390600	0.48767900
C	-2.76526200	-0.82913200	0.05519400
H	6.29222200	1.33696900	-0.63520100

H	3.892921000	1.038212000	-0.568989000
H	4.399935000	-2.916692000	1.070024000
H	6.835463000	-2.619233000	1.005454000
H	2.221029000	-2.172718000	0.719407000
H	1.822976000	0.629535000	-0.464256000
H	-0.328437000	1.393369000	-0.852286000
H	0.093534000	-2.556318000	0.811464000
H	-2.761965000	1.148304000	-0.825812000
H	-2.331698000	-2.788747000	0.857864000
C	8.212569000	-0.542495000	0.186209000
C	9.076913000	0.452790000	-0.199345000
H	8.707937000	-1.434522000	0.564129000
C	-4.192862000	-1.063871000	0.083162000
C	-5.232822000	-0.166855000	-0.027232000
H	-4.473038000	-2.108753000	0.181590000
C	-7.728945000	-0.073705000	0.260603000
C	-6.746311000	-1.907361000	-0.988777000
H	-8.058167000	0.859215000	-0.216703000
H	-7.557836000	0.144472000	1.321022000
H	-6.470077000	-2.734749000	-0.314336000
H	-6.153953000	-2.014830000	-1.903325000
N	-6.504541000	-0.597091000	-0.378405000
C	-8.771464000	-1.185974000	0.042933000
C	-8.260946000	-1.911529000	-1.212474000
H	-9.785813000	-0.789564000	-0.063166000

H	-8.770443000	-1.875602000	0.895509000
H	-8.666040000	-2.921775000	-1.323411000
H	-8.512853000	-1.342253000	-2.115324000
C	-4.408507000	1.757925000	1.375346000
C	-5.651035000	2.242957000	-0.665963000
H	-3.377774000	1.396615000	1.443638000
H	-4.920777000	1.476508000	2.306432000
H	-6.629939000	1.979806000	-1.074348000
H	-4.975888000	2.405379000	-1.522920000
N	-5.129038000	1.195918000	0.221293000
C	-4.454776000	3.277677000	1.134917000
C	-5.687308000	3.479513000	0.238011000
H	-3.551049000	3.597478000	0.601673000
H	-4.502173000	3.842984000	2.070345000
H	-6.603572000	3.473360000	0.841110000
H	-5.660824000	4.415809000	-0.327765000
C	10.487874000	0.236749000	-0.075123000
N	11.633025000	0.053828000	0.028863000
C	8.692036000	1.723809000	-0.729063000
N	8.397779000	2.764165000	-1.162094000

TSBD-12



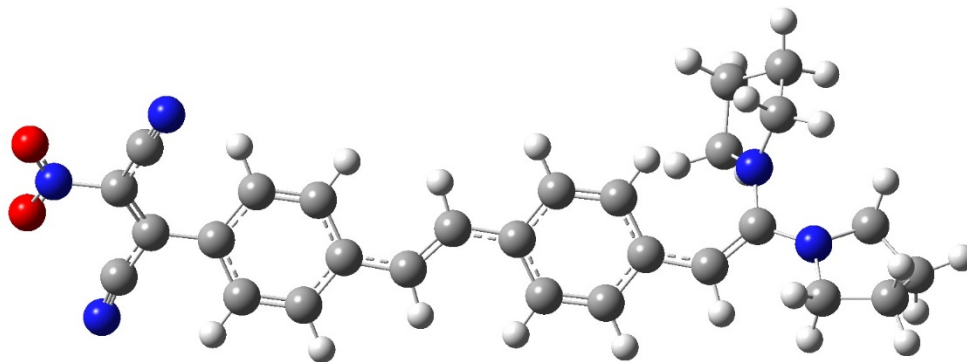
C	-4.767390000	0.490101000	-0.111836000
C	-3.398011000	0.315498000	-0.098607000
C	-2.808521000	-0.952185000	-0.325394000
C	-3.687259000	-2.027333000	-0.593122000
C	-5.058761000	-1.857756000	-0.625739000
C	-5.638476000	-0.596479000	-0.363239000
C	1.025787000	-0.501799000	-0.048458000
C	1.885912000	0.587376000	0.212243000
C	1.636960000	-1.760742000	-0.256637000
C	3.263014000	0.444642000	0.252756000
C	-1.380532000	-1.197791000	-0.310408000
C	-0.404642000	-0.280383000	-0.076271000
C	3.009118000	-1.906522000	-0.212609000
C	3.880994000	-0.811560000	0.032461000
H	-5.162004000	1.489451000	0.028673000
H	-2.770036000	1.181885000	0.080742000
H	-3.270617000	-3.013290000	-0.781212000
H	-5.696953000	-2.707734000	-0.842642000
H	-1.094699000	-2.229159000	-0.507187000



H	-0.700988000	0.749640000	0.118271000
H	1.449081000	1.566473000	0.399055000
H	1.023203000	-2.635043000	-0.453940000
H	3.878873000	1.304204000	0.495471000
H	3.444274000	-2.889848000	-0.375433000
C	-7.097304000	-0.447286000	-0.387546000
C	-7.810996000	0.479243000	0.315532000
N	-9.243288000	0.666891000	0.245470000
O	-9.849391000	0.118680000	-0.673954000
O	-9.748592000	1.354685000	1.134411000
N	-7.197486000	1.372358000	1.315137000
O	-7.126116000	2.560015000	1.014752000
O	-6.802151000	0.857844000	2.352206000
C	5.301724000	-1.059699000	0.104286000
C	6.352202000	-0.164383000	0.086330000
H	5.569884000	-2.105977000	0.219143000
C	8.863162000	-0.146844000	-0.074644000
C	7.780306000	-1.684658000	1.461195000
H	9.185298000	0.856948000	0.233785000
H	8.754946000	-0.135553000	-1.165053000
H	7.519250000	-2.630207000	0.958552000
H	7.142023000	-1.593723000	2.346096000
N	7.594868000	-0.526868000	0.579925000
C	9.869391000	-1.204325000	0.414138000
C	9.281664000	-1.657146000	1.760455000

H	10.884984000	-0.804911000	0.492937000
H	9.897134000	-2.050612000	-0.282671000
H	9.660390000	-2.627808000	2.093813000
H	9.499331000	-0.919717000	2.542396000
C	5.620678000	1.433073000	-1.718036000
C	6.793726000	2.323197000	0.224025000
H	4.575982000	1.107855000	-1.744865000
H	6.146967000	0.925822000	-2.538418000
H	7.735806000	2.131581000	0.742439000
H	6.078237000	2.692031000	0.978004000
N	6.278429000	1.117870000	-0.438143000
C	5.732133000	2.965521000	-1.825330000
C	6.929343000	3.322626000	-0.928490000
H	4.821407000	3.433903000	-1.432586000
H	5.852455000	3.298702000	-2.860291000
H	7.872100000	3.149525000	-1.461873000
H	6.918241000	4.362622000	-0.588518000
C	-7.791309000	-1.394764000	-1.219780000
N	-8.189957000	-2.243764000	-1.907769000

TSBD-13



<b>C</b>	<b>-5.042596000</b>	<b>0.594845000</b>	<b>0.043744000</b>
<b>C</b>	<b>-3.675983000</b>	<b>0.405546000</b>	<b>0.029436000</b>
<b>C</b>	<b>-3.103085000</b>	<b>-0.863001000</b>	<b>-0.235539000</b>
<b>C</b>	<b>-3.999293000</b>	<b>-1.922304000</b>	<b>-0.512361000</b>
<b>C</b>	<b>-5.367840000</b>	<b>-1.737352000</b>	<b>-0.518653000</b>
<b>C</b>	<b>-5.935094000</b>	<b>-0.474705000</b>	<b>-0.218902000</b>
<b>C</b>	<b>0.736995000</b>	<b>-0.460049000</b>	<b>0.000036000</b>
<b>C</b>	<b>1.611277000</b>	<b>0.612184000</b>	<b>0.285163000</b>
<b>C</b>	<b>1.333517000</b>	<b>-1.716982000</b>	<b>-0.259564000</b>
<b>C</b>	<b>2.987000000</b>	<b>0.456199000</b>	<b>0.300418000</b>
<b>C</b>	<b>-1.679720000</b>	<b>-1.124569000</b>	<b>-0.248649000</b>
<b>C</b>	<b>-0.690156000</b>	<b>-0.224296000</b>	<b>0.000221000</b>
<b>C</b>	<b>2.704423000</b>	<b>-1.876157000</b>	<b>-0.240466000</b>
<b>C</b>	<b>3.590277000</b>	<b>-0.797518000</b>	<b>0.028404000</b>
<b>H</b>	<b>-5.422694000</b>	<b>1.590314000</b>	<b>0.230937000</b>
<b>H</b>	<b>-3.036311000</b>	<b>1.261042000</b>	<b>0.219417000</b>
<b>H</b>	<b>-3.597196000</b>	<b>-2.908677000</b>	<b>-0.728158000</b>
<b>H</b>	<b>-6.015853000</b>	<b>-2.576939000</b>	<b>-0.744094000</b>
<b>H</b>	<b>-1.407799000</b>	<b>-2.152348000</b>	<b>-0.480636000</b>

H	-0.973463000	0.801503000	0.232345000
H	1.186125000	1.588048000	0.511484000
H	0.708851000	-2.578479000	-0.477744000
H	3.614157000	1.301656000	0.562581000
H	3.128276000	-2.857078000	-0.442834000
C	-7.388518000	-0.310760000	-0.218349000
C	-8.087852000	0.665491000	0.464452000
N	-9.540697000	0.818053000	0.334728000
O	-10.130654000	0.128460000	-0.494522000
O	-10.069257000	1.645496000	1.077156000
C	5.008603000	-1.060607000	0.068986000
C	6.067413000	-0.173663000	0.071069000
H	5.268459000	-2.112981000	0.137326000
C	8.576481000	-0.159374000	-0.117275000
C	7.502867000	-1.764757000	1.355306000
H	8.914624000	0.819826000	0.248383000
H	8.452472000	-0.079028000	-1.202864000
H	7.220870000	-2.682781000	0.814946000
H	6.883116000	-1.707731000	2.256085000
N	7.313208000	-0.566075000	0.530664000
C	9.576968000	-1.254461000	0.292057000
C	9.010204000	-1.768221000	1.625460000
H	10.599813000	-0.873793000	0.369493000
H	9.576478000	-2.063111000	-0.448587000
H	9.383747000	-2.758413000	1.902203000

H	9.251936000	-1.073260000	2.438578000
C	5.326396000	1.496367000	-1.661496000
C	6.527394000	2.304450000	0.299867000
H	4.281477000	1.172586000	-1.691612000
H	5.844881000	1.023576000	-2.507101000
H	7.476896000	2.089194000	0.794989000
H	5.825418000	2.645009000	1.079280000
N	5.996027000	1.128448000	-0.401636000
C	5.438448000	3.031531000	-1.706656000
C	6.649201000	3.349414000	-0.813428000
H	4.534288000	3.483926000	-1.281436000
H	5.544303000	3.407291000	-2.728515000
H	7.583785000	3.196238000	-1.366858000
H	6.645801000	4.374672000	-0.431261000
C	-8.095221000	-1.298294000	-0.992803000
N	-8.474802000	-2.190204000	-1.637188000
C	-7.521604000	1.572748000	1.399263000
N	-7.041763000	2.305187000	2.166878000

**Table 1: Comparison of previously reported geometries with optimized geometries in present study**

Parameters		TSBD-2		TSB	
		B3LYP/6-31G(d)	B3LYP/6-311G(d, p) <sup>a</sup>	B3LYP/6-31G(d)	B3LYP/6-311G(d, p) <sup>a</sup>
Bond Length (Angstrom)	C1-C1'	1.354	1.350	1.349 (1.326) <sup>b</sup>	1.345
	C1-C2	1.458	1.458	1.466 (1.471) <sup>b</sup>	1.465
	C5-N1	1.461	1.469	-----	-----
	C5'-N1'	1.380	1.378	-----	-----
	N1'-C9'	1.453	1.454	-----	-----
	C1-H1	1.089	1.086	1.089	1.087
	C3-H2	1.085	1.083	1.086	1.084

	N1-O1	1.234	1.227	-----	-----
Angle (Degree)	C1'-C1-C2	126.686	126.689	127.166	127.198
	C1-C1'-C2'	127.638	127.694	127.166 (126.4) <sup>b</sup>	127.199
	C1-C2-C7	118.708	118.744	118.677 (119.0) <sup>b</sup>	118.705
	C6-C5-N1	119.387	119.392	-----	-----

<sup>a</sup> M. M. Alam, M. Chattopadhyaya and S. Chakrabarti, *J. Phys. Chem. A*, 2012, **116**, 11034-11040.

<sup>b</sup> K. Ogawa, J. Harada and S. Tomoda, *Acta Crystallogr.*, 1995, **B51**, 240-248.

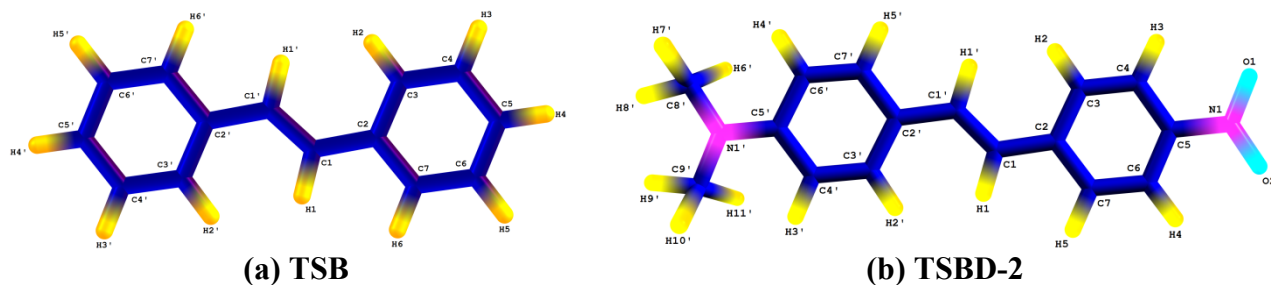


Figure 1. Representation of (a) TSB and (b) TSBD-2 geometries.

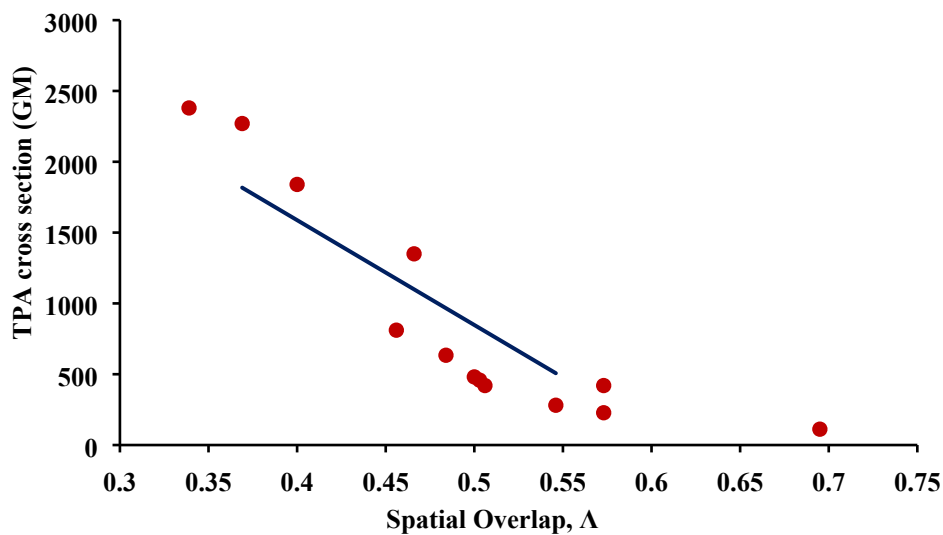


Figure 2. Scatter diagram of spatial overlap and TPA  
Values which appear to have a linear relationship.