

Study on the Inter- and Intra-Salt-bridge Mechanism of A β ₂₃₋₂₈ Oligomer interaction with small molecules: QM/MM

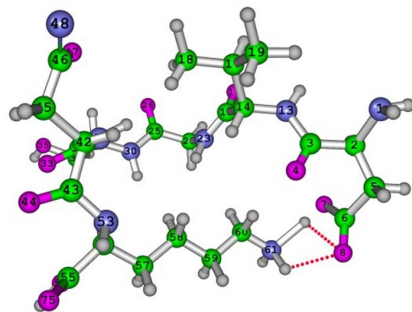
Method

*Subramaniam Boopathi, Ponmalai Kolandaivel**

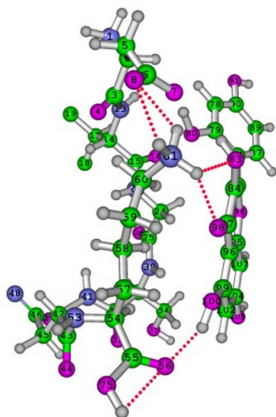
Department of Physics, Bharathiar University, Coimbatore-46, Tamilnadu, India.

*Corresponding author: ponkvel@hotmail.com

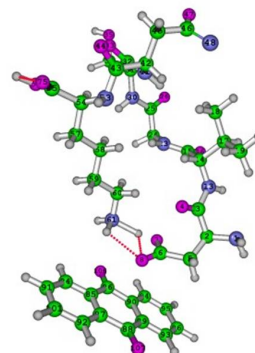
Fax: +91-422-2422387



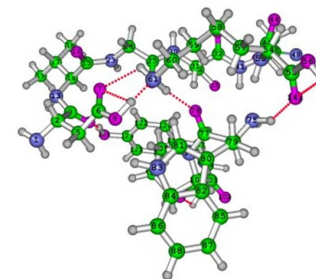
Monomer



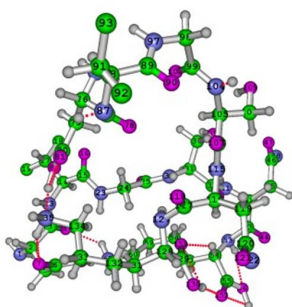
Monomer...Morin



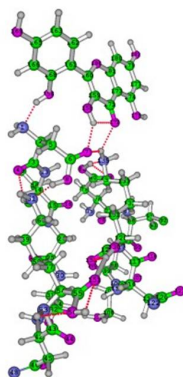
Monomer...AQ



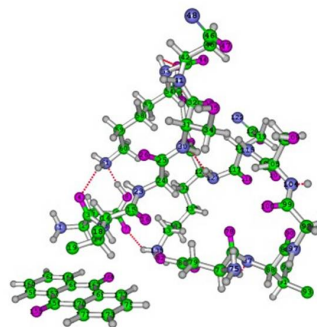
Monomer...TPT



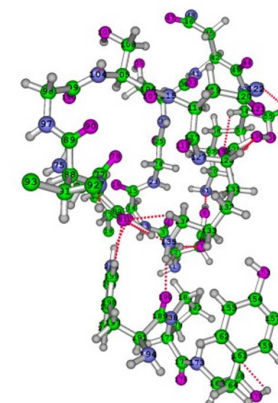
Dimer-i



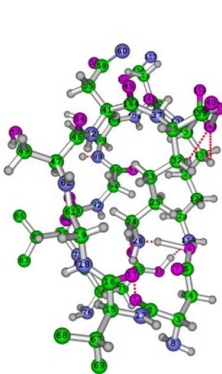
Dimer-i...Morin



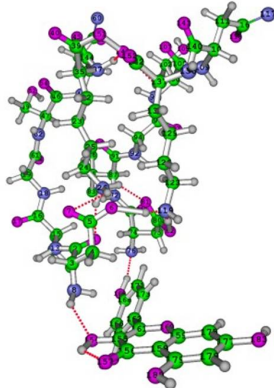
Dimer-i...AQ



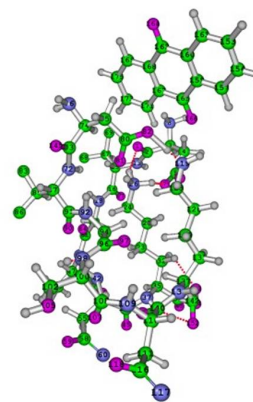
Dimer-i...TPT



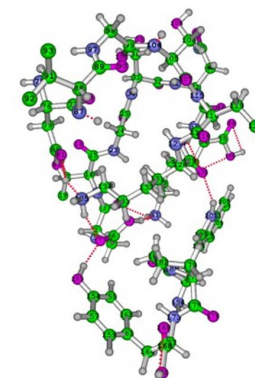
Dimer-ii



Dimer-ii...Morin



Dimer-ii...AQ



Dimer-ii...TPT

● → Oxygen
 ● → Nitrogen
 ● → Carbon
 ● → Hydrogen

Fig. S1 Optimized structure of monomer, dimer-i and dimer-ii structure with Morin, AQ and TPT molecules at ONIOM(M05-2X/6-31G*:UFF) level of theory.

Input file preparation for dimer structure are given below

```
#ONIOM(M052X/6-31++G(d,p):UFF) OPT
```

```
dimer
```

```
0 1 0 1 0 1
```

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6 6.969078158 -3.451724415 -0.188625115 H
6 6.068866158 -2.843277415 -1.269442115 H
8 6.403511158 -1.799517415 -1.789425115 H
6 6.944567158 -2.514988415 1.029276885 H
6 5.555780158 -2.533880415 1.647138885 H
8 5.159726158 -3.536378415 2.207913885 H
8 4.796018158 -1.467264415 1.490736885 H
1 8.606761158 -2.708707415 -1.110612115 H
1 6.607284158 -4.428977415 0.129938885 H
1 7.652454158 -2.908363415 1.756775885 H
1 7.250510158 -1.514620415 0.719758885 H
7 4.852452158 -3.517539415 -1.670575115 L H 3
6 4.092353158 -3.133841415 -2.866262115 L
6 2.751710158 -2.576727415 -2.433518115 L
8 1.714008158 -3.067717415 -2.848693115 L
6 3.978474158 -4.343281415 -3.827594115 L
6 3.343218158 -3.948469415 -5.119895115 L
6 5.326720158 -4.903905415 -4.136083115 L
1 4.520593158 -4.333953415 -1.108096115 L
1 4.622846158 -2.318403415 -3.407763115 L
1 3.368139158 -5.143967415 -3.357215115 L
7 2.713798158 -1.508379415 -1.594611115 L
6 1.477752158 -0.831910415 -1.195005115 L
6 1.215292158 0.366534585 -2.066574115 L
8 1.991032158 0.641836585 -2.968480115 L
1 3.613350158 -1.084853415 -1.278273115 L
1 0.609708158 -1.523947415 -1.245017115 L
1 1.579735158 -0.501368415 -0.141624115 L
```

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1	-0.544016842	0.849768585	-1.084609115	L
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1	-1.504299842	0.921940585	-3.932316115	L
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8	-0.359302842	6.693069585	0.406511885	L
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1	2.267004158	2.787030585	-0.665418115	H
1	2.962084158	3.957879585	-1.778527115	H
1	4.301869158	1.944594585	-1.951437115	H
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6	-2.248127842	-5.135300415	-1.161920115	H
6	-2.809502842	-4.217454415	-0.068607115	H
8	-2.670197842	-3.020955415	-0.171456115	H
6	-0.803777842	-4.735395415	-1.449004115	H
6	0.066256158	-4.905263415	-0.224812115	H
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6	-4.895592842	-5.221590415	0.613500885	L
6	-5.731221842	-4.032960415	0.172089885	L
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6	-5.388994842	1.851948585	-1.375579115	L
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6	-2.399940842	1.522838585	1.920614885	L
6	-1.775653842	0.220873585	2.389108885	L H 127
8	-2.475315842	-0.654060415	2.875746885	L
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6	-2.579589842	2.630980585	4.177032885	L
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8	1.192103158	2.220431585	1.550872885	H
1	2.573613158	7.499875585	2.680239885	H
1	1.688674158	3.609346585	3.366608885	H

--link1--

#ONIOM(M052X/6-31++G(d,p):UFF) OPT

Morin-dimer

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8	-2.990019130	-3.147157358	-3.058504019	H
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6	-3.633211130	-2.184829358	0.401705981	H
8	-4.104854130	-1.307393358	1.098977981	H
8	-2.329722130	-2.329656358	0.276351981	H
1	-5.223369130	-4.107757358	-2.807679019	H
1	-5.345948130	-1.459920358	-1.573937019	H
1	-5.466977130	-3.234804358	0.086774981	H
1	-4.037200130	-4.045651358	-0.639237019	H
7	-2.930699130	-0.872869358	-2.611748019	L H 3
6	-1.729343130	-0.588204358	-3.403664019	L
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1	1.510437870	-1.041207358	-0.442744019	L
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8	7.465612870	-0.284052358	-2.717266019	L
1	4.018361870	-0.336246358	-0.429159019	L
1	5.261609870	-1.698251358	-2.870930019	L
1	5.693887870	0.780714642	-2.806189019	L
1	6.430324870	0.587636642	-1.184057019	L
1	7.283918870	-0.498417358	-3.669404019	L

7	6.457002870	-3.342703358	-1.304114019	L
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6	6.513692870	-4.623871358	0.791739981	L H 53
8	7.004419870	-4.402349358	1.891516981	L
6	8.664620870	-3.680516358	-0.205451019	L
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8	9.719740870	-2.237904358	-1.747935019	L
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1	7.390979870	-5.207871358	-1.037202019	L
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1	9.262596870	-4.417385358	0.373835981	L
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6	2.706210870	-4.360272358	-0.526810019	H
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1	4.292004870	-3.599945358	1.483028981	H
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1	3.524310870	-4.714439358	-1.154948019	H
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1	1.246357870	-5.736593358	-1.347706019	H
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6	-1.021688130	5.441164642	-2.245191019	H
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6	-2.653651130	3.677905642	-1.528669019	H
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8	-3.290205130	2.564407642	-1.791420019	H
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1	-2.454656130	4.422136642	-3.530327019	H
1	-1.119957130	3.417918642	-2.972592019	H
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6	0.641071870	7.167419642	-0.130450019	L
6	2.118504870	6.823774642	-0.193779019	L
8	2.676803870	6.388829642	0.801169981	L
6	0.342460870	8.257638642	0.932739981	L
6	0.616890870	7.789922642	2.324574981	L
6	1.124686870	9.501855642	0.671004981	L
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1	0.321143870	7.599709642	-1.106495019	L
1	-0.733839130	8.526477642	0.874556981	L
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6	4.246648870	6.709871642	-1.467008019	L
6	4.534070870	5.246283642	-1.273320019	L
8	4.060359870	4.440774642	-2.057862019	L
1	2.317589870	7.327706642	-2.206205019	L
1	4.601297870	7.011352642	-2.476219019	L
1	4.795858870	7.330690642	-0.726362019	L
7	5.309035870	4.831937642	-0.234114019	L
6	5.650956870	3.425428642	0.028899981	L
6	5.047103870	2.968220642	1.337547981	L
8	4.540016870	3.785679642	2.089331981	L
6	7.179910870	3.271088642	0.063347981	L
8	7.740406870	3.661219642	-1.161303019	L
1	5.692491870	5.549378642	0.423641981	L
1	5.249371870	2.768430642	-0.773364019	L
1	7.601331870	3.914370642	0.865636981	L
1	7.469295870	2.221402642	0.294808981	L
1	7.546205870	2.933017642	-1.807517019	L
7	5.060507870	1.645863642	1.666769981	L
6	4.536124870	1.091538642	2.922472981	L
6	3.073807870	1.464993642	3.098850981	L H 127
8	2.740445870	2.279096642	3.948281981	L
6	5.432933870	1.505385642	4.108970981	L
6	5.071181870	0.767340642	5.366826981	L
8	4.669210870	1.378758642	6.340463981	L
7	5.202965870	-0.571693358	5.430271981	L
1	5.513372870	0.972617642	1.009643981	L
1	4.584107870	-0.017600358	2.846741981	L
1	6.492591870	1.276439642	3.863060981	L
1	5.362920870	2.601739642	4.279941981	L

7	2.060786870	0.866001642	2.269117981	H
6	1.398335870	-0.204739358	2.984363981	H
6	2.030856870	-1.566634358	2.765870981	H
8	1.752601870	-2.411076358	3.750626981	H
6	-0.082549130	-0.237192358	2.491897981	H
6	-0.809989130	1.021427642	2.969424981	H
6	-2.259803130	1.127199642	2.494925981	H
6	-2.375856130	1.348247642	0.989977981	H
7	-3.729752695	1.735146967	0.360061547	H
1	2.513816870	0.408466642	1.469694981	H
1	1.337523870	-0.040630358	4.066311981	H
1	-0.087144130	-0.313044358	1.401961981	H
1	-0.568264130	-1.134376358	2.885521981	H
1	-0.788208130	1.030921642	4.063803981	H
1	-0.249866130	1.897999642	2.635469981	H
1	-2.827153130	0.233867642	2.767395981	H
1	-2.729599130	1.975880642	3.002504981	H
1	-1.729430130	2.173145642	0.681496981	H
1	-2.066832130	0.451978642	0.450902981	H
1	-4.072629695	2.543289967	0.872588547	H
1	-3.643880565	2.089926318	-0.650004584	H
1	-4.369349130	0.900822642	0.799305981	H
1	-5.966015130	-2.805182358	-3.435305019	H
1	-0.545188130	6.130927642	-4.110308019	H
8	3.368737870	-4.645322358	3.749524981	H
8	2.710211870	-1.854424358	1.798316981	H
1	4.771850870	-6.333932358	4.191354981	H
1	2.265049870	-3.242140358	3.620299981	H
1	-7.312232130	-3.026564358	-1.636602019	H
8	-7.873011130	-2.406508358	-1.116588019	H
1	-5.981695130	-1.201082358	1.512685981	H
8	-6.841084130	-1.649694358	1.356374981	H
6	-7.796808130	-0.705997358	1.306138981	H
6	-9.068655130	-0.993915358	0.956973981	H
6	-9.558787130	-2.306902358	0.528508981	H
6	-10.691191130	-2.876220358	1.108814981	H
6	-11.139352130	-4.138201358	0.745567981	H
1	-12.013480130	-4.572207358	1.216628981	H
6	-10.433154130	-4.848998358	-0.226023019	H
6	-9.318768130	-4.294129358	-0.845065019	H
1	-8.812956130	-4.850198358	-1.623930019	H
6	-8.890989130	-3.017453358	-0.487001019	H
8	-10.803651130	-6.098108358	-0.622490019	H

1	-11.589507130	-6.363001358	-0.129507019	H
6	-7.382752130	0.655870642	1.652978981	H
8	-6.200102130	0.861057642	1.922922981	H
6	-8.449906130	1.647777642	1.643088981	H
6	-8.249826130	3.022382642	1.931232981	H
8	-6.993599130	3.435218642	2.195996981	H
1	-7.006600130	4.388038642	2.354303981	H
6	-9.311962130	3.908315642	1.934876981	H
1	-9.169318130	4.958891642	2.153460981	H
6	-10.602028130	3.449309642	1.644895981	H
6	-10.841564130	2.119323642	1.346512981	H
6	-9.758347130	1.240032642	1.344563981	H
8	-11.589848130	4.377124642	1.666709981	H
1	-12.429544130	3.955788642	1.446040981	H
1	-11.827035130	1.744844642	1.103807981	H
1	-11.216632130	-2.318900358	1.874044981	H
8	-10.051856130	-0.036432358	1.017644981	H

--Link1--

#ONIOM(M052X/6-31++G(d,p):UFF) Opt

AQ-dimer

0 1 0 1 0 1

7	6.828788267	-3.764472796	-0.803233307	H
6	5.752543267	-2.840652796	-1.141341307	H
6	4.782816267	-2.666968796	0.031987693	H
8	4.309587267	-3.655483796	0.553311693	H
6	4.959554267	-3.407197796	-2.330063307	H
6	3.967826267	-2.360203796	-2.809312307	H
8	4.366706267	-1.340905796	-3.334369307	H
8	2.685432267	-2.572546796	-2.570573307	H
1	6.427616267	-4.558201796	-0.313125307	H
1	6.176850267	-1.886196796	-1.449815307	H
1	5.671782267	-3.600074796	-3.130657307	H
1	4.476423267	-4.339539796	-2.034556307	H
7	4.454204267	-1.343171796	0.517675693	L H 3
6	3.759436267	-1.116730796	1.790662693	L
6	2.418247267	-0.470753796	1.508465693	L
8	2.153948267	0.632258204	1.960336693	L
6	4.660084267	-0.288490796	2.739210693	L
6	4.034107267	-0.136876796	4.085943693	L
6	5.981832267	-0.955364796	2.925082693	L

1	4.770937267	-0.512071796	-0.031356307	L
1	3.550915267	-2.089769796	2.290057693	L
1	4.833277267	0.720289204	2.310178693	L
7	1.498858267	-1.140487796	0.765096693	L
6	0.131718267	-0.659794796	0.551137693	L
6	-0.785899733	-1.113392796	1.653620693	L
8	-0.339587733	-1.753467796	2.592765693	L
1	1.731127267	-2.098285796	0.421661693	L
1	0.111486267	0.449314204	0.475432693	L
1	-0.244606733	-1.067045796	-0.407460307	L
7	-2.109502733	-0.807154796	1.593058693	L
6	-3.075703733	-1.144526796	2.647347693	L
6	-4.192286733	-1.987944796	2.075921693	L
8	-4.827248733	-1.571167796	1.120752693	L
6	-3.634143733	0.147892204	3.260946693	L
8	-4.500485733	-0.138775796	4.325762693	L
1	-2.455503733	-0.260824796	0.771245693	L
1	-2.575667733	-1.706270796	3.466390693	L
1	-2.796793733	0.792775204	3.613209693	L
1	-4.194201733	0.719793204	2.493843693	L
1	-3.929911733	-0.406644796	5.092719693	L
7	-4.504717733	-3.188511796	2.639170693	L
6	-5.687241733	-3.990064796	2.286447693	L
6	-5.659346733	-4.381295796	0.825570693	L H 53
8	-6.576438733	-4.070406796	0.076095693	L
6	-6.991388733	-3.268313796	2.694341693	L
6	-7.018736733	-2.955898796	4.162600693	L
8	-7.073415733	-1.799561796	4.540797693	L
7	-7.000720733	-3.951950796	5.068932693	L
1	-3.945688733	-3.518804796	3.458392693	L
1	-5.643415733	-4.942991796	2.860005693	L
1	-7.108700733	-2.330125796	2.109238693	L
1	-7.862935733	-3.917921796	2.460780693	L
7	-4.594858733	-5.186858796	0.352799693	H
6	-3.957830733	-4.655649796	-0.845667307	H
6	-4.597012733	-5.053928796	-2.166290307	H
8	-5.558016733	-5.980085796	-2.059908307	H
6	-2.485495733	-5.103477796	-0.912567307	H
6	-1.683275733	-4.488982796	0.229519693	H
6	-0.205999733	-4.885262796	0.196485693	H
6	0.497528267	-4.400581796	-1.068761307	H
7	1.955306267	-4.621477796	-1.074684307	H
1	-4.946078733	-6.122201796	0.193573693	H

1	-3.928707733	-3.563071796	-0.843507307	H
1	-2.440451733	-6.198051796	-0.866099307	H
1	-2.082995733	-4.786626796	-1.874546307	H
1	-1.765240733	-3.401885796	0.152543693	H
1	-2.134649733	-4.788638796	1.176042693	H
1	0.300923267	-4.448266796	1.063181693	H
1	-0.102031733	-5.972865796	0.281932693	H
1	0.098125267	-4.894074796	-1.955068307	H
1	0.313713267	-3.331922796	-1.202965307	H
1	2.164694267	-5.600742796	-1.233530307	H
1	2.314297733	-3.864790204	-1.727834693	H
1	2.364169267	-4.383919796	-0.174334307	H
7	0.627003267	5.954483204	1.829495693	H
6	1.328234267	5.353687204	0.694298693	H
6	0.233202267	5.051138204	-0.337567307	H
8	-0.505365733	4.112696204	-0.153714307	H
6	2.058202267	4.053020204	1.020465693	H
6	2.700634267	3.463255204	-0.214293307	H
8	2.540151267	3.960481204	-1.319679307	H
8	3.402264267	2.376393204	0.014354693	H
1	-0.040436733	5.277981204	2.185436693	H
1	2.032190267	6.082653204	0.292357693	H
1	2.814431267	4.200426204	1.796180693	H
1	1.340217267	3.321853204	1.399629693	H
7	0.042188267	5.906346204	-1.492702307	L H 77
6	-0.546912733	7.201967204	-1.105644307	L
6	-1.961561733	6.993043204	-0.595007307	L
8	-2.797881733	6.494097204	-1.331767307	L
6	-0.499784733	8.193891204	-2.296309307	L
6	-1.211537733	7.673176204	-3.501826307	L
6	-1.075538733	9.519356204	-1.922302307	L
1	0.981521267	6.066050204	-1.925248307	L
1	0.073560267	7.657054204	-0.299468307	L
1	0.561406267	8.362137204	-2.578338307	L
7	-2.285268733	7.317052204	0.686060693	L
6	-3.581680733	6.988357204	1.279525693	L
6	-3.708718733	5.499680204	1.444222693	L
8	-2.921221733	4.916763204	2.171467693	L
1	-1.556307733	7.724297204	1.314405693	L
1	-3.666591733	7.470195204	2.277326693	L
1	-4.396393733	7.397237204	0.643225693	L
7	-4.675523733	4.813982204	0.776422693	L
6	-4.802050733	3.348474204	0.797503693	L

6	-4.685805733	2.783389204	-0.601547307	L
8	-4.670105733	3.536600204	-1.561969307	L
6	-6.150917733	2.960391204	1.423007693	L
8	-6.246260733	3.456990204	2.730836693	L
1	-5.361586733	5.349026204	0.195602693	L
1	-3.989556733	2.894681204	1.405561693	L
1	-6.979064733	3.390663204	0.819650693	L
1	-6.281142733	1.854372204	1.429745693	L
1	-5.666167733	2.882223204	3.295696693	L
7	-4.590488733	1.436726204	-0.781811307	L
6	-4.546086733	0.762708204	-2.086719307	L
6	-3.337669733	1.220613204	-2.886863307	L H 127
8	-3.460427733	2.069892204	-3.757681307	L
6	-5.884009733	0.933468204	-2.837319307	L
6	-5.953344733	0.056017204	-4.055045307	L
8	-6.034237733	0.553737204	-5.163666307	L
7	-5.940545733	-1.284925796	-3.927288307	L
1	-4.591683733	0.823969204	0.062897693	L
1	-4.425997733	-0.325442796	-1.892650307	L
1	-6.721348733	0.658289204	-2.159861307	L
1	-6.031401733	1.995648204	-3.129728307	L
7	-2.033637733	0.664386204	-2.632964307	H
6	-1.762888733	-0.414847796	-3.563438307	H
6	-2.308348733	-1.752378796	-3.098403307	H
8	-2.698217733	-2.525685796	-4.101494307	H
6	-0.214618733	-0.557041796	-3.673382307	H
6	0.410544267	0.700699204	-4.282245307	H
6	1.921888267	0.795566204	-4.060013307	H
6	2.272421267	0.974060204	-2.583419307	H
7	3.659432760	1.478450657	-2.130146732	H
1	-2.039337733	0.220864204	-1.706973307	H
1	-2.132912733	-0.213785796	-4.573602307	H
1	0.178816267	-0.745069796	-2.674179307	H
1	0.021078267	-1.436971796	-4.278402307	H
1	0.190077267	0.720121204	-5.353341307	H
1	-0.067824733	1.579315204	-3.843197307	H
1	2.440398267	-0.083760796	-4.447857307	H
1	2.296390267	1.666388204	-4.608925307	H
1	1.620094267	1.732170204	-2.143525307	H
1	2.128417267	0.041910204	-2.037359307	H
1	3.858185760	2.305671657	-2.685031732	H
1	3.640658774	1.848968752	-1.146054882	H
1	4.304935267	0.659916204	-2.621854307	H

1	7.486971267	-3.320386796	-0.171810307	H
1	1.281611267	6.157252204	2.575825693	H
8	-4.259097733	-4.634472796	-3.256679307	H
8	-2.362792733	-2.078274796	-1.927104307	H
1	-5.857485733	-6.173535796	-2.964002307	H
1	-3.124260733	-3.335283796	-3.735462307	H
8	9.897067000	-0.204767000	2.898073000	H
6	9.222763000	-0.062700000	1.894973000	H
6	9.409445000	-0.949891000	0.710163000	H
6	10.384588000	-1.943224000	0.762844000	H
1	10.968679000	-2.042134000	1.668058000	H
6	10.586691000	-2.774074000	-0.333453000	H
1	11.342558000	-3.547798000	-0.290844000	H
6	9.820177000	-2.612654000	-1.487504000	H
1	9.975370000	-3.264604000	-2.336839000	H
6	8.845515000	-1.623679000	-1.545304000	H
1	8.233701000	-1.482983000	-2.426937000	H
6	8.632062000	-0.794591000	-0.445208000	H
6	7.556318000	0.234613000	-0.516974000	H
8	6.826102000	0.309152000	-1.491038000	H
6	7.389490000	1.137449000	0.652003000	H
6	8.180554000	0.995305000	1.800725000	H
6	7.977100000	1.837112000	2.890870000	H
1	8.595903000	1.703612000	3.767981000	H
6	6.987714000	2.812566000	2.836524000	H
1	6.825810000	3.461976000	3.687293000	H
6	6.197862000	2.948281000	1.696127000	H
1	5.412506000	3.691406000	1.657550000	H
6	6.400183000	2.114649000	0.603227000	H
1	5.786544000	2.194264000	-0.281613000	H

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#ONIOM(M052X/6-31++G(d,p):UFF) OPT

TPT-dimer

0 1 0 1 0 1

7	4.757922431	-3.640601955	3.691377281	H
6	3.741053431	-2.977419955	2.882131281	H
6	2.496134431	-2.660319955	3.724724281	H
8	1.881588431	-3.579999955	4.224202281	H
6	3.324179431	-3.907534955	1.731375281	H

6	2.520436431	-3.117016955	0.717978281	H
8	3.078748431	-2.304038955	-0.002151719	H
8	1.221194431	-3.280063955	0.690200281	H
1	4.316184431	-4.369423955	4.242924281	H
1	4.183545431	-2.073320955	2.460796281	H
1	4.231347431	-4.266118955	1.248655281	H
1	2.763895431	-4.750918955	2.137157281	H
7	2.100340431	-1.335314955	3.922636281	L H 3
6	0.945885431	-0.952361955	4.746715281	L
6	-0.115987569	-0.373609955	3.836526281	L
8	-0.484359569	0.782608045	3.968920281	L
6	1.399341431	0.016959045	5.865905281	L
6	0.267645431	0.357356045	6.778373281	L
6	2.477611431	-0.601155955	6.691566281	L
1	2.643512431	-0.574544955	3.455590281	L
1	0.501891431	-1.848971955	5.235605281	L
1	1.794926431	0.954240045	5.418342281	L
7	-0.657208569	-1.158165955	2.868464281	L
6	-1.652187569	-0.692637955	1.900636281	L
6	-3.039459569	-1.120729955	2.294830281	L
8	-3.211214569	-1.768524955	3.315414281	L
1	-0.357484569	-2.155274955	2.804588281	L
1	-1.625401569	0.413270045	1.800311281	L
1	-1.405936569	-1.122159955	0.908334281	L
7	-4.095862569	-0.764639955	1.516188281	L
6	-5.499406569	-1.024270955	1.870305281	L
6	-6.231196569	-1.644445955	0.701108281	L
8	-6.108532569	-1.155318955	-0.408997719	L
6	-6.170349569	0.294396045	2.283844281	L
8	-7.492738569	0.074071045	2.695763281	L
1	-3.904290569	-0.195341955	0.660812281	L
1	-5.556461569	-1.716096955	2.739269281	L
1	-5.589998569	0.770495045	3.107005281	L
1	-6.178218569	1.004624045	1.431058281	L
1	-7.444949569	-0.340561955	3.596511281	L
7	-7.048917569	-2.717094955	0.889627281	L
6	-7.902353569	-3.301742955	-0.157761719	L
6	-7.060220569	-3.824681955	-1.300084719	L H 53
8	-7.204168569	-3.397749955	-2.438520719	L
6	-8.994741569	-2.308595955	-0.615903719	L
6	-9.830906569	-1.830065955	0.535425281	L
8	-9.850575569	-0.647649955	0.826708281	L
7	-10.575671569	-2.701792955	1.241951281	L

1	-7.150183569	-3.109088955	1.853389281	L
1	-8.422046569	-4.186706955	0.273058281	L
1	-8.534136569	-1.437680955	-1.130710719	L
1	-9.663981569	-2.809366955	-1.348956719	L
7	-6.122429569	-4.851190955	-1.040043719	H
6	-4.754746569	-4.467186955	-1.356580719	H
6	-4.331673569	-4.907557955	-2.747063719	H
8	-4.843160569	-5.796652955	-3.358352719	H
6	-3.781784569	-5.222037955	-0.419960719	H
6	-3.823440569	-4.655474955	0.997551281	H
6	-2.669703569	-5.159977955	1.873464281	H
6	-1.324519569	-4.697538955	1.317305281	H
7	-0.145015569	-4.927483955	2.172951281	H
1	-6.378786569	-5.673861955	-1.574372719	H
1	-4.574442569	-3.402062955	-1.220057719	H
1	-4.073453569	-6.276712955	-0.419449719	H
1	-2.776932569	-5.146565955	-0.828082719	H
1	-3.751920569	-3.566350955	0.933776281	H
1	-4.787880569	-4.890363955	1.449448281	H
1	-2.789251569	-4.764617955	2.887295281	H
1	-2.693448569	-6.252258955	1.949777281	H
1	-1.106915569	-5.182588955	0.366273281	H
1	-1.370480569	-3.630183955	1.100845281	H
1	0.039870431	-5.918503955	2.280996281	H
1	0.501448569	-4.333305045	1.641799719	H
1	-0.268845569	-4.545537955	3.105724281	H
7	-1.351594569	5.553207045	2.206809281	H
6	-0.327538569	4.778520045	1.499387281	H
6	-0.866403569	4.604714045	0.075566281	H
8	-1.771470569	3.827032045	-0.127841719	H
6	-0.053555569	3.402493045	2.096159281	H
6	1.004579431	2.650058045	1.302830281	H
8	1.367210431	3.124500045	0.209351281	H
8	1.452676431	1.565161045	1.811795281	H
1	-2.192236569	4.986801045	2.249356281	H
1	0.594608431	5.359492045	1.479528281	H
1	0.263096431	3.483076045	3.139202281	H
1	-0.976017569	2.816747045	2.077227281	H
7	-0.353135569	5.411699045	-1.015561719	L H 77
6	-0.769209569	6.821774045	-0.887938719	L
6	-2.277694569	6.932701045	-1.020268719	L
8	-2.823075569	6.506646045	-2.026325719	L
6	-0.031804569	7.695678045	-1.934508719	L

6	-0.284723569	7.242873045	-3.335219719	L
6	-0.414044569	9.133059045	-1.808330719	L
1	0.691293431	5.355923045	-0.986258719	L
1	-0.457051569	7.203227045	0.111436281	L
1	1.061498431	7.626900045	-1.750233719	L
7	-3.021485569	7.461761045	-0.010849719	L
6	-4.481675569	7.374304045	0.014847281	L
6	-4.891551569	5.956618045	0.292644281	L
8	-4.662271569	5.480791045	1.392136281	L
1	-2.544658569	7.805603045	0.853224281	L
1	-4.882767569	8.035178045	0.813257281	L
1	-4.896800569	7.734229045	-0.951723719	L
7	-5.470145569	5.204790045	-0.681363719	L
6	-5.690441569	3.755022045	-0.566827719	L
6	-4.923868569	3.016079045	-1.642496719	L
8	-4.407433569	3.637769045	-2.556596719	L
6	-7.192105569	3.451483045	-0.675484719	L
8	-7.899467569	4.105136045	0.343464281	L
1	-5.710822569	5.660278045	-1.591824719	L
1	-5.328889569	3.378671045	0.415702281	L
1	-7.574536569	3.806461045	-1.656678719	L
1	-7.377316569	2.354339045	-0.619293719	L
1	-7.723085569	3.600042045	1.180018281	L
7	-4.818487569	1.659819045	-1.583032719	L
6	-4.183976569	0.801212045	-2.595689719	L
6	-2.680519569	1.003270045	-2.608679719	L H 127
8	-2.205899569	2.044332045	-3.035632719	L
6	-4.826319569	1.014431045	-3.985267719	L
6	-4.550739569	-0.129085955	-4.916653719	L
8	-3.837152569	0.032223045	-5.890417719	L
7	-5.114715569	-1.332026955	-4.696373719	L
1	-5.241648569	1.179598045	-0.760839719	L
1	-4.378631569	-0.252622955	-2.296217719	L
1	-5.928396569	1.109600045	-3.872957719	L
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1	0.116619431	-1.866688955	-1.977279719	H
1	-0.082740569	-2.488385955	-3.605536719	H
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1	2.465866431	-1.126879955	-2.421920719	H
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6	5.206019431	-1.020536955	-4.880704719	H
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