

Is this how bromine spiropyran salt is converted to merocyanine under UV irradiation? A look through the prism of quantum chemical calculations

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Supplementary information

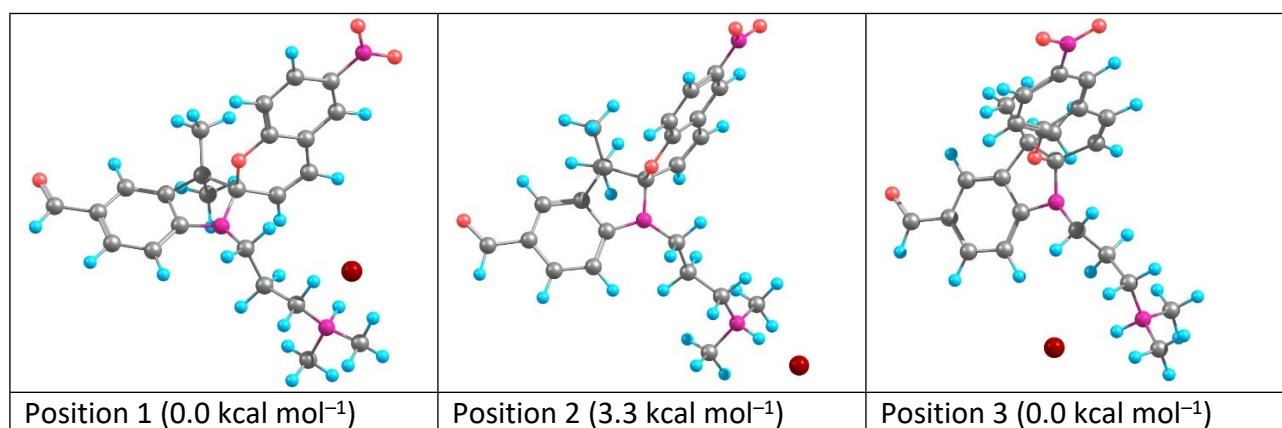


Fig. 1. Position of bromine ion relative to $\text{NH}^+(\text{CH}_3)_2$ group of propyl fragment.

Cartesian coordinates of spiropyran and merocyanine forms

Spiropyran

6	0.509669000	3.832646000	0.301942000
6	0.179824000	2.534312000	0.602612000
6	1.708085000	4.083715000	-0.396519000
6	1.028761000	1.477322000	0.219344000
6	2.542090000	3.025138000	-0.763820000
1	3.461867000	3.239409000	-1.303769000
6	2.222214000	1.700921000	-0.464013000
1	2.880378000	0.888125000	-0.764313000
1	-0.125879000	4.669304000	0.581572000
6	-0.985239000	1.957968000	1.380274000
6	-0.917810000	0.458883000	0.922185000
7	0.483422000	0.266461000	0.623461000
6	-0.681408000	2.071955000	2.883378000
1	-0.590376000	3.128815000	3.150024000
1	-1.488084000	1.633591000	3.480018000
1	0.258738000	1.572539000	3.138893000
6	-2.335856000	2.596791000	1.071731000
1	-2.351111000	3.624592000	1.447446000
1	-2.536292000	2.618949000	-0.001893000
1	-3.142542000	2.048740000	1.572886000
6	-1.433018000	-0.533063000	1.925118000
6	-2.612273000	-1.142955000	1.785918000
6	-3.427574000	-0.914742000	0.597320000
6	-4.706665000	-1.433020000	0.432523000
6	-2.854049000	-0.167481000	-0.446962000
1	-5.172311000	-2.018079000	1.217618000
6	-5.384481000	-1.196475000	-0.756892000

6	-3.542674000	0.047265000	-1.642923000
1	-3.064969000	0.621073000	-2.428952000
6	-4.819731000	-0.466298000	-1.800001000
1	-5.380023000	-0.305215000	-2.712523000
8	-1.608773000	0.336951000	-0.353111000
1	-0.804891000	-0.700833000	2.794103000
1	-2.980789000	-1.831472000	2.540770000
7	-6.727703000	-1.738461000	-0.920442000
8	-7.311360000	-1.519287000	-1.969743000
8	-7.201878000	-2.385292000	-0.000014000
6	2.087449000	5.459192000	-0.743088000
8	1.432406000	6.446858000	-0.469079000
1	3.046136000	5.556282000	-1.291794000
6	0.957199000	-1.001321000	0.097420000
1	0.110625000	-1.696120000	0.075500000
1	1.306685000	-0.872605000	-0.936724000
6	2.096414000	-1.569758000	0.944046000
1	1.768520000	-1.660035000	1.984314000
1	2.935937000	-0.864752000	0.909365000
7	3.976601000	-3.199630000	0.700510000
1	4.492397000	-2.393453000	0.264502000
6	4.246917000	-3.273608000	2.158162000
1	3.947334000	-2.337011000	2.626419000
1	3.676960000	-4.105088000	2.576670000
1	5.314064000	-3.436054000	2.305933000
6	4.452405000	-4.408915000	-0.021316000
1	3.837153000	-5.261744000	0.268504000
1	4.368068000	-4.207543000	-1.089788000
1	5.495252000	-4.586080000	0.241427000
35	4.698581000	-1.096011000	-1.519502000
6	2.542437000	-2.913777000	0.380338000
1	1.946607000	-3.749536000	0.757848000
1	2.494690000	-2.896024000	-0.711283000

CCC

6	-4.102579000	-1.972789000	-0.144720000
6	-2.809570000	-1.798235000	0.301568000
6	-4.682477000	-0.949101000	-0.909465000
6	-2.124397000	-0.621420000	-0.005933000
6	-3.973643000	0.217854000	-1.207487000
1	-4.449831000	0.992277000	-1.803296000
6	-2.668088000	0.410571000	-0.756486000
1	-2.121253000	1.321921000	-0.992007000
1	-4.677017000	-2.869809000	0.070468000
6	-1.905415000	-2.687473000	1.116120000
6	-0.638276000	-1.850329000	1.174361000
7	-0.832198000	-0.691103000	0.572462000
6	-2.477432000	-2.939389000	2.522594000
1	-3.431387000	-3.465823000	2.428552000

1	-1.801847000	-3.565889000	3.111246000
1	-2.650814000	-2.000177000	3.054991000
6	-1.600455000	-4.013844000	0.398987000
1	-2.530087000	-4.574800000	0.265049000
1	-1.143059000	-3.824859000	-0.574795000
1	-0.911148000	-4.613443000	1.000840000
6	0.531400000	-2.290929000	1.862769000
6	1.858925000	-2.191834000	1.544615000
6	2.543535000	-1.820054000	0.341099000
6	1.885890000	-1.768645000	-0.968277000
6	3.930240000	-1.619089000	0.431441000
6	2.740398000	-1.432966000	-2.096616000
6	4.675844000	-1.294638000	-0.681947000
6	4.072883000	-1.193789000	-1.963440000
1	4.690096000	-0.935414000	-2.816124000
1	0.301385000	-2.854837000	2.764331000
1	2.524627000	-2.530170000	2.338744000
6	-6.066399000	-1.104271000	-1.410752000
8	-6.757939000	-2.076108000	-1.193891000
1	-6.448704000	-0.257217000	-2.012382000
6	0.102967000	0.425658000	0.498102000
1	0.124270000	0.787433000	-0.535790000
1	1.094914000	0.058546000	0.754845000
6	-0.318228000	1.559466000	1.434692000
1	-0.461604000	1.173603000	2.448297000
1	-1.271732000	1.972294000	1.086863000
7	0.164626000	4.013811000	1.518313000
1	-0.507074000	4.063212000	0.713135000
6	-0.532851000	4.237247000	2.810144000
1	-1.295429000	3.471341000	2.945017000
1	0.202430000	4.183260000	3.614701000
1	-0.997754000	5.222433000	2.789109000
6	1.186648000	5.060251000	1.245056000
1	2.011356000	4.943216000	1.949062000
1	1.524006000	4.928435000	0.216436000
1	0.722678000	6.039113000	1.362647000
35	-0.746051000	3.559275000	-1.463377000
6	0.758314000	2.645164000	1.401561000
1	1.492130000	2.532163000	2.203555000
1	1.271119000	2.639886000	0.436873000
1	4.427559000	-1.701743000	1.392940000
8	0.670381000	-2.005247000	-1.126756000
1	2.256550000	-1.374051000	-3.066253000
7	6.086708000	-1.065260000	-0.543396000
8	6.596084000	-1.167310000	0.568963000
8	6.730229000	-0.774105000	-1.546871000

CCT

6	4.550831000	-1.118053000	0.347740000
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6	3.272176000	-0.663353000	0.590380000
6	4.864317000	-1.562130000	-0.944565000
6	2.322101000	-0.660467000	-0.432746000
6	3.902990000	-1.548520000	-1.957337000
1	4.170870000	-1.896086000	-2.951403000
6	2.606094000	-1.097212000	-1.719648000
1	1.876092000	-1.092556000	-2.519834000
1	5.314761000	-1.139879000	1.120560000
6	2.638821000	-0.137235000	1.850370000
6	1.232847000	0.200693000	1.368464000
7	1.096626000	-0.157936000	0.081643000
6	2.605844000	-1.222473000	2.942646000
1	3.632094000	-1.519159000	3.176709000
1	2.146622000	-0.841632000	3.858818000
1	2.055793000	-2.105577000	2.606758000
6	3.337353000	1.132239000	2.364566000
1	4.362754000	0.888600000	2.657507000
1	3.370949000	1.904985000	1.591200000
1	2.810362000	1.528667000	3.237303000
6	0.265963000	0.708441000	2.260031000
6	-0.894507000	1.426465000	2.034208000
6	-1.229265000	2.286456000	0.960014000
6	-0.241055000	2.937088000	0.193447000
6	-2.651648000	2.602871000	0.764882000
1	0.812327000	2.737106000	0.367962000
6	-0.604091000	3.878539000	-0.737908000
6	-2.947412000	3.630145000	-0.221394000
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1	-2.199496000	4.987141000	-1.689981000
8	-3.548156000	1.979051000	1.364888000
1	0.473028000	0.456784000	3.297718000
1	-1.638250000	1.397273000	2.831781000
7	0.422599000	4.560351000	-1.486792000
8	0.076826000	5.416482000	-2.291494000
8	1.592761000	4.253156000	-1.291944000
6	6.228476000	-2.054530000	-1.242354000
8	7.120632000	-2.103690000	-0.423735000
1	6.393841000	-2.387552000	-2.285033000
6	-0.137558000	-0.183821000	-0.704199000
1	-0.487918000	0.844518000	-0.833849000
1	0.116047000	-0.564337000	-1.692010000
6	-1.226280000	-1.055775000	-0.066753000
1	-1.208952000	-0.922336000	1.014876000
1	-1.051173000	-2.114211000	-0.281089000
7	-3.742378000	-1.300001000	0.022590000
1	-3.685909000	-2.317406000	-0.275995000
6	-3.693929000	-1.284268000	1.509502000
1	-2.908794000	-1.963549000	1.840455000

1	-3.514542000	-0.257105000	1.838938000
1	-4.654271000	-1.642371000	1.880756000
6	-5.009343000	-0.702989000	-0.473335000
1	-5.066145000	0.322479000	-0.100131000
1	-5.001910000	-0.716304000	-1.563438000
1	-5.844505000	-1.295083000	-0.099630000
35	-3.004765000	-4.244829000	-0.752947000
6	-2.576275000	-0.623144000	-0.623654000
1	-2.729392000	0.449377000	-0.482383000
1	-2.648212000	-0.853439000	-1.690897000

TCT

6	-4.219121000	0.057047000	0.268883000
6	-3.065634000	-0.350594000	-0.368910000
6	-4.214825000	1.308957000	0.898803000
6	-1.941397000	0.475674000	-0.363791000
6	-3.084690000	2.130321000	0.866550000
1	-3.120441000	3.104326000	1.347448000
6	-1.912451000	1.731441000	0.224481000
1	-1.051638000	2.395598000	0.176200000
1	-5.119406000	-0.550650000	0.290469000
6	-2.754606000	-1.592650000	-1.160488000
6	-1.318104000	-1.335123000	-1.570846000
7	-0.904673000	-0.174594000	-1.098625000
6	-2.833251000	-2.868599000	-0.300949000
1	-3.875531000	-3.039885000	-0.017681000
1	-2.481399000	-3.732690000	-0.872912000
1	-2.238891000	-2.773906000	0.612676000
6	-3.657931000	-1.719790000	-2.402267000
1	-4.697712000	-1.791917000	-2.072905000
1	-3.559626000	-0.849931000	-3.057173000
1	-3.415373000	-2.625156000	-2.964907000
6	-0.584275000	-2.187462000	-2.479913000
6	0.703463000	-2.573976000	-2.336572000
6	1.462486000	-2.484267000	-1.102183000
6	2.843952000	-2.026956000	-1.191463000
6	0.897454000	-2.843688000	0.110042000
6	3.591393000	-2.048356000	0.051596000
6	1.651985000	-2.782285000	1.279618000
6	3.011783000	-2.396870000	1.241253000
1	3.577518000	-2.385303000	2.166783000
1	-1.156724000	-2.513568000	-3.345616000
1	1.199449000	-3.037142000	-3.188312000
6	-5.435788000	1.780532000	1.596374000
8	-6.460289000	1.137831000	1.663075000
1	-5.357164000	2.780008000	2.064658000
6	0.373109000	0.497829000	-1.364475000
1	0.888700000	-0.059086000	-2.150064000
1	0.128726000	1.501600000	-1.732992000

6	1.249959000	0.640136000	-0.118955000
1	1.393540000	-0.321093000	0.376868000
1	0.760822000	1.320877000	0.584810000
7	3.187659000	2.057768000	0.546255000
1	2.454267000	2.773929000	0.762759000
6	3.513631000	1.251124000	1.751003000
1	2.614632000	0.743458000	2.099984000
1	4.274025000	0.517073000	1.479595000
1	3.888102000	1.920185000	2.525132000
6	4.362297000	2.826119000	0.052484000
1	5.093165000	2.129719000	-0.360365000
1	4.003258000	3.517871000	-0.710201000
1	4.793356000	3.379875000	0.886246000
35	0.931657000	4.140726000	-0.241570000
6	2.581778000	1.247964000	-0.556832000
1	3.306060000	0.492271000	-0.873025000
1	2.420098000	1.958603000	-1.370685000
1	-0.121280000	-3.213143000	0.157726000
8	3.306350000	-1.576474000	-2.262055000
1	4.635763000	-1.751843000	0.006983000
7	1.048021000	-3.153295000	2.519168000
8	1.732860000	-3.127797000	3.538982000
8	-0.140001000	-3.476534000	2.525649000

CTC

6	-5.390539000	-0.617092000	0.149615000
6	-4.035628000	-0.793551000	-0.025613000
6	-5.912600000	0.682364000	0.046357000
6	-3.220411000	0.305612000	-0.306714000
6	-5.080159000	1.769165000	-0.229788000
1	-5.510062000	2.764495000	-0.302995000
6	-3.707916000	1.601122000	-0.412731000
1	-3.068533000	2.451433000	-0.622760000
1	-6.060969000	-1.445219000	0.364071000
6	-3.181634000	-2.035234000	0.021757000
6	-1.790480000	-1.467049000	-0.243852000
7	-1.888343000	-0.139862000	-0.456203000
6	-3.235682000	-2.707747000	1.403002000
1	-4.258811000	-3.039829000	1.602550000
1	-2.576605000	-3.579825000	1.430738000
1	-2.934771000	-2.012144000	2.191098000
6	-3.576952000	-3.030715000	-1.083603000
1	-4.605130000	-3.363399000	-0.913380000
1	-3.519050000	-2.566405000	-2.071642000
1	-2.924183000	-3.907807000	-1.065101000
6	-0.668242000	-2.299078000	-0.256890000
6	0.668433000	-1.923667000	-0.195688000
6	1.796217000	-2.764571000	-0.178566000
6	3.056707000	-2.143198000	-0.023553000

6	1.715060000	-4.232556000	-0.303721000
1	3.117311000	-1.062686000	0.062246000
6	4.207266000	-2.883001000	0.018973000
6	2.991505000	-4.944453000	-0.248047000
1	2.942802000	-6.024729000	-0.337368000
6	4.178100000	-4.306765000	-0.096658000
1	5.114036000	-4.852329000	-0.059340000
8	0.646738000	-4.843550000	-0.448451000
1	-0.876333000	-3.361755000	-0.236567000
1	0.912824000	-0.870076000	-0.094532000
7	5.469854000	-2.209883000	0.184771000
8	6.488835000	-2.889733000	0.195679000
8	5.475363000	-0.989640000	0.309711000
6	-7.362650000	0.907869000	0.233443000
8	-8.157367000	0.025048000	0.475428000
1	-7.693932000	1.959900000	0.137010000
6	-0.826215000	0.768363000	-0.866315000
1	-0.109220000	0.195884000	-1.459668000
1	-1.271186000	1.508919000	-1.536760000
6	-0.165701000	1.458992000	0.331000000
1	0.173387000	0.704684000	1.049594000
1	-0.914827000	2.073524000	0.840716000
7	1.805682000	2.926312000	0.938846000
1	2.370296000	3.679008000	0.435104000
6	2.733062000	1.971978000	1.596834000
1	2.163330000	1.171175000	2.071291000
1	3.409659000	1.563973000	0.845234000
1	3.304316000	2.513147000	2.351096000
6	0.985487000	3.687573000	1.916516000
1	1.662238000	4.271905000	2.539858000
1	0.332251000	4.360715000	1.359839000
1	0.407986000	2.997747000	2.532316000
35	2.677483000	5.388685000	-0.715197000
6	0.993476000	2.316137000	-0.158798000
1	1.692181000	1.732270000	-0.766386000
1	0.647182000	3.157508000	-0.766971000

CTT

6	-5.303350000	-0.860897000	0.070281000
6	-3.934728000	-0.875104000	-0.087880000
6	-5.976752000	0.364607000	-0.056721000
6	-3.254595000	0.311152000	-0.374167000
6	-5.277711000	1.540796000	-0.337058000
1	-5.822450000	2.477094000	-0.425018000
6	-3.892995000	1.537170000	-0.500690000
1	-3.356947000	2.456591000	-0.708033000
1	-5.871758000	-1.760254000	0.291537000
6	-2.936628000	-2.002910000	-0.009820000
6	-1.619679000	-1.268926000	-0.250875000

7	-1.876506000	0.031274000	-0.496332000
6	-2.944840000	-2.674371000	1.372572000
1	-3.922671000	-3.133723000	1.543805000
1	-2.183867000	-3.457971000	1.426414000
1	-2.757610000	-1.945465000	2.165473000
6	-3.178710000	-3.041343000	-1.120935000
1	-4.164332000	-3.493923000	-0.978901000
1	-3.146925000	-2.575494000	-2.109466000
1	-2.427209000	-3.834763000	-1.078170000
6	-0.396068000	-1.940790000	-0.207001000
6	0.874692000	-1.381500000	-0.188153000
6	2.115336000	-2.032782000	-0.124889000
6	2.264897000	-3.437082000	-0.102724000
6	3.301119000	-1.155977000	-0.082770000
1	1.402204000	-4.093751000	-0.135489000
6	3.515340000	-3.988867000	-0.036386000
6	4.592045000	-1.829333000	-0.013395000
1	5.474109000	-1.198746000	0.018405000
6	4.694107000	-3.181622000	0.008494000
1	5.658210000	-3.674138000	0.060950000
8	3.212385000	0.084185000	-0.106620000
1	-0.489799000	-3.019232000	-0.116918000
1	0.990688000	-0.304726000	-0.183997000
7	3.650777000	-5.427037000	-0.008838000
8	2.636571000	-6.112850000	-0.041564000
8	4.779951000	-5.896731000	0.047674000
6	-7.445234000	0.414229000	0.114172000
8	-8.127659000	-0.554369000	0.371054000
1	-7.902229000	1.414959000	-0.008450000
6	-0.916885000	1.061633000	-0.872346000
1	-0.152349000	0.592420000	-1.497107000
1	-1.438825000	1.781201000	-1.507372000
6	-0.316027000	1.757523000	0.354803000
1	-0.046626000	1.005213000	1.104654000
1	-1.079422000	2.402534000	0.801303000
7	1.589834000	3.256969000	1.063004000
1	2.322395000	3.853055000	0.572749000
6	2.263424000	2.335388000	2.014626000
1	1.509921000	1.811712000	2.605327000
1	2.862461000	1.622811000	1.444947000
1	2.894412000	2.932884000	2.673246000
6	0.724139000	4.247657000	1.751129000
1	1.349197000	4.823713000	2.433861000
1	0.301161000	4.913811000	0.998244000
1	-0.060071000	3.733375000	2.306781000
35	3.057374000	5.357817000	-0.685161000
6	0.909704000	2.555251000	-0.067773000
1	1.667397000	1.898086000	-0.508489000
1	0.660518000	3.335406000	-0.793807000

TTC

6	1.230827000	4.976923000	0.193737000
6	0.811420000	3.689175000	-0.057128000
6	2.602651000	5.261790000	0.101064000
6	1.744243000	2.705174000	-0.398173000
6	3.520026000	4.263099000	-0.233460000
1	4.577018000	4.508844000	-0.292241000
6	3.106676000	2.956852000	-0.489448000
1	3.826665000	2.185923000	-0.739296000
1	0.539724000	5.772444000	0.460585000
6	-0.573675000	3.080525000	-0.030921000
6	-0.267321000	1.629515000	-0.392932000
7	1.057668000	1.495598000	-0.608153000
6	-1.178838000	3.203562000	1.379140000
1	-1.261562000	4.262939000	1.639127000
1	-2.175681000	2.760275000	1.429105000
1	-0.540984000	2.713890000	2.120007000
6	-1.467746000	3.745923000	-1.094383000
1	-1.550936000	4.813266000	-0.870176000
1	-1.034925000	3.634053000	-2.091933000
1	-2.473132000	3.319590000	-1.100021000
6	-1.123477000	0.532585000	-0.477712000
6	-2.493390000	0.574240000	-0.260458000
6	-3.353931000	-0.539372000	-0.205207000
6	-4.738233000	-0.286674000	-0.060852000
6	-2.866607000	-1.931808000	-0.255660000
1	-5.097062000	0.736558000	-0.007199000
6	-5.637349000	-1.317219000	0.003734000
6	-3.893653000	-2.965952000	-0.183718000
1	-3.545489000	-3.992583000	-0.230236000
6	-5.213555000	-2.677818000	-0.060975000
1	-5.961796000	-3.460141000	-0.005951000
8	-1.663074000	-2.237166000	-0.339196000
1	-0.704177000	-0.440320000	-0.686832000
1	-2.975969000	1.538915000	-0.118760000
7	-7.042391000	-1.023338000	0.143888000
8	-7.396632000	0.148570000	0.191766000
8	-7.823700000	-1.964642000	0.208802000
6	3.086381000	6.633836000	0.365154000
8	2.363147000	7.559507000	0.665423000
1	4.180287000	6.775572000	0.270489000
6	1.704978000	0.245697000	-0.992925000
1	1.109872000	-0.208770000	-1.790462000
1	2.678240000	0.492892000	-1.421017000
6	1.854204000	-0.713665000	0.191055000
1	0.864560000	-0.911124000	0.617198000
1	2.462832000	-0.237495000	0.966074000
7	2.327776000	-3.149154000	0.662623000

1	3.012255000	-3.877258000	0.296882000
6	0.954592000	-3.716760000	0.665101000
1	0.237552000	-2.977082000	1.021527000
1	0.693438000	-4.002177000	-0.353715000
1	0.950254000	-4.593630000	1.312733000
6	2.819316000	-2.837744000	2.029112000
1	2.821203000	-3.761333000	2.608022000
1	3.838584000	-2.458515000	1.944948000
1	2.164048000	-2.102868000	2.497546000
35	4.878302000	-4.645097000	-0.276562000
6	2.497180000	-2.008485000	-0.288743000
1	2.061080000	-2.341384000	-1.235420000
1	3.575912000	-1.904383000	-0.436582000

TTT

6	5.315055000	-0.192379000	0.168542000
6	3.976244000	0.016244000	-0.078028000
6	5.814511000	-1.502016000	0.080822000
6	3.151059000	-1.061711000	-0.413124000
6	4.972448000	-2.567318000	-0.246015000
1	5.382966000	-3.571940000	-0.303294000
6	3.616331000	-2.367422000	-0.499385000
1	2.970350000	-3.202453000	-0.745079000
1	5.991222000	0.617702000	0.429411000
6	3.155964000	1.288268000	-0.045321000
6	1.769611000	0.756133000	-0.406382000
7	1.848558000	-0.577519000	-0.622045000
6	3.188707000	1.895203000	1.369350000
1	4.225977000	2.120743000	1.633477000
1	2.613917000	2.822002000	1.424709000
1	2.790144000	1.190510000	2.104135000
6	3.670146000	2.283049000	-1.102812000
1	4.709225000	2.537644000	-0.874932000
1	3.632914000	1.841594000	-2.102350000
1	3.086067000	3.205881000	-1.106109000
6	0.565197000	1.443164000	-0.493223000
6	0.408628000	2.804381000	-0.246164000
6	-0.803551000	3.499524000	-0.169654000
6	-2.060659000	2.853911000	-0.226646000
6	-0.729643000	4.961151000	0.047969000
1	-2.135074000	1.780722000	-0.363515000
6	-3.212551000	3.574326000	-0.081826000
6	-2.014779000	5.652573000	0.173999000
1	-1.977447000	6.725997000	0.327035000
6	-3.196210000	4.993966000	0.112378000
1	-4.141577000	5.514185000	0.214761000
8	0.345924000	5.564517000	0.118911000
1	-0.319467000	0.867226000	-0.739492000
1	1.282937000	3.428052000	-0.079988000

7	-4.477652000	2.880851000	-0.103351000
8	-5.500716000	3.545960000	-0.013666000
8	-4.479003000	1.657668000	-0.207861000
6	7.246632000	-1.760037000	0.340509000
8	8.047806000	-0.896630000	0.628709000
1	7.559230000	-2.818808000	0.254810000
6	0.716700000	-1.418217000	-0.990891000
1	0.154135000	-0.900417000	-1.773124000
1	1.109035000	-2.333248000	-1.438421000
6	-0.176760000	-1.732764000	0.213619000
1	-0.444171000	-0.792763000	0.708409000
1	0.386303000	-2.331892000	0.935802000
7	-2.551890000	-2.434441000	0.727799000
1	-3.238366000	-3.149271000	0.335022000
6	-3.221848000	-1.111832000	0.821468000
1	-2.553575000	-0.390077000	1.293716000
1	-3.490572000	-0.776205000	-0.179963000
1	-4.121583000	-1.224831000	1.426564000
6	-2.177656000	-2.977381000	2.058427000
1	-3.084107000	-3.054806000	2.659008000
1	-1.749862000	-3.969873000	1.911709000
1	-1.464208000	-2.309176000	2.541906000
35	-3.898716000	-5.013628000	-0.339869000
6	-1.425337000	-2.470450000	-0.254720000
1	-1.821522000	-2.036074000	-1.177549000
1	-1.232449000	-3.530020000	-0.444154000