

Supporting Information

Thermally Activated Delayed Fluorescence Poly(dendrimer)s – Detrapping Excitons for Reverse Intersystem Crossing

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Table S1. Thermal stability of **Da**, **Pa**, **Db** and **Pb**.

Compound	T_{decomp} (°C) ^a
Da	443
Pa	430
Db	536
Pb	440

^a decomposition temperature determined by 5 wt% loss.

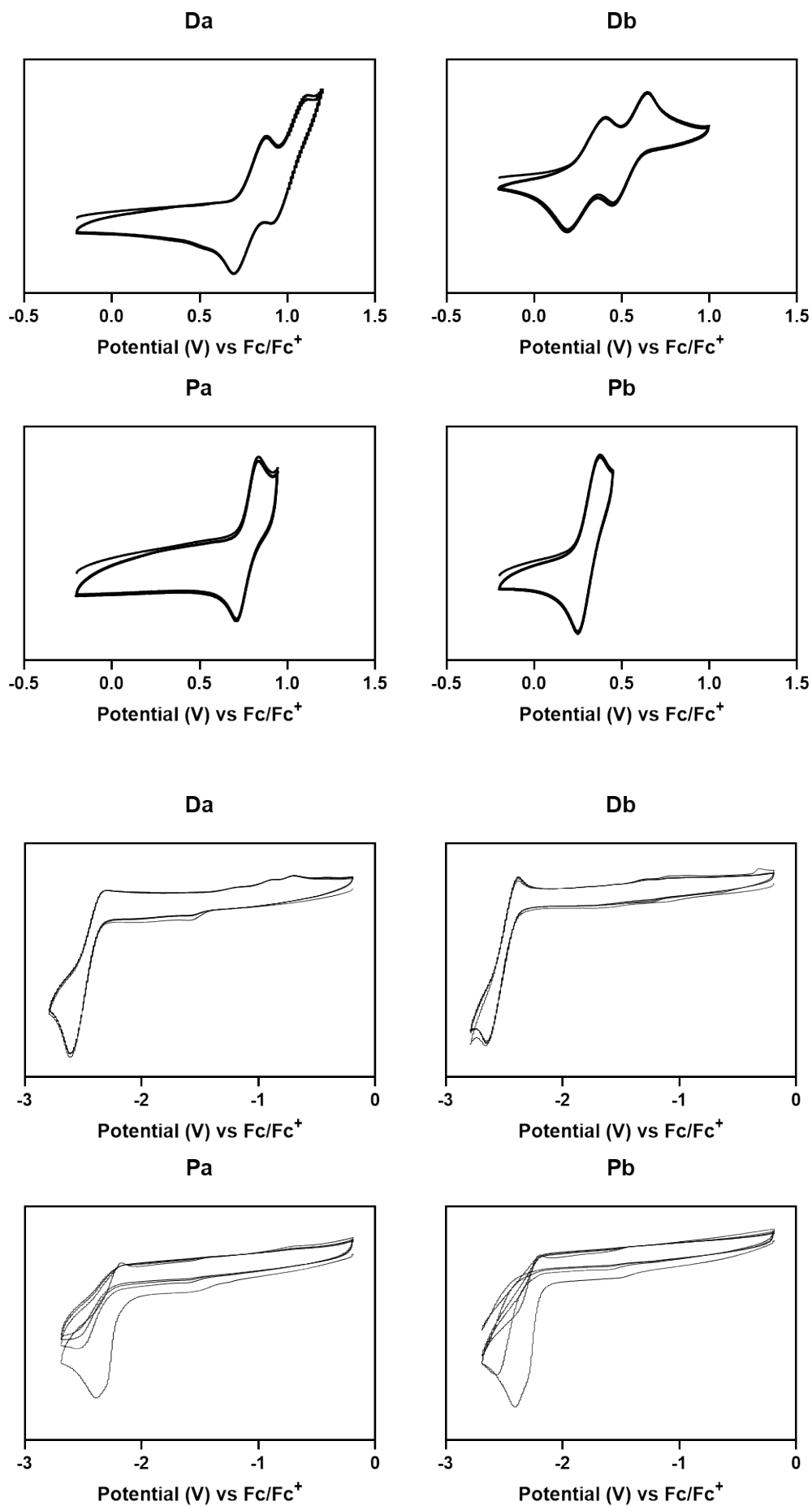


Figure S1. Cyclic voltammograms of **Da**, **Pa**, **Db** and **Pb** in dichloromethane (top) or tetrahydrofuran (bottom) in the presence of 0.1 M tetra-*n*-butylammonium perchlorate at room temperature.

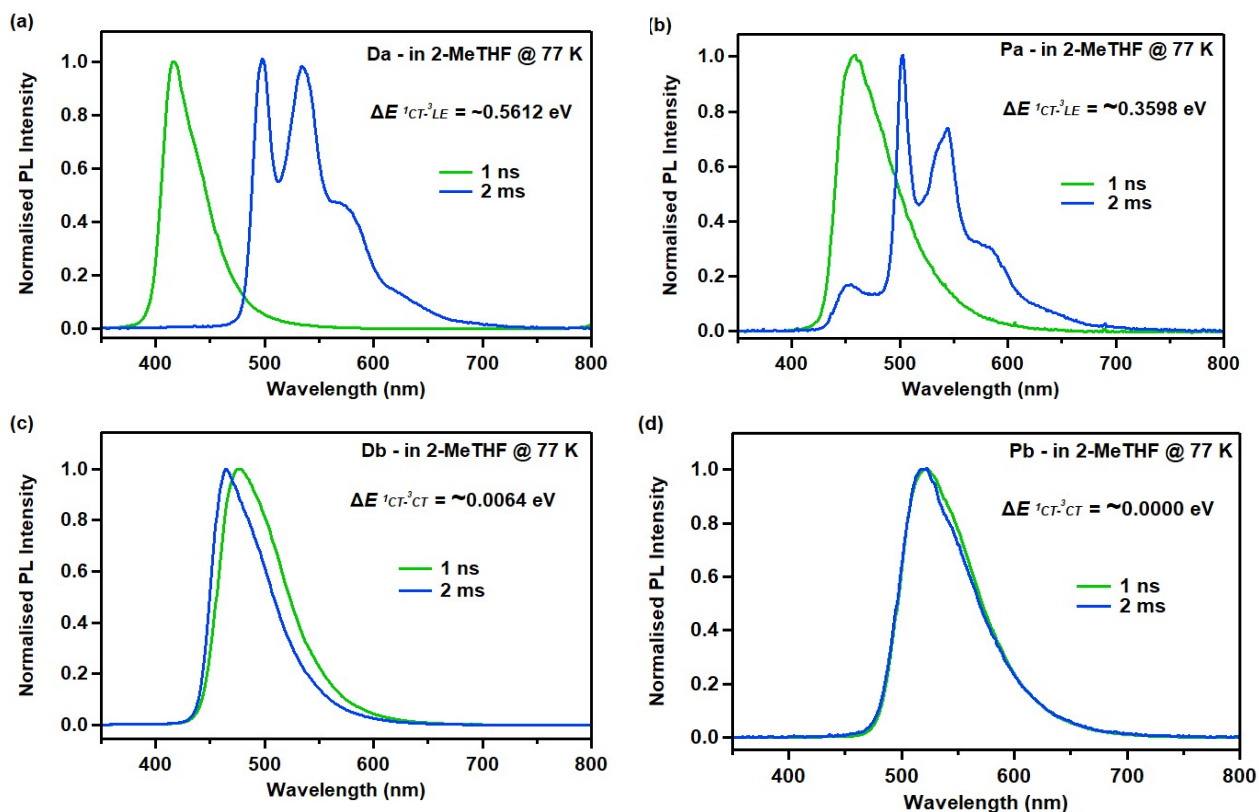


Figure S2. Solution PL spectra measured at 77 K and the estimated energy difference estimated using the difference in energy between the onset of the prompt PL and the phosphorescence of (a) **Da**, (b) **Pa** (c) **Db** and (d) **Pb**.

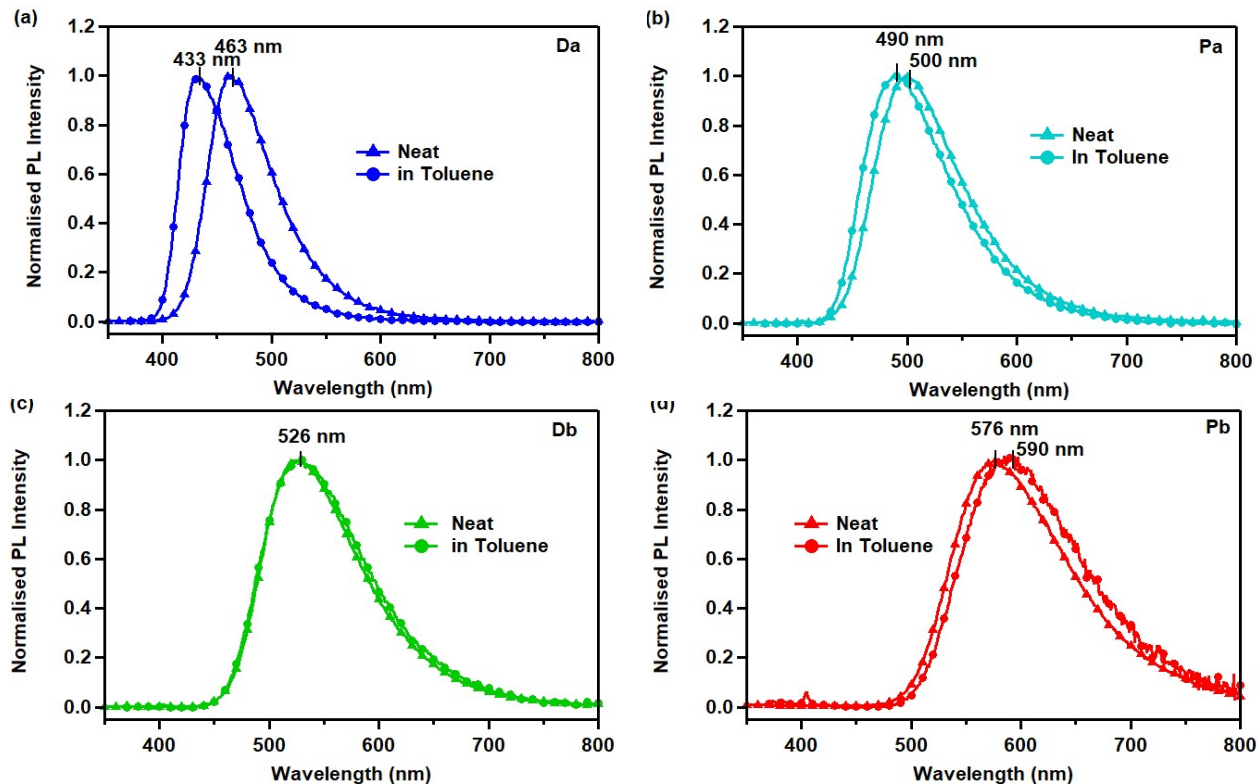


Figure S3. The steady-state PL spectra in toluene and neat films of (a) **Da**, (b) **Pa** (c) **Db** and (d) **Pb** measured at 300 K.

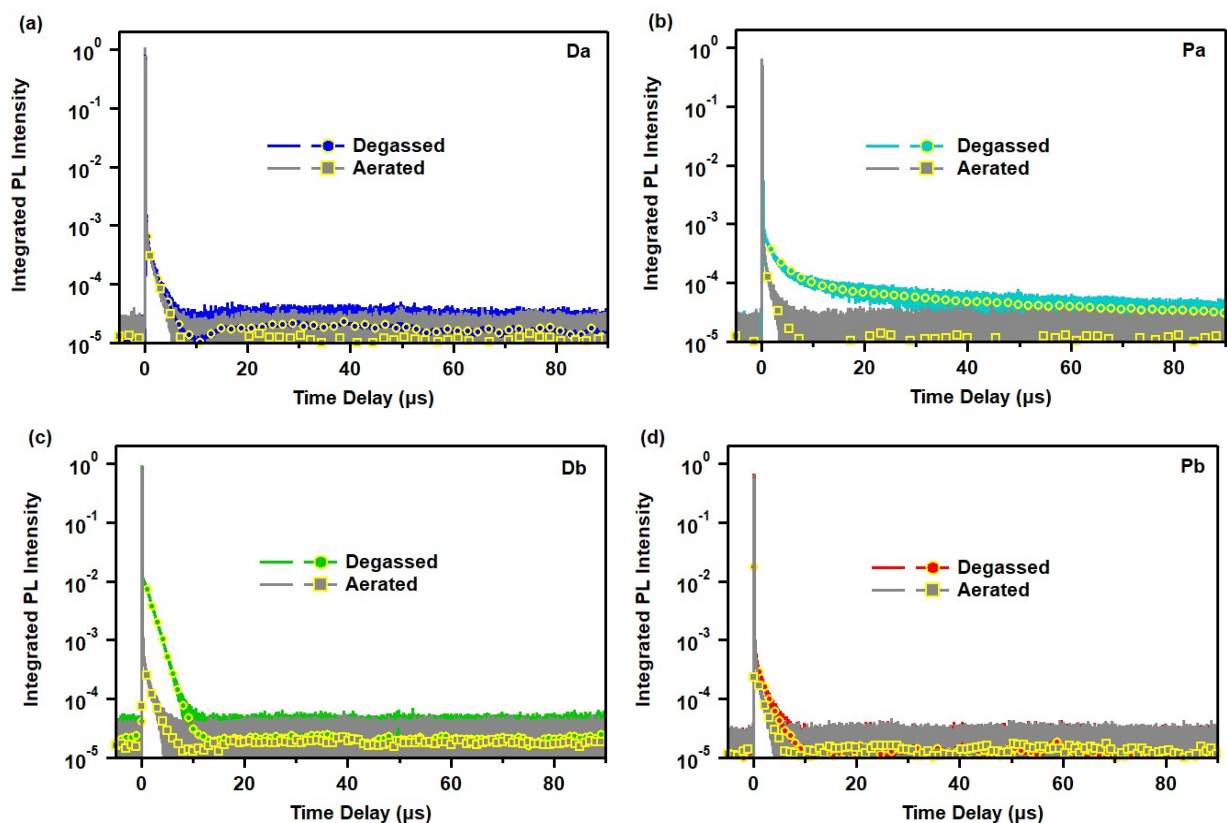


Figure S4. PL decay of (a) **Da**, (b) **Pa**, (c) **Db** and (d) **Pb** in deoxygenated and aerated toluene solution at 300 K.

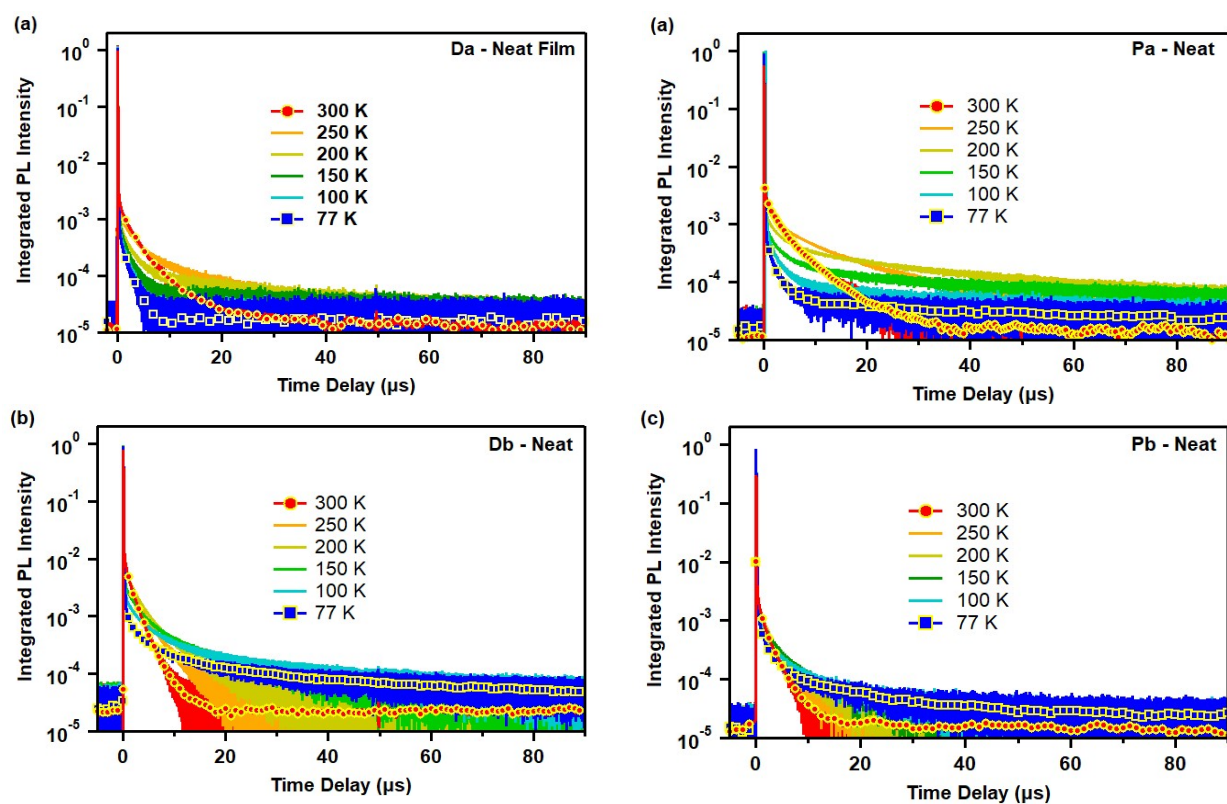


Figure S5. PL decay curves of neat films of (a) **Pa**, (b) **Db** and (c) **Pb** at temperatures varying between 77–300 K.

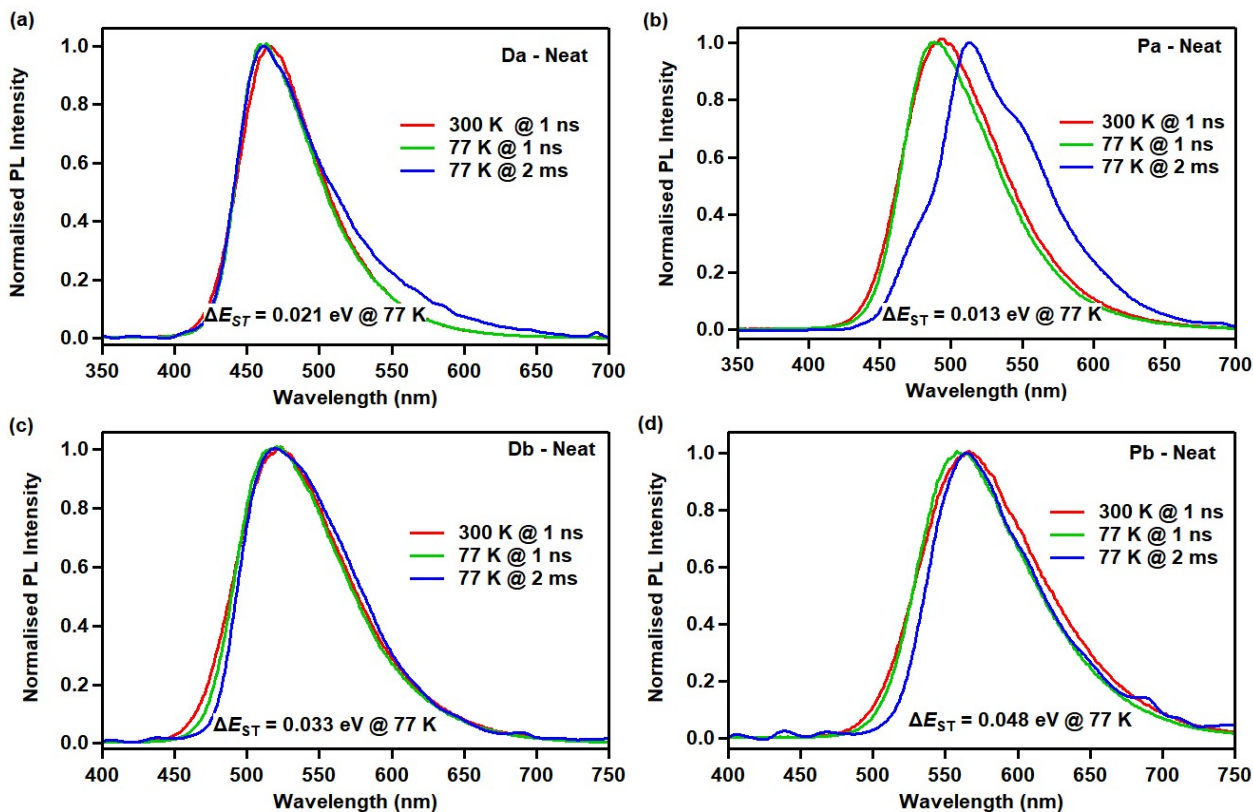
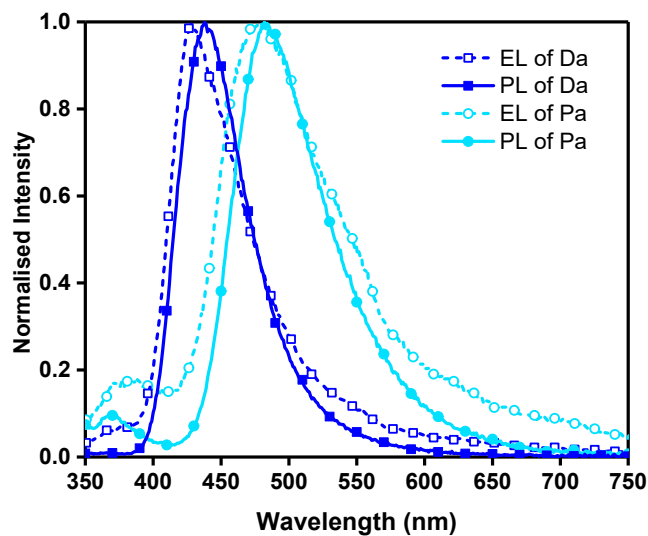


Figure S6. PL spectra of the neat films measured at 300 K (prompt) and 77 K (prompt and delayed) and the estimated energy difference calculated using the short wavelength onsets for the prompt and delayed components at 77 K for (a) **Da**, (b) **Pa** (c) **Db** and (d) **Pb**.

(a)



(b)

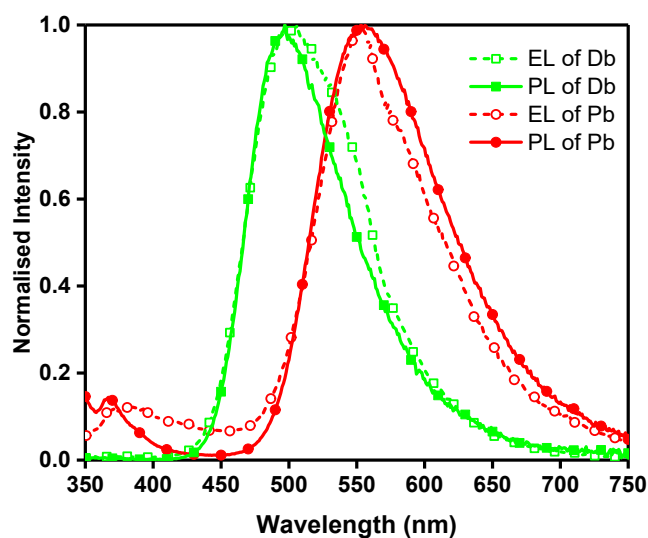


Figure S7. Comparison of EL and PL spectra of MCP blended film with (a) **Da** and **Pa**, (b) **Db** and **Pb**

Atom coordinates for all optimized geometries and the energies of all optimized ground-state structures of the compounds Da, Ma, Db and Mb.

Atom coordinates for optimized S0 structure of Da at B3LYP/6-31G(d) level of theory (energy=-3672.4636 a.u.)

C	-0.04246800	-1.22218500	-2.19705100
C	-0.03616500	-1.20864900	-3.59450800
C	0.00000000	0.00000000	-4.28658000
C	0.03616500	1.20864800	-3.59450800
C	0.04246800	1.22218500	-2.19705100
C	0.00000000	0.00000000	-1.48411400
C	0.00000000	0.00000000	-0.05235900

N	0.00000000	0.00000000	1.11045700
C	-2.82789700	4.66075800	-2.29511700
C	-2.39824400	5.82295800	-1.61306800
C	-1.16728700	5.79225100	-0.94322100
C	-0.38600500	4.63502800	-0.96326100
C	-0.84520600	3.49256700	-1.66072900
C	-2.07214700	3.49269700	-2.32549200
C	0.89469100	4.28519300	-0.37875200
C	1.16488500	2.94523700	-0.74483100
N	0.09225800	2.45939500	-1.51238300
C	1.82603900	4.99697100	0.38004800
C	3.02507400	4.38828800	0.77345800
C	3.26745800	3.05220800	0.37777800
C	2.35784700	2.32156800	-0.37958300
C	4.02367400	5.12983400	1.58418700
C	-3.23649800	7.04849200	-1.60805800
C	-2.64534100	8.32509900	-1.69547800
C	-3.43770700	9.46400700	-1.68611200
C	-4.83942700	9.35922100	-1.59424200
C	-5.44141000	8.10270800	-1.50840300
C	-4.63896500	6.96289300	-1.51413700
C	3.60979400	6.02225900	2.59200700
C	4.52948400	6.73641000	3.35798900
C	5.89400500	6.55768800	3.12421000
C	6.32660700	5.66421000	2.12474400
C	5.40536800	4.96080000	1.36200000
C	7.07271900	7.15985100	3.75675800
C	8.22656500	6.63457600	3.14030800
H	8.07714100	3.50073100	1.60873500
C	-3.00618600	10.92821000	-1.77792600
C	-4.35824400	11.63977800	-1.71862400
C	-5.41231700	10.70959100	-1.61292000
C	-4.62918700	13.00297100	-1.75597200
C	-5.95858200	13.43732000	-1.68828000
C	-7.00347600	12.51318700	-1.58423900
C	-6.73833500	11.14249600	-1.54571100
C	7.18145700	8.09519700	4.78819200
C	8.45277200	8.50175200	5.19941000
C	9.59846500	7.98137700	4.58856600
C	9.48907100	7.04358900	3.55450500
H	1.56565300	-8.40541100	-1.79590100
H	6.52113100	-8.00513500	-1.42681900
H	10.38621700	6.64490600	3.08625100
H	3.82400000	-13.72988100	-1.83614500
H	6.18015000	-14.50089900	-1.71666000
H	8.03054700	-12.86484600	-1.53247900
H	7.55409000	-10.42842600	-1.46425200
H	5.10351000	-5.98573400	-1.41624300
H	-2.54837900	-6.13459300	2.79402800
H	-4.17963900	-7.41271800	4.13396400
H	-5.74033200	-4.29460100	0.57063700
C	2.82789700	-4.66075800	-2.29511700
C	2.39824500	-5.82295900	-1.61306800
C	1.16728700	-5.79225100	-0.94322100
C	0.38600500	-4.63502800	-0.96326100

C	0.84520600	-3.49256700	-1.66072900
C	2.07214700	-3.49269700	-2.32549200
C	-0.89469100	-4.28519300	-0.37875200
C	-1.16488400	-2.94523700	-0.74483200
N	-0.09225800	-2.45939500	-1.51238300
C	-1.82603800	-4.99697100	0.38004800
C	-3.02507400	-4.38828800	0.77345800
C	-3.26745800	-3.05220800	0.37777800
C	-2.35784700	-2.32156800	-0.37958300
C	-4.02367400	-5.12983300	1.58418700
C	3.23649800	-7.04849200	-1.60805800
C	2.64534100	-8.32509900	-1.69547800
C	3.43770700	-9.46400700	-1.68611200
C	4.83942700	-9.35922100	-1.59424200
C	5.44141000	-8.10270800	-1.50840300
C	4.63896500	-6.96289400	-1.51413700
C	-3.60979400	-6.02225900	2.59200700
C	-4.52948400	-6.73641000	3.35798900
C	-5.89400500	-6.55768700	3.12421000
C	-6.32660700	-5.66421000	2.12474400
C	-5.40536800	-4.96080000	1.36200000
C	-7.07271900	-7.15985000	3.75675800
C	-8.22656500	-6.63457600	3.14030800
C	7.85346400	5.63341100	2.04653600
C	3.00618600	-10.92821000	-1.77792600
C	4.35824300	-11.63977800	-1.71862400
C	5.41231700	-10.70959100	-1.61292000
C	4.62918700	-13.00297100	-1.75597200
C	5.95858200	-13.43732000	-1.68828000
C	7.00347600	-12.51318800	-1.58423900
C	6.73833400	-11.14249700	-1.54571100
C	-7.18145700	-8.09519700	4.78819200
C	-8.45277200	-8.50175100	5.19941000
C	-9.59846500	-7.98137600	4.58856600
C	-9.48907100	-7.04358800	3.55450500
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H	3.77074500	-4.68709200	-2.83318300
H	-4.18370600	-2.56742100	0.70070800
H	-2.57283400	-1.29504300	-0.65702600
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H	0.83456700	-6.66228100	-0.38428600
H	-6.29425600	-8.50271900	5.26645500
H	-8.55265000	-9.22865700	6.00121200
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H	0.00000000	0.00000000	-5.37248500
H	0.07631200	2.15350100	-4.12602700
H	-3.77074400	4.68709200	-2.83318300
H	-0.83456700	6.66228100	-0.38428600
H	-2.42925700	2.61664700	-2.85768200
H	1.63581000	6.03429100	0.64009500
H	4.18370700	2.56742100	0.70070800
H	2.57283400	1.29504300	-0.65702600
H	-1.56565300	8.40541100	-1.79590100

H	-6.52113100	8.00513500	-1.42681900
H	-5.10351000	5.98573400	-1.41624300
H	2.54837900	6.13459300	2.79402800
H	4.17963900	7.41271900	4.13396400
H	5.74033300	4.29460100	0.57063700
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H	-8.03054800	12.86484600	-1.53247900
H	-7.55409000	10.42842500	-1.46425200
H	6.29425600	8.50271900	5.26645500
H	8.55265000	9.22865800	6.00121200
H	10.58118600	8.30714800	4.91910400
C	-2.27464700	11.21713200	-3.10806000
H	-2.02391900	12.28119800	-3.18924100
H	-2.89688100	10.94592500	-3.96686300
C	-8.40295700	-4.22434600	2.36517100
H	-8.05397200	-3.87713900	3.34287900
H	-8.07714100	-3.50073100	1.60873500
C	8.35950700	6.09550700	0.66194100
H	8.03182900	5.40262500	-0.12186200
H	9.45501700	6.13072100	0.64242600
H	-2.60611000	11.12527200	0.36819100
C	-2.10726500	11.32533900	-0.58544000
H	-1.16685500	10.76219700	-0.60494200
H	-1.86039900	12.39262600	-0.62516800
H	-9.49916700	-4.22929800	2.37534100
C	2.27464700	-11.21713200	-3.10806100
H	-8.03182900	-5.40262500	-0.12186100
H	7.98089800	7.09291500	0.41683800
C	8.40295700	4.22434700	2.36517100
H	9.49916700	4.22929900	2.37534100
H	8.05397200	3.87714000	3.34287900
H	1.16685500	-10.76219700	-0.60494200
C	2.10726500	-11.32534000	-0.58544100
H	2.60611000	-11.12527200	0.36819100
H	1.34079900	-10.64618500	-3.16765400
H	2.89688100	-10.94592600	-3.96686400
H	1.86039800	-12.39262600	-0.62516800
H	2.02391900	-12.28119800	-3.18924100
C	-8.35950700	-6.09550600	0.66194100
H	-9.45501700	-6.13072100	0.64242600
H	-7.98089800	-7.09291400	0.41683800
C	-7.85346400	-5.63341000	2.04653600
H	-1.34079900	10.64618500	-3.16765300

Atom coordinates for optimized T1 structure Da at UCAM-B3LYP/6-31G(d) level of theory

C	-0.15747800	-1.26246700	-2.73866500
C	-0.12661900	-1.22363400	-4.09514100
C	0.00026500	-0.00002100	-4.80853400
C	0.12705300	1.22360500	-4.09508400
C	0.15766200	1.26243300	-2.73862000
C	0.00000600	-0.00001100	-1.94736500
C	-0.00006600	-0.00000800	-0.56851600
N	-0.00013100	0.00000300	0.60628900

C	-2.69691700	4.71152900	-2.81055300
C	-2.34558400	5.79061800	-1.97806700
C	-1.17472700	5.70467900	-1.22264000
C	-0.37823900	4.56920700	-1.30607600
C	-0.75464600	3.51034700	-2.15209700
C	-1.91939700	3.56843000	-2.90907900
C	0.85951900	4.17020700	-0.65933200
C	1.17526900	2.88864900	-1.14435000
N	0.18447600	2.47790200	-2.03987200
C	1.71635300	4.80207300	0.23315200
C	2.88990800	4.16404300	0.63917500
C	3.18758900	2.89036700	0.11811100
C	2.35223400	2.24428700	-0.77775400
C	3.81660600	4.82126100	1.59231600
C	-3.20601600	6.99667200	-1.90538900
C	-2.63664600	8.27487100	-1.81274000
C	-3.44946900	9.39137200	-1.74049500
C	-4.84384300	9.25776500	-1.76231500
C	-5.42426800	7.99883400	-1.85538700
C	-4.60245200	6.88060400	-1.92471800
C	3.31875200	5.56757100	2.66892700
C	4.16875800	6.19508000	3.57124800
C	5.54230800	6.07470500	3.39939000
C	6.05635900	5.33075600	2.32934100
C	5.20547100	4.71014500	1.43320900
C	6.66639300	6.61389000	4.17402800
C	7.85971000	6.19735800	3.56762900
H	7.88711600	3.30593200	1.63384600
C	-3.04365600	10.85613600	-1.64412500
C	-4.40526400	11.53739200	-1.60724600
C	-5.44130900	10.59564500	-1.67693500
C	-4.69607700	12.88904500	-1.51880700
C	-6.02972200	13.29632700	-1.50045900
C	-7.05814100	12.35837100	-1.56995500
C	-6.77137800	10.99937500	-1.65894400
C	6.68858900	7.40516200	5.31676300
C	7.91885200	7.77763800	5.85042000
C	9.10631300	7.36465500	5.24910300
C	9.08176300	6.57104700	4.10262300
H	1.55518300	-8.37999300	-1.82182000
H	6.50383900	-7.88115100	-1.86482800
H	10.01273200	6.25351100	3.64061900
H	3.90069000	-13.62788200	-1.46399200
H	6.26872100	-14.35330300	-1.43130600
H	8.09137500	-12.69103700	-1.55446100
H	7.57532000	-10.27137500	-1.71281400
H	5.05088700	-5.89342600	-1.97046800
H	-2.24511900	-5.63429000	2.81377400
H	-3.75683100	-6.76048300	4.40194500
H	-5.60472900	-4.15349000	0.58975900
C	2.69697000	-4.71166300	-2.81063400
C	2.34560100	-5.79073700	-1.97814600
C	1.17474800	-5.70475700	-1.22271200
C	0.37830100	-4.56926100	-1.30614900
C	0.75474000	-3.51041700	-2.15217600

C	1.91948700	-3.56853700	-2.90915900
C	-0.85944100	-4.17021500	-0.65939500
C	-1.17514900	-2.88864600	-1.14441000
N	-0.18434100	-2.47793000	-2.03993500
C	-1.71629200	-4.80205400	0.23308500
C	-2.88983000	-4.16398400	0.63910800
C	-3.18747700	-2.89030400	0.11803700
C	-2.35210300	-2.24425300	-0.77783200
C	-3.81654500	-4.82117100	1.59225100
C	3.20599100	-6.99681900	-1.90546800
C	2.63657600	-8.27499700	-1.81280000
C	3.44936100	-9.39152500	-1.74055600
C	4.84374000	-9.25796600	-1.76239300
C	5.42420800	-7.99905700	-1.85548200
C	4.60243100	-6.88079900	-1.92481400
C	-3.31870900	-5.56750600	2.66885300
C	-4.16873100	-6.19498400	3.57118100
C	-5.54227700	-6.07455400	3.39933400
C	-6.05631000	-5.33058200	2.32929300
C	-5.20540700	-4.70999900	1.43315700
C	-6.66637500	-6.61369900	4.17398200
C	-7.85968200	-6.19711900	3.56759600
C	7.57920800	5.34477900	2.33735800
C	3.04349900	-10.85627400	-1.64417000
C	4.40508400	-11.53757700	-1.60730200
C	5.44116000	-10.59586700	-1.67700900
C	4.69585200	-12.88923900	-1.51885500
C	6.02948300	-13.29656600	-1.50051900
C	7.05793300	-12.35864600	-1.57003500
C	6.77121600	-10.99964100	-1.65903100
C	-6.68859000	-7.40497200	5.31671500
C	-7.91886100	-7.77740200	5.85038400
C	-9.10631300	-7.36437200	5.24907900
C	-9.08174400	-6.57076200	4.10260000
H	-1.49175900	-5.80175800	0.59138900
H	3.59561900	-4.78583600	-3.41406300
H	-4.09297700	-2.38908100	0.44311500
H	-2.60703600	-1.26513800	-1.16702800
H	-10.01270500	-6.25318900	3.64060700
H	2.20863300	-2.75351300	-3.56270700
H	0.90297300	-6.51313900	-0.55119200
H	-5.76524100	-7.72862100	5.78831200
H	-7.95387100	-8.39473300	6.74281200
H	-10.05841400	-7.66280300	5.67709000
H	-0.21361400	-2.15641700	-4.64266200
H	0.00034300	-0.00000900	-5.89081700
H	0.21415300	2.15639200	-4.64258200
H	-3.59557000	4.78567200	-3.41398100
H	-0.90297400	6.51307400	-0.55112600
H	-2.20851400	2.75339800	-3.56263200
H	1.49178600	5.80176900	0.59145900
H	4.09310200	2.38917000	0.44319600
H	2.60719100	1.26517200	-1.16693800
H	-1.55525600	8.37990400	-1.82177400
H	-6.50389500	7.88089100	-1.86472000

H	-5.05087400	5.89321600	-1.97035800
H	2.24516200	5.63431200	2.81385700
H	3.75684400	6.76056100	4.40201800
H	5.60480600	4.15365500	0.58980500
H	-3.90094000	13.62771600	-1.46395900
H	-6.26899500	14.35305700	-1.43125100
H	-8.09159400	12.69072600	-1.55437300
H	-7.57545700	10.27108100	-1.71271300
H	5.76523200	7.72877400	5.78837100
H	7.95384700	8.39496800	6.74285000
H	10.05840700	7.66312100	5.67710600
C	-2.23163300	11.29448000	-2.87329500
H	-2.00278700	12.36387600	-2.82243700
H	-2.78412500	11.10634700	-3.79805000
C	-8.15054900	-3.92664500	2.49617700
H	-7.76187800	-3.44388300	3.39706900
H	-7.88699800	-3.30568600	1.63382100
C	8.14053400	5.99806100	1.06442000
H	7.87661400	5.40955000	0.17978200
H	9.23244900	6.06089600	1.11306300
H	-2.80477300	10.82550300	0.52650800
C	-2.24408500	11.13212600	-0.36086400
H	-1.29510400	10.58625100	-0.37265400
H	-2.01658800	12.19917000	-0.27058200
H	-9.24258700	-3.95690600	2.56756300
C	2.23144700	-11.29460100	-2.87332800
H	-7.87658900	-5.40929900	0.17975100
H	7.74511200	7.00914600	0.93330100
C	8.15065300	3.92689900	2.49620100
H	9.24269100	3.95720100	2.56757500
H	7.76201000	3.44412000	3.39709600
H	1.29496900	-10.58632100	-0.37268200
C	2.24393300	-11.13222800	-0.36089800
H	2.80464100	-10.82561500	0.52646500
H	1.28311400	-10.74988900	-2.92378000
H	2.78393500	-11.10649300	-3.79809100
H	2.01640300	-12.19926300	-0.27060500
H	2.00256600	-12.36398800	-2.82245900
C	-8.14052200	-5.99780400	1.06439000
H	-9.23244000	-6.06059700	1.11304400
H	-7.74514000	-7.00890300	0.93326400
C	-7.57916000	-5.34454700	2.33732400
H	-1.28328300	10.74980000	-2.92375400

Atom coordinates for optimized S1 structure of Da at CAM-B3LYP/6-31G(d) level of theory

C	0.87720400	0.21773700	3.44566800
C	0.79427900	0.54002100	4.78173700
C	-0.44545600	0.71069300	5.42266300
C	-1.61156300	0.53090000	4.66398900
C	-1.55771900	0.20664300	3.32531900
C	-0.30109800	0.03417200	2.62305600
C	-0.23278700	-0.10660900	1.23746400
N	-0.17922900	-0.26153100	0.07622500
C	-4.73656900	3.19851300	2.41876700

C	-5.81550300	2.71567700	1.65640800
C	-5.80959100	1.37349500	1.24280100
C	-4.75481700	0.55191800	1.59329500
C	-3.69442900	1.06378400	2.37004800
C	-3.66884300	2.39282400	2.78249600
C	-4.42594100	-0.84032300	1.31805600
C	-3.19270700	-1.09204300	1.95504200
N	-2.76020400	0.06017900	2.59423200
C	-5.06664800	-1.85591700	0.63459200
C	-4.48605300	-3.13402400	0.58006200
C	-3.25936600	-3.35466400	1.23205400
C	-2.60010900	-2.35211600	1.92397900
C	-5.16020500	-4.23081700	-0.14744800
C	-6.93530700	3.60918700	1.28741800
C	-6.70314600	4.95898200	0.98018300
C	-7.75948100	5.78109900	0.63676800
C	-9.06734100	5.27862500	0.59337400
C	-9.31486800	3.94450700	0.89452300
C	-8.24967700	3.12225700	1.23736600
C	-5.11471500	-5.54561700	0.33904800
C	-5.74588700	-6.58702800	-0.32795500
C	-6.43473000	-6.31556900	-1.50437000
C	-6.48787000	-5.00769100	-2.00581400
C	-5.86040600	-3.97423000	-1.33665700
C	-7.18186000	-7.19269300	-2.41189500
C	-7.68137800	-6.41422100	-3.46545900
H	-6.06190100	-3.45628400	-4.31725200
C	-7.72962400	7.25582800	0.25822600
C	-9.20681300	7.52419600	0.00395600
C	-9.97096200	6.36556700	0.20175400
C	-9.81985300	8.70756400	-0.37445600
C	-11.20243700	8.72737500	-0.55489000
C	-11.96022400	7.57410300	-0.35813800
C	-11.34961400	6.38297100	0.02196300
C	-7.42860100	-8.55999300	-2.35805600
C	-8.18270700	-9.14465600	-3.37073600
C	-8.68050000	-8.37256400	-4.41908400
C	-8.43158700	-7.00149900	-4.47131000
H	5.71287500	-2.92030900	-1.16371100
H	5.42403300	-7.54230400	0.65283400
H	-8.82359600	-6.40834800	-5.29304500
H	9.03370700	-6.33776500	-4.39521400
H	9.49578200	-8.76659100	-4.25030200
H	8.45486200	-10.13841500	-2.47989400
H	6.93156700	-9.10214600	-0.82117200
H	4.18391100	-5.70496700	1.72610800
H	6.22992600	4.68787700	3.85575900
H	8.12978500	6.20710200	3.46984800
H	6.86414000	2.84531100	0.02845100
C	2.81997700	-3.32872000	1.53718800
C	4.10422300	-3.09539800	1.01205900
C	4.66041300	-1.81236800	1.12155000
C	3.94178100	-0.80156800	1.73493400
C	2.65411400	-1.06608600	2.24517200
C	2.08277400	-2.33285500	2.15616200

C	4.22508800	0.59419200	2.03446100
C	3.09148500	1.09424800	2.70818300
N	2.14801900	0.08265200	2.83775200
C	5.30523400	1.42532000	1.79422200
C	5.26512500	2.76145700	2.21850400
C	4.11421200	3.23293800	2.87698500
C	3.02036000	2.41987200	3.12730800
C	6.41379200	3.66186700	1.97334000
C	4.86069500	-4.18702900	0.35948100
C	5.66905100	-3.92700500	-0.75784500
C	6.37310800	-4.95475000	-1.35635500
C	6.28846800	-6.26089000	-0.85541600
C	5.49235200	-6.53603600	0.25013700
C	4.78638100	-5.49983900	0.84711400
C	6.78263300	4.62478900	2.92393200
C	7.85960000	5.47600500	2.71357800
C	8.58459400	5.36772300	1.53277400
C	8.22835700	4.41228300	0.57122500
C	7.15608400	3.56714100	0.78599100
C	9.74710000	6.11390900	1.03930700
C	10.08939800	5.61179000	-0.22412300
C	-7.27940600	-4.95416900	-3.30564600
C	7.28770100	-4.89573000	-2.57251300
C	7.72059500	-6.35131800	-2.68624300
C	7.13090500	-7.13201500	-1.68205500
C	8.57140600	-6.93278600	-3.61220100
C	8.83072500	-8.30050200	-3.52977600
C	8.24327400	-9.07478800	-2.53073200
C	7.38781500	-8.49585400	-1.59832300
C	10.47460100	7.15002700	1.61399700
C	11.55202600	7.68170300	0.91197200
C	11.89421400	7.18387000	-0.34415700
C	11.16298000	6.14478800	-0.91885200
H	6.19161300	1.04252900	1.29860400
H	2.38053700	-4.31433300	1.42910700
H	4.06907700	4.27579600	3.17172100
H	2.13420400	2.80384200	3.61846500
H	11.43745300	5.76348500	-1.89870100
H	1.09040300	-2.52602200	2.54456000
H	5.66379500	-1.62575800	0.75250300
H	10.21084800	7.53993200	2.59283600
H	12.13108600	8.49094200	1.34610600
H	12.73749500	7.60894800	-0.87975900
H	1.71744600	0.64339400	5.34386000
H	-0.49843700	0.96024400	6.47392700
H	-2.58698200	0.62682300	5.13149800
H	-4.74924100	4.23061100	2.75165200
H	-6.61691000	0.99614300	0.62367300
H	-2.84513900	2.78024300	3.36986900
H	-6.02937800	-1.68030900	0.16574200
H	-2.79953800	-4.33452400	1.16679800
H	-1.65000600	-2.53413000	2.41046100
H	-5.68707000	5.34289800	0.98677700
H	-10.32435600	3.54479300	0.87280300
H	-8.44175700	2.08671600	1.49925700

H	-4.59750100	-5.74840200	1.27123100
H	-5.70336000	-7.59460900	0.07490300
H	-5.87877600	-2.96596100	-1.74047200
H	-9.23769200	9.61172200	-0.53050800
H	-11.69327600	9.64921600	-0.85144600
H	-13.03572000	7.60576000	-0.50270900
H	-11.94302300	5.48613200	0.17448300
H	-7.04218300	-9.16438500	-1.54257100
H	-8.38502600	-10.21094400	-3.34445100
H	-9.26708000	-8.84317200	-5.20210300
C	-6.89224500	7.49095300	-1.00918100
H	-5.84296900	7.23392800	-0.83210300
H	-7.25776000	6.88321300	-1.84148800
C	9.91115300	3.16823600	-0.84641900
H	10.47288100	2.89148300	0.05009300
H	10.61657000	3.25761800	-1.67879400
C	-8.51082400	-4.04391800	-3.17531400
H	-9.10621900	-4.06766400	-4.09361000
H	-9.14912600	-4.36008500	-2.34550500
H	-7.23903400	9.18149600	1.14981600
C	-7.19287600	8.11935300	1.41074900
H	-7.77544000	7.96559400	2.32335500
H	-6.14817300	7.87134100	1.62437500
H	9.21662400	2.35506200	-1.08102800
C	6.52292300	-4.44008600	-3.82555000
H	9.05392300	4.96724900	-2.76100000
H	-8.20703400	-3.00689000	-2.99942700
C	-6.39989600	-4.48527100	-4.47599700
H	-5.51750700	-5.12167200	-4.58536500
H	-6.96184500	-4.51397600	-5.41504300
H	9.17206800	-3.98835000	-3.18100200
C	8.48985000	-3.97074500	-2.32503200
H	8.15802400	-2.93730000	-2.18158200
H	6.15970400	-3.41448200	-3.70484100
H	7.17507600	-4.46508400	-4.70448400
H	9.04790300	-4.27821500	-1.43623300
H	5.66255100	-5.08656900	-4.01894600
C	8.37128400	4.85086100	-1.91312400
H	7.65309200	4.06396100	-2.16491800
H	7.82157900	5.78741800	-1.78520100
C	9.15008600	4.48714800	-0.63875400
H	-6.93494300	8.54302900	-1.30863000

Atom coordinates for optimized S0 structure of **Ma** at B3LYP/6-31G(d) level of theory (energy= -3942.8402 a.u.)

C	0.85593800	-0.75437800	2.98546000
C	0.77662200	-0.95056600	4.36327900
C	-0.45682200	-0.96977200	5.03286500
C	-1.62324500	-0.78849100	4.27277300
C	-1.57200100	-0.60130600	2.89283700
C	-0.32463900	-0.58091100	2.22653700
C	-0.25971000	-0.38964800	0.81050000
N	-0.20734700	-0.23500300	-0.34104900
C	-4.58731400	2.71265700	3.09589100

C	-5.74794500	2.51937100	2.31078300
C	-5.84938800	1.35653200	1.53468400
C	-4.81987600	0.41298700	1.54699100
C	-3.67368000	0.63945800	2.34689300
C	-3.54528300	1.79116200	3.12422700
C	-4.61391700	-0.85083000	0.86519700
C	-3.35228500	-1.34181100	1.27821500
N	-2.77774700	-0.42321200	2.16983100
C	-5.39161800	-1.60193200	-0.01901700
C	-4.92728600	-2.83755700	-0.48861800
C	-3.66656800	-3.30136400	-0.04536300
C	-2.87169100	-2.57351900	0.83378300
C	-5.74133800	-3.64726900	-1.42985300
C	-6.83157800	3.53443700	2.30787000
C	-6.52933600	4.91093600	2.33570400
C	-7.55029700	5.85045300	2.32992600
C	-8.89795500	5.44229500	2.29413300
C	-9.21494000	4.08306700	2.26521100
C	-8.18421500	3.14450400	2.27414900
C	-5.80020000	-5.04915000	-1.31081800
C	-6.56207400	-5.82476900	-2.18327000
C	-7.28573900	-5.19551100	-3.19766100
C	-7.23844700	-3.79399600	-3.33166800
C	-6.47569600	-3.02838100	-2.46148400
C	-8.15717100	-5.73702700	-4.24639100
C	-8.63845000	-4.66407700	-5.02408300
H	-6.78458200	-1.71038100	-5.19138300
C	-7.44341800	7.37565400	2.34451500
C	-8.91888100	7.77614100	2.32254400
C	-9.74924600	6.63716300	2.29228300
C	-9.47728500	9.04929200	2.32702400
C	-10.87074800	9.18436500	2.30125400
C	-11.69343300	8.05348600	2.27103500
C	-11.13902300	6.77153900	2.26612600
C	-8.53029500	-7.05052400	-4.53974200
C	-9.38938900	-7.28400100	-5.61594200
C	-9.86848300	-6.22025500	-6.38756900
C	-9.49393600	-4.90347700	-6.09343700
H	6.92837400	-3.82779400	0.02234200
H	7.81788800	-7.09020400	3.68557000
H	-9.87237300	-4.08334900	-6.69944900
H	11.48740700	-7.05076600	-1.48608900
H	12.62460600	-8.91696400	-0.30934700
H	11.83188400	-9.67090800	1.91257400
H	9.88695000	-8.56935600	2.99534400
H	5.97189300	-5.46531100	3.88454500
H	4.65059800	4.92229800	1.34900800
H	6.07623800	6.66766900	0.34246200
H	6.18149100	2.00392500	-1.41663000
C	3.96766500	-3.97178200	2.68186200
C	5.19303500	-3.57000500	2.10031900
C	5.32013700	-2.25050700	1.64480300
C	4.25320200	-1.35839700	1.77109500
C	3.04331900	-1.79460800	2.36288900
C	2.88826800	-3.10458500	2.81832500

C	4.06875000	0.03551900	1.41405600
C	2.75193300	0.38816000	1.79467200
N	2.12570600	-0.73529100	2.35760300
C	4.90341000	0.99759500	0.84073900
C	4.44047400	2.30607800	0.65004100
C	3.12222200	2.62458100	1.05211500
C	2.27041900	1.68622100	1.62488400
C	5.31340500	3.34117200	0.04092500
C	6.31682000	-4.53168400	1.97108500
C	7.14140300	-4.52636300	0.82785800
C	8.18990400	-5.42843500	0.71844500
C	8.44043700	-6.36182300	1.74354700
C	7.63248500	-6.38213600	2.88163700
C	6.58341000	-5.47019200	2.98659700
C	5.29543400	4.66794700	0.51251300
C	6.10739800	5.65312500	-0.04710600
C	6.96092600	5.31478800	-1.09851200
C	6.99353600	3.99206200	-1.58199500
C	6.18006300	3.01719700	-1.02233700
C	7.90849300	6.12119500	-1.87561300
C	8.51691100	5.28984900	-2.83807000
C	-8.08997000	-3.33104800	-4.51443000
C	9.18739700	-5.59889600	-0.42799400
C	10.04255600	-6.75444100	0.09247400
C	9.59216600	-7.18432900	1.35728900
C	11.13157400	-7.37366400	-0.51025300
C	11.77258000	-8.42652000	0.15393800
C	11.32459600	-8.85228600	1.40879600
C	10.23114800	-8.23468000	2.01990000
C	8.24646000	7.47353400	-1.78924200
C	9.19764100	7.98933300	-2.67233000
C	9.80212800	7.16563600	-3.62763400
C	9.46324700	5.80977300	-3.71390000
H	5.92427000	0.74125400	0.57188800
H	3.85412200	-5.00199600	3.00580400
H	2.75070900	3.63042400	0.88142200
H	1.26098500	1.96108500	1.91255700
H	9.93952600	5.17818100	-4.46044700
H	1.95447900	-3.44686100	3.25323300
H	6.25996200	-1.91572100	1.21490200
H	7.77935100	8.11814400	-1.04876100
H	9.47035500	9.03997500	-2.61682600
H	10.54056500	7.58108400	-4.30826000
H	1.69912700	-1.09962000	4.91379000
H	-2.59431600	-0.77958000	4.75579900
H	-4.51654800	3.60068900	3.71693800
H	-6.71809100	1.20558200	0.90009400
H	-2.66795900	1.96475600	3.73943600
H	-6.37215100	-1.24322600	-0.31935100
H	-3.29181000	-4.24641900	-0.42676800
H	-1.90366000	-2.95259200	1.14499200
H	-5.48914500	5.22761700	2.33347700
H	-10.25010600	3.75118200	2.24653600
H	-8.42833600	2.08589200	2.28110100
H	-5.25862400	-5.53383300	-0.50329700

H	-6.59402900	-6.90474400	-2.06207200
H	-6.41436100	-1.94973100	-2.58349200
H	-8.84633600	9.93500200	2.34961500
H	-11.31632700	10.17560200	2.30446000
H	-12.77347500	8.17329500	2.25099600
H	-11.78292500	5.89585500	2.24229200
H	-8.16062400	-7.88091700	-3.94323800
H	-9.68816500	-8.30109200	-5.85585600
H	-10.53656600	-6.41705900	-7.22188800
C	-6.69948200	7.89980500	1.09550200
H	-5.66014500	7.55128700	1.08854900
H	-7.18175400	7.55393300	0.17577600
C	9.11594800	2.86189300	-2.39957000
H	9.63069900	3.14721600	-1.47651000
H	9.85587500	2.82777200	-3.20762400
C	-9.22616500	-2.38942000	-4.05720100
H	-9.86490000	-2.11229500	-4.90400900
H	-9.85330300	-2.86822700	-3.29831600
H	-6.72880300	8.97439700	3.65626700
C	-6.74105000	7.87865600	3.62560600
H	-7.25269300	7.51736200	4.52342100
H	-5.70207000	7.53037000	3.65963100
H	8.71375800	1.85040000	-2.26922000
C	8.47365700	-5.97591200	-1.74560000
H	7.98668700	3.39888000	-4.87657900
H	-8.81571200	-1.46686300	-3.63042700
C	-7.22568400	-2.63207600	-5.58824600
H	-6.41188100	-3.28279500	-5.92361400
H	-7.83294300	-2.36577800	-6.46127000
H	10.78911600	-4.47803100	-1.41067000
C	10.03241600	-4.32148400	-0.63311700
H	9.39827100	-3.48363500	-0.94563200
H	7.81521400	-5.16416500	-2.07576000
H	9.20386300	-6.16181100	-2.54185800
H	10.54596300	-4.03584200	0.29051800
H	7.86701400	-6.87849100	-1.62102100
C	7.27655700	3.42956400	-4.04198200
H	6.84040400	2.42973100	-3.93424000
H	6.47319000	4.12601300	-4.30209400
C	7.98552400	3.85968100	-2.73798800
H	-6.68671900	8.99593300	1.08401700
C	-0.52442900	-1.17392800	6.49954100
C	-1.57830100	-1.89555800	7.08358000
C	0.46238200	-0.64820700	7.35029700
C	-1.63794700	-2.08512800	8.46175600
H	-2.34637200	-2.33496500	6.45317300
C	0.39422900	-0.83778900	8.72753000
H	1.27384700	-0.05724000	6.93472300
C	-0.65354400	-1.56310100	9.31093200
H	-2.46232000	-2.65441600	8.88480200
H	1.16479200	-0.40630700	9.36223000
C	-0.70537200	-1.79380300	10.80216400
H	-0.12471700	-2.68193300	11.08542600
H	-0.28763600	-0.94493400	11.35382600
H	-1.73185700	-1.95222200	11.14837600

Atom coordinates for optimized T1 structure of **Ma** at UCAM-B3LYP/6-31G(d) level of theory

C	0.82702200	-0.82023700	2.86521800
C	0.77425700	-1.01602000	4.23842700
C	-0.44128400	-1.00983800	4.92661300
C	-1.61519600	-0.80685100	4.19656700
C	-1.58655800	-0.61964400	2.82188400
C	-0.35889100	-0.62192800	2.13825200
C	-0.31914900	-0.42752300	0.72036000
N	-0.28885300	-0.27024200	-0.42486400
C	-4.58959700	2.67337300	3.14966000
C	-5.75385600	2.49914400	2.37676500
C	-5.86366700	1.36635300	1.57179600
C	-4.83477900	0.42950900	1.54605700
C	-3.68606800	0.63279600	2.33247100
C	-3.54928500	1.75835800	3.13865000
C	-4.63829100	-0.81669600	0.83153900
C	-3.38068400	-1.31462900	1.21744200
N	-2.79576800	-0.42114000	2.11909500
C	-5.42418500	-1.54041000	-0.06065200
C	-4.96602500	-2.75693200	-0.56260000
C	-3.70751400	-3.23273600	-0.14643300
C	-2.90628600	-2.53171800	0.73950700
C	-5.78924700	-3.54078000	-1.51663800
C	-6.84128400	3.50817500	2.42029500
C	-6.54467800	4.87734600	2.47920400
C	-7.56836800	5.80649300	2.51928800
C	-8.90627600	5.39187500	2.49821900
C	-9.21770800	4.03919500	2.43791300
C	-8.18471300	3.11032600	2.40188200
C	-5.85062100	-4.93793300	-1.42917800
C	-6.61873600	-5.68754700	-2.31189500
C	-7.34342900	-5.03205500	-3.29962000
C	-7.29361900	-3.63576100	-3.40040200
C	-6.52404400	-2.89551100	-2.52138000
C	-8.22582000	-5.54391200	-4.35522800
C	-8.70530900	-4.45432600	-5.09567400
H	-6.85999600	-1.50740000	-5.19428600
C	-7.46912600	7.32510900	2.57703900
C	-8.94074700	7.71646500	2.59419800
C	-9.76355300	6.58246000	2.54730900
C	-9.50007400	8.98281100	2.64669500
C	-10.88871700	9.11159300	2.65222800
C	-11.70491100	7.98300100	2.60531000
C	-11.14787400	6.70856600	2.55223000
C	-8.60383100	-6.84246700	-4.67647300
C	-9.46892900	-7.04342700	-5.74818600
C	-9.94670700	-5.96170000	-6.48549100
C	-9.56599100	-4.65973400	-6.16166700
H	7.61422100	-3.27416200	0.83429900
H	6.92127700	-7.95480500	2.52239900
H	-9.94298700	-3.82227400	-6.74261300
H	12.42331800	-6.19136900	-0.11086100
H	13.02782500	-8.54828200	0.38070300

H	11.40391300	-10.06434400	1.46337900
H	9.14646500	-9.26472000	2.07834100
H	5.12796400	-6.36551200	2.72185600
H	4.65553100	4.74847400	1.04465500
H	6.08379500	6.44686900	-0.02804600
H	6.03289900	1.77026600	-1.72122000
C	3.86186700	-4.07805500	2.54772100
C	5.11282000	-3.72391300	1.92856600
C	5.22257000	-2.38299900	1.44618700
C	4.17429600	-1.49305900	1.58709600
C	2.97510300	-1.89356700	2.20995800
C	2.81560800	-3.19968200	2.68816000
C	3.99614100	-0.10220000	1.20549600
C	2.70261600	0.27199000	1.61119800
N	2.07710300	-0.83006600	2.20722300
C	4.82515900	0.83169300	0.59353600
C	4.37461300	2.13585800	0.39140400
C	3.07953600	2.48065900	0.82126200
C	2.23428200	1.56841800	1.43265300
C	5.24507400	3.14493700	-0.26109700
C	6.17355600	-4.65152500	1.80404400
C	7.46368100	-4.28399800	1.19614900
C	8.45868800	-5.17902800	1.08975300
C	8.31032900	-6.54638700	1.56498800
C	7.05643100	-6.93900500	2.16382000
C	6.05765500	-6.04120900	2.27265200
C	5.26868900	4.47023800	0.19322600
C	6.07978900	5.42774400	-0.40369200
C	6.88587100	5.05701800	-1.47291700
C	6.87452500	3.73609700	-1.93906400
C	6.06269000	2.78832700	-1.34281700
C	7.82771900	5.83121500	-2.29039800
C	8.38176300	4.97619000	-3.25336100
C	-8.15256900	-3.14156000	-4.55680500
C	9.85511500	-4.99625500	0.50096400
C	10.44651000	-6.38702600	0.70159900
C	9.50140500	-7.25374500	1.32726500
C	11.69938100	-6.84715000	0.36552500
C	12.04166800	-8.17917900	0.64325400
C	11.11984600	-9.03676600	1.25700100
C	9.85570900	-8.59423300	1.60297700
C	8.19774800	7.16986000	-2.23182000
C	9.13044500	7.64844500	-3.14741100
C	9.68251200	6.80016100	-4.10538100
C	9.30957200	5.45755400	-4.16264700
H	5.83269300	0.55513700	0.29848200
H	3.72124300	-5.08100000	2.92719600
H	2.72019800	3.48942000	0.64690000
H	1.23927800	1.86315500	1.74663900
H	9.74470200	4.80368600	-4.91370500
H	1.89155800	-3.51713900	3.15910800
H	6.12724600	-2.04744000	0.95681000
H	7.76930100	7.83416500	-1.48687200
H	9.43027500	8.69145200	-3.11526500
H	10.40868400	7.18796400	-4.81322800

H	1.70330100	-1.18309300	4.77117100
H	-2.57500400	-0.78296500	4.69952500
H	-4.51256200	3.54458600	3.79198200
H	-6.74134000	1.22807000	0.94802500
H	-2.66521800	1.91581900	3.74671900
H	-6.40473300	-1.17127100	-0.34516000
H	-3.34094200	-4.16978500	-0.55232900
H	-1.93846800	-2.92103700	1.03538600
H	-5.50734400	5.20057200	2.46930400
H	-10.25069100	3.70351200	2.42873600
H	-8.42153100	2.05118100	2.38137200
H	-5.30239600	-5.44309400	-0.64014800
H	-6.65311100	-6.76916200	-2.21852000
H	-6.46300000	-1.81488600	-2.61638700
H	-8.87132100	9.86843400	2.68294300
H	-11.33778500	10.09922200	2.69314800
H	-12.78440800	8.09892900	2.61002800
H	-11.78717900	5.83123400	2.51557100
H	-8.23330200	-7.68819700	-4.10440300
H	-9.77387500	-8.05145700	-6.01220300
H	-10.62061000	-6.13412600	-7.31910200
C	-6.75529800	7.88723500	1.33739100
H	-5.71601300	7.54497200	1.30204500
H	-7.25233100	7.56679600	0.41762100
C	8.93139200	2.55013200	-2.80442300
H	9.48191200	2.83410700	-1.90315700
H	9.64255800	2.48604600	-3.63429300
C	-9.27891300	-2.21970400	-4.06317100
H	-9.92736600	-1.92404400	-4.89423000
H	-9.89457300	-2.71843000	-3.30937100
H	-6.74433700	8.88380900	3.91533700
C	-6.75052800	7.79079700	3.85326800
H	-7.24344100	7.40013800	4.74788200
H	-5.71068600	7.44808400	3.85713900
H	8.50728400	1.55296000	-2.64782700
C	9.78959600	-4.62674800	-0.98892100
H	7.74708900	3.08634000	-5.24263800
H	-8.86464700	-1.30842500	-3.61977300
C	-7.30503400	-2.41544400	-5.61358500
H	-6.49672700	-3.05541800	-5.97796700
H	-7.92320900	-2.12343100	-6.46870000
H	11.67450800	-3.86049300	0.88358300
C	10.65323300	-3.93367800	1.27185900
H	10.18180400	-2.95056400	1.17213900
H	9.30347300	-3.65496300	-1.12324400
H	10.79586200	-4.56418300	-1.41630000
H	10.70901300	-4.17866200	2.33611200
H	9.22360000	-5.37192700	-1.55463200
C	7.06534000	3.14144300	-4.38777600
H	6.61197800	2.15394500	-4.25452900
H	6.27052900	3.85263100	-4.62894400
C	7.82207200	3.56619300	-3.11914100
H	-6.74866700	8.98179800	1.35987100
C	-0.48401400	-1.21298500	6.39315100
C	-1.53070700	-1.92079600	6.99054900

C	0.51951000	-0.69834000	7.21885300
C	-1.56780000	-2.10812000	8.36482500
H	-2.31487500	-2.34943900	6.37423000
C	0.47442900	-0.88617200	8.59272700
H	1.33012300	-0.11919400	6.78759400
C	-0.56629300	-1.59735500	9.19113100
H	-2.38951400	-2.66678200	8.80407000
H	1.25966300	-0.46442700	9.21384000
C	-0.59498400	-1.82646700	10.67880900
H	-0.06212900	-2.74700400	10.94382800
H	-0.11474100	-1.00543300	11.21802400
H	-1.61944300	-1.92482300	11.04786900

*Atom coordinates for optimized SI structure of **Ma** at CAM-B3LYP/6-31G(d) level of theory*

C	0.88043800	0.22344400	3.38721300
C	0.80057400	0.56168200	4.71731100
C	-0.43395200	0.76698000	5.37935300
C	-1.59508600	0.58416100	4.58831400
C	-1.53880200	0.24107900	3.25883100
C	-0.29034300	0.04202400	2.56334300
C	-0.21803700	-0.10604200	1.17559400
N	-0.15823100	-0.26259900	0.01717000
C	-4.75629600	3.20454600	2.39978200
C	-5.84218600	2.71237000	1.65290900
C	-5.82906400	1.37172900	1.23816400
C	-4.76085800	0.55922800	1.57230100
C	-3.69406600	1.07966300	2.33378200
C	-3.67558800	2.40917400	2.74631700
C	-4.42531200	-0.82891400	1.28973500
C	-3.17954000	-1.07263000	1.90366300
N	-2.74575800	0.08423800	2.53776200
C	-5.07310900	-1.84889500	0.61717800
C	-4.48772800	-3.12268700	0.55204400
C	-3.24853200	-3.33614400	1.18280400
C	-2.58241700	-2.33002400	1.86264600
C	-5.16868200	-4.22410200	-0.16303000
C	-6.97537200	3.59622600	1.30089800
C	-6.75954800	4.94792100	0.99054000
C	-7.82785100	5.76072200	0.66211000
C	-9.13161100	5.24664200	0.63667700
C	-9.36308000	3.91049400	0.94153400
C	-8.28594500	3.09781300	1.26974600
C	-5.11092600	-5.53745900	0.32565900
C	-5.74819800	-6.58287100	-0.32938800
C	-6.45612800	-6.31671300	-1.49557100
C	-6.52199600	-5.01020100	-1.99888100
C	-5.88779100	-3.97292800	-1.34187400
C	-7.21380900	-7.19870600	-2.38969700
C	-7.73264000	-6.42439400	-3.43697000
H	-6.13977200	-3.46108200	-4.31975100
C	-7.81631100	7.23575400	0.28378400
C	-9.29901200	7.49068100	0.04848300
C	-10.05008600	6.32537800	0.25686800
C	-9.92749300	8.66829300	-0.32248500

C	-11.31244500	8.67565400	-0.48480800
C	-12.05723500	7.51580000	-0.27747500
C	-11.43106700	6.33040400	0.09522700
C	-7.45425800	-8.56683900	-2.32944800
C	-8.22151300	-9.15655000	-3.32929400
C	-8.73842600	-8.38860700	-4.37138200
C	-8.49582800	-7.01665700	-4.43004700
H	5.75514200	-2.91621200	-1.18219200
H	5.38840200	-7.55306600	0.58209100
H	-8.90280400	-6.42669300	-5.24680200
H	9.09482400	-6.33563500	-4.39187000
H	9.52924500	-8.77028200	-4.26343400
H	8.44468600	-10.14866700	-2.52471000
H	6.90422500	-9.11309500	-0.88147800
H	4.14860500	-5.71468500	1.65283200
H	6.25460200	4.65430300	3.88913900
H	8.17051200	6.16067000	3.53644100
H	6.93442000	2.81780400	0.06575200
C	2.81520600	-3.32463600	1.47143200
C	4.10739100	-3.09749000	0.96383700
C	4.67229200	-1.81890100	1.09001500
C	3.95388500	-0.80768700	1.70133000
C	2.65747100	-1.06566800	2.19228500
C	2.07794300	-2.32752400	2.08830300
C	4.24564700	0.58338700	2.01687100
C	3.10859800	1.08788500	2.68157600
N	2.15462200	0.08340800	2.78815400
C	5.33481800	1.40652900	1.79568800
C	5.30116900	2.74035900	2.23100700
C	4.14667300	3.21643300	2.87948500
C	3.04274200	2.41119300	3.10970900
C	6.45978400	3.63227400	2.00629400
C	4.86389200	-4.18966400	0.31338600
C	5.69406500	-3.92632100	-0.78723200
C	6.39747200	-4.95506600	-1.38440000
C	6.29102400	-6.26533300	-0.89822300
C	5.47354000	-6.54360100	0.19091300
C	4.76775000	-5.50655300	0.78627800
C	6.82058200	4.58991400	2.96547400
C	7.90651200	5.43387700	2.77395500
C	8.64816700	5.32415600	1.60357800
C	8.30018400	4.37384900	0.63373900
C	7.21951600	3.53524900	0.82999500
C	9.82242900	6.06430900	1.12982900
C	10.18042200	5.56368000	-0.12980900
C	-7.33426500	-4.96239200	-3.28609500
C	7.33316100	-4.89336100	-2.58423400
C	7.75285900	-6.35219800	-2.70536900
C	7.13837400	-7.13673000	-1.71923000
C	8.61323000	-6.93333800	-3.62269200
C	8.85694500	-8.30439800	-3.54955000
C	8.24483600	-9.08248100	-2.56833200
C	7.37973200	-8.50398500	-1.64472800
C	10.54724700	7.09448800	1.71853100
C	11.63807100	7.62166900	1.03421500

C	11.99594900	7.12528600	-0.21819200
C	11.26737500	6.09227400	-0.80691600
H	6.22338700	1.02028100	1.30697000
H	2.36949100	-4.30590700	1.35157300
H	4.10625000	4.25705300	3.18208800
H	2.15423300	2.80044400	3.59211500
H	11.55412400	5.71236800	-1.78376100
H	1.08033800	-2.51742800	2.46448300
H	5.68199500	-1.63766500	0.73618800
H	10.27100200	7.48327100	2.69434800
H	12.21535400	8.42624600	1.47917400
H	12.84956400	7.54694100	-0.73992400
H	1.73112800	0.68140800	5.26155800
H	-2.57556400	0.66301300	5.04550700
H	-4.77349300	4.23619000	2.73394900
H	-6.64152500	0.98655400	0.63065200
H	-2.84699500	2.80605500	3.32042700
H	-6.04531000	-1.67777000	0.16647100
H	-2.78517200	-4.31397000	1.11131800
H	-1.62429500	-2.50971500	2.33407400
H	-5.74691500	5.34085700	0.98295500
H	-10.36918600	3.50181900	0.93394200
H	-8.46503700	2.06067900	1.53455100
H	-4.57877400	-5.73604300	1.25033100
H	-5.69569400	-7.58935000	0.07506900
H	-5.91623300	-2.96548900	-1.74725000
H	-9.35551100	9.57750900	-0.48664300
H	-11.81534200	9.59287700	-0.77542200
H	-13.13477900	7.53775000	-0.40791100
H	-12.01440200	5.42841600	0.25598600
H	-7.05296300	-9.16809100	-1.51882900
H	-8.41915900	-10.22357800	-3.29776400
H	-9.33509600	-8.86311300	-5.14436600
C	-6.99701400	7.47927300	-0.99376800
H	-5.94323700	7.23202500	-0.82987800
H	-7.36714800	6.86850000	-1.82181300
C	9.99640200	3.12285300	-0.76126500
H	10.54215600	2.83995000	0.14315000
H	10.71537900	3.21004000	-1.58213700
C	-8.56734900	-4.05715600	-3.13763300
H	-9.17714800	-4.08490000	-4.04632200
H	-9.19100500	-4.37472500	-2.29729700
H	-7.33267200	9.16544600	1.17062400
C	-7.27332900	8.10361700	1.43016700
H	-7.84307900	7.94385500	2.34979700
H	-6.22382200	7.86520700	1.63074700
H	9.30045000	2.31488000	-1.00927600
C	6.59456700	-4.41708000	-3.84529900
H	9.18021600	4.93227300	-2.68392200
H	-8.26526100	-3.01856700	-2.96809600
C	-6.47573100	-4.49184100	-4.47121000
H	-5.59243300	-5.12461700	-4.59359200
H	-7.05253700	-4.52471300	-5.40106900
H	9.23705400	-4.00011700	-3.15110100
C	8.54045200	-3.98365400	-2.30681800

H	8.21712900	-2.94815400	-2.15880000
H	6.23964400	-3.38910000	-3.72014300
H	7.26151500	-4.43960200	-4.71309800
H	9.07989600	-4.30580600	-1.41176300
H	5.73127200	-5.05276200	-4.06022500
C	8.48377600	4.81799700	-1.84707000
H	7.76475100	4.03621700	-2.11211200
H	7.93802200	5.75765400	-1.72520300
C	9.24060500	4.44609100	-0.56188100
H	-7.05321400	8.53102900	-1.29211100
C	-0.50811100	1.13589100	6.79374100
C	-1.62779700	1.79839100	7.32611000
C	0.53282400	0.84242600	7.69222500
C	-1.69912000	2.14040000	8.66801600
H	-2.45076400	2.07324300	6.67384100
C	0.45752500	1.19577700	9.03049900
H	1.40528700	0.29762600	7.34577300
C	-0.65784400	1.85380300	9.55149200
H	-2.58399800	2.65378400	9.03656000
H	1.28192800	0.94032400	9.69200000
C	-0.72301300	2.25921200	11.00058400
H	-0.17668300	1.55648600	11.63696000
H	-0.28195500	3.25068800	11.16104800
H	-1.75635400	2.30333200	11.35712200

Atom coordinates for optimized S0 structure of Db at B3LYP/6-31G(d) level of theory (energy=-3426.8148 a.u.)

C	-1.18129300	0.85152700	-2.01545100
C	-1.14095500	1.40881700	-3.29638700
C	0.08079800	1.71483200	-3.89269000
C	1.27660700	1.46325200	-3.22301000
C	1.26467400	0.89368100	-1.94675600
C	0.02828200	0.58583700	-1.32937900
C	0.00085200	0.00936500	-0.01896500
N	-0.02157200	-0.45858100	1.04535700
C	4.49083400	3.72739900	-0.65294400
C	5.62862500	3.10648600	-0.09133900
C	5.66761900	1.71398700	0.03510000
C	4.58361900	0.95398600	-0.41188800
C	3.44925800	1.59933400	-0.96061800
C	3.39019300	2.98932200	-1.07564600
C	4.30550100	-0.46915700	-0.42293800
C	3.01136200	-0.63337500	-0.97124200
N	2.48675600	0.63174300	-1.28593500
C	5.03749300	-1.58820700	-0.01590700
C	4.49228300	-2.86354600	-0.19080000
C	3.21352300	-3.00425700	-0.77466800
C	2.45991800	-1.90141100	-1.15932900
N	5.21699000	-4.02358100	0.20952700
N	6.72722200	3.90432700	0.34208100
C	4.56773100	-5.02479700	0.97972100
C	6.59237700	-4.14345800	-0.12327600
C	6.48840700	5.04584900	1.15247600
C	8.05197700	3.52740800	-0.00516100

C	4.84332500	-6.38557500	0.76156300
C	4.20176400	-7.36362200	1.51844000
C	3.26231800	-7.01044500	2.48977100
C	2.97835200	-5.65989000	2.70131400
C	3.62820900	-4.67248400	1.96303400
C	7.51773600	-4.63679300	0.81170300
C	8.86444800	-4.75593200	0.47389900
C	9.31879900	-4.37011700	-0.78894300
C	8.40350100	-3.86894500	-1.71704400
C	7.05208000	-3.76253100	-1.39512700
C	5.49988400	5.01895000	2.15027900
C	5.25490300	6.14817300	2.92953700
C	5.99759100	7.31585500	2.74394300
C	6.98702500	7.34322000	1.75841200
C	7.22746100	6.22582300	0.96171900
C	9.09471600	3.62508600	0.93122200
C	10.39239800	3.25772700	0.58054700
C	10.67368100	2.76972700	-0.69721500
C	9.63741000	2.66122000	-1.62704300
C	8.33994600	3.04279700	-1.29201700
C	-3.23718900	2.65862800	1.57370400
C	-4.53217600	2.15036200	1.82018600
C	-5.05831300	1.16096100	0.98417200
C	-4.29349800	0.69215800	-0.08759300
C	-2.98570900	1.19171000	-0.29358300
C	-2.45152800	2.18350900	0.53002000
C	-4.54653100	-0.27797700	-1.13524900
C	-3.38397400	-0.32534300	-1.94182600
N	-2.42918500	0.55929800	-1.41833000
C	-5.63100100	-1.10865100	-1.42886900
C	-5.56382300	-1.95976800	-2.53679400
C	-4.39764700	-1.98183500	-3.33357100
C	-3.29676400	-1.18429000	-3.03884400
N	-6.66134500	-2.80653300	-2.86808900
N	-5.29289600	2.65720500	2.91325000
C	-6.42925600	-4.18127300	-3.13836700
C	-7.98127000	-2.28206900	-2.86698000
C	-6.66197700	2.98573500	2.72818700
C	-4.68588300	2.78290400	4.19157900
C	-7.14114800	-4.84018700	-4.15525500
C	-6.90881100	-6.18873600	-4.41694600
C	-5.95360900	-6.90159900	-3.68860500
C	-5.23758500	-6.24746900	-2.68427400
C	-5.47539300	-4.90346800	-2.40207100
C	-9.04926500	-3.02529300	-2.33703000
C	-10.34155000	-2.50377900	-2.34324800
C	-10.59298200	-1.23012600	-2.85732500
C	-9.53192200	-0.48445700	-3.37544600
C	-8.23927200	-1.00406800	-3.39049200
C	-7.08567000	3.63941900	1.55879800
C	-8.43123700	3.94897900	1.37238100
C	-9.37677200	3.63177800	2.34996200
C	-8.95824200	2.98922300	3.51694800
C	-7.61753200	2.65880800	3.70492300
C	-4.96951400	3.88923200	5.01030400

C	-4.37174900	4.00913400	6.26304100
C	-3.46825900	3.04501200	6.71584500
C	-3.17576100	1.95039300	5.89990500
C	-3.78269100	1.81097200	4.65295600
H	-2.07641500	1.61377100	-3.80612500
H	0.10111300	2.15218700	-4.88644600
H	2.23197900	1.68681000	-3.68585900
H	4.47847900	4.80844200	-0.74584800
H	6.53666600	1.23620200	0.47632900
H	2.52014600	3.48815700	-1.49084000
H	6.02333700	-1.47709600	0.42447800
H	2.81145700	-4.00202100	-0.91621400
H	1.47795800	-2.03649800	-1.60045000
H	5.56002400	-6.66906600	-0.00253700
H	4.42863300	-8.41076200	1.33456600
H	2.75832000	-7.77657300	3.07203900
H	2.25356300	-5.36617800	3.45613800
H	3.40930400	-3.62493500	2.14261800
H	7.17438500	-4.92509400	1.80000200
H	9.56487000	-5.13950600	1.21141100
H	10.37069600	-4.45749600	-1.04555600
H	8.73923600	-3.56948300	-2.70664700
H	6.34390500	-3.38408600	-2.12546300
H	4.92869700	4.11014300	2.31001100
H	4.48622800	6.10695400	3.69699400
H	5.80847500	8.19169900	3.35800400
H	7.56923100	8.24665300	1.59555800
H	7.98755700	6.25939800	0.18773300
H	8.88089800	3.98918500	1.93093000
H	11.18539600	3.33981400	1.31945800
H	11.68509800	2.47681000	-0.96393500
H	9.83996600	2.28856000	-2.62790700
H	7.54164700	2.96768100	-2.02346300
H	-2.84875300	3.43594700	2.22336900
H	-6.05580800	0.77367700	1.16603200
H	-1.45826200	2.58770600	0.36492500
H	-6.52225600	-1.09852200	-0.80933900
H	-4.36335800	-2.64662000	-4.19054300
H	-2.40506100	-1.22788500	-3.65629900
H	-7.87465100	-4.28954300	-4.73565700
H	-7.47011600	-6.68042900	-5.20743500
H	-5.77034400	-7.95101400	-3.90089200
H	-4.49589700	-6.78860200	-2.10234700
H	-4.92538700	-4.40674200	-1.60924800
H	-8.85954600	-4.00962100	-1.92133600
H	-11.15416500	-3.09415400	-1.92769700
H	-11.60041700	-0.82397900	-2.85305300
H	-9.71097100	0.50665600	-3.78446300
H	-7.42155800	-0.42394000	-3.80618800
H	-6.35431100	3.90057600	0.80056600
H	-8.73863900	4.45483900	0.46061300
H	-10.42402700	3.88059900	2.20402300
H	-9.68207500	2.72685500	4.28433200
H	-7.30269900	2.14574100	4.60788600
H	-5.65873200	4.65015100	4.65825700

H	-4.60393000	4.87211800	6.88199600
H	-2.99810100	3.14622600	7.68987900
H	-2.47852500	1.18828700	6.23811600
H	-3.55885900	0.95067900	4.03042500

Atom coordinates for optimized T1 strcuture of Db at UCAM-B3LYP/6-31G(d) level of theory

C	-1.20185500	1.01968700	-2.09343700
C	-1.12662400	1.59740900	-3.35463500
C	0.11084700	1.88606000	-3.91541900
C	1.28005300	1.59178000	-3.22749600
C	1.22408400	1.00276400	-1.96830400
C	-0.02451500	0.71675400	-1.38953800
C	-0.09181500	0.11695900	-0.08884300
N	-0.13372100	-0.37729000	0.95538100
C	4.46089200	3.71234700	-0.50510400
C	5.57019500	3.05045700	0.05109300
C	5.57984600	1.66199300	0.13201000
C	4.49156800	0.94428500	-0.35772600
C	3.38757000	1.62688400	-0.90058500
C	3.35748600	3.01670500	-0.97041900
C	4.18619700	-0.47060800	-0.42932200
C	2.90924000	-0.58414800	-1.00746400
N	2.41828000	0.69635400	-1.28141900
C	4.88418600	-1.61566200	-0.05238200
C	4.31896900	-2.86356100	-0.28929300
C	3.05373100	-2.95499000	-0.89706800
C	2.33354600	-1.82737500	-1.25153500
N	5.01360400	-4.05118900	0.07072700
N	6.67657100	3.80815500	0.52537800
C	4.34467300	-5.05094300	0.81564100
C	6.37738700	-4.19514000	-0.27828400
C	6.45129700	4.89240200	1.40559500
C	7.98906900	3.44095100	0.14453200
C	4.59031600	-6.40628100	0.57056300
C	3.92816300	-7.38265800	1.30230500
C	2.99713300	-7.03095500	2.27460500
C	2.74240900	-5.68458500	2.51203200
C	3.41363100	-4.70025100	1.79824200
C	7.29109200	-4.75714200	0.61896400
C	8.62692100	-4.89564100	0.26564200
C	9.08084900	-4.46102600	-0.97528200
C	8.17643100	-3.89127700	-1.86553700
C	6.83562800	-3.76540500	-1.52773200
C	5.45246800	4.81792000	2.38138200
C	5.21885900	5.89212500	3.23020800
C	5.98352200	7.04987300	3.13540000
C	6.98294000	7.12403400	2.17020000
C	7.21155100	6.06253900	1.30523200
C	9.04158100	3.48936000	1.06413800
C	10.32620400	3.12828800	0.67982600
C	10.58308900	2.69487600	-0.61670400
C	9.53592500	2.63480100	-1.53037800
C	8.25182100	3.01124100	-1.16006900
C	-3.20814200	2.86001900	1.44279300

C	-4.45816000	2.33628200	1.74174900
C	-5.08552100	1.28922400	0.88856500
C	-4.29445300	0.81215800	-0.20082800
C	-3.03413700	1.35592500	-0.44076100
C	-2.46158200	2.41174400	0.34484500
C	-4.51445200	-0.19078500	-1.19805800
C	-3.36727100	-0.21964700	-2.02600000
N	-2.46872100	0.73578500	-1.53048400
C	-5.56071400	-1.08115100	-1.46751800
C	-5.45124700	-1.94966300	-2.54793500
C	-4.30123700	-1.94986300	-3.35862900
C	-3.24094400	-1.09153100	-3.09451200
N	-6.51239400	-2.85310600	-2.84653300
N	-5.16209300	2.72997600	2.86292400
C	-6.22448700	-4.22612800	-3.02062200
C	-7.83786200	-2.37018300	-2.93162000
C	-6.58178100	2.70995900	2.86963100
C	-4.48826800	3.26016400	4.00413000
C	-6.89355600	-4.98134100	-3.99003900
C	-6.60064000	-6.32823800	-4.15645900
C	-5.62569800	-6.94363000	-3.37767200
C	-4.95107600	-6.19287500	-2.42062400
C	-5.24961900	-4.84943500	-2.23490400
C	-8.90899800	-3.11862900	-2.43199000
C	-10.20754300	-2.63525500	-2.52414200
C	-10.46354600	-1.39331200	-3.09576600
C	-9.39930000	-0.64119200	-3.58278400
C	-8.09970300	-1.12386100	-3.51069600
C	-7.29249300	3.10193800	1.73278800
C	-8.68222800	3.05308400	1.73696500
C	-9.36804000	2.63560800	2.87057700
C	-8.65631000	2.26092300	4.00932200
C	-7.27074400	2.29291500	4.01234900
C	-4.89670000	4.47404000	4.55474400
C	-4.25003000	4.97468200	5.67822100
C	-3.19526000	4.27307000	6.25159000
C	-2.78927000	3.06174400	5.69759200
C	-3.43254700	2.55145300	4.57883000
H	-2.04616100	1.82801400	-3.88010100
H	0.16390900	2.34080600	-4.89858000
H	2.24998700	1.80096800	-3.66418300
H	4.47451800	4.79540500	-0.55995700
H	6.43209200	1.15210800	0.56887500
H	2.50583200	3.54511400	-1.38468900
H	5.86258000	-1.54362600	0.41090200
H	2.63506700	-3.93784300	-1.08325400
H	1.35794300	-1.92238100	-1.71497900
H	5.30273400	-6.68913400	-0.19662100
H	4.13328900	-8.42928700	1.09789400
H	2.47536500	-7.79717600	2.83879300
H	2.02130800	-5.39123200	3.26894500
H	3.21635100	-3.65281900	1.99775000
H	6.94794500	-5.08492900	1.59405600
H	9.32078800	-5.33506700	0.97601600
H	10.12697700	-4.56390800	-1.24480500

H	8.51278000	-3.55087400	-2.84032000
H	6.13338400	-3.33117300	-2.23095300
H	4.86096800	3.91338700	2.47072800
H	4.43828600	5.81468500	3.98110900
H	5.80288400	7.88463400	3.80484300
H	7.58450100	8.02330800	2.07717900
H	7.98239200	6.13404700	0.54574700
H	8.84696000	3.81125300	2.08123100
H	11.13013900	3.17299600	1.40840500
H	11.58679800	2.40586700	-0.91099000
H	9.71934100	2.30274500	-2.54785600
H	7.44227900	2.97292700	-1.88071100
H	-2.81532900	3.66191400	2.05666600
H	-5.89199200	0.69578200	1.30022700
H	-1.51150000	2.85995000	0.08709500
H	-6.45096200	-1.09911800	-0.84805900
H	-4.24869200	-2.63547300	-4.19659300
H	-2.35294600	-1.10091000	-3.71798000
H	-7.64396500	-4.50575300	-4.61199400
H	-7.13172000	-6.89705400	-4.91396300
H	-5.39432100	-7.99489900	-3.51562900
H	-4.19056900	-6.65776800	-1.80032400
H	-4.72847600	-4.27317700	-1.47849100
H	-8.71772000	-4.08108000	-1.97049100
H	-11.02468100	-3.23245400	-2.13041900
H	-11.47902800	-1.01587500	-3.15971400
H	-9.58057500	0.32890500	-4.03608600
H	-7.27604500	-0.53686900	-3.90159400
H	-6.75337600	3.45581800	0.86219100
H	-9.22846000	3.35628200	0.84950900
H	-10.45276400	2.60474800	2.87180200
H	-9.18484500	1.93078900	4.89789400
H	-6.71407600	1.98565200	4.89083600
H	-5.71599100	5.01990000	4.09969800
H	-4.56953600	5.92175400	6.10120900
H	-2.69112900	4.66712300	7.12808800
H	-1.97159900	2.50466500	6.14342500
H	-3.12536100	1.60678800	4.14426400

Atom coordinates for optimized SI structure of Db at CAM-B3LYP/6-31G(d) level of theory

C	-0.79170400	-0.92690000	-2.32140300
C	-0.78233400	-0.91714600	-3.69710600
C	-0.00013800	0.00008000	-4.41945500
C	0.78210400	0.91727400	-3.69712100
C	0.79156500	0.92697700	-2.32141700
C	-0.00004900	0.00002600	-1.54270300
C	-0.00001200	0.00000200	-0.15022400
N	1.58355300	1.89476100	-1.63982400
N	-1.58365000	-1.89470800	-1.63979400
C	-2.96903400	-1.94497000	-1.63512600
C	-3.39692100	-3.03732600	-0.85019000
C	-2.19022500	-3.67719000	-0.35095800
C	-1.10539300	-2.93464900	-0.86725600
C	2.96893600	1.94500200	-1.63520800

C	3.39687200	3.03734100	-0.85027500
C	2.19020500	3.67721800	-0.35098900
C	1.10534200	2.93470200	-0.86725500
C	-3.88466300	-1.09658600	-2.25286400
C	-5.23241500	-1.36338900	-2.08670300
C	-5.68021400	-2.44431900	-1.30376300
C	-4.74855800	-3.28225500	-0.67718000
C	-1.95937600	-4.76944100	0.46590100
C	-0.63729600	-5.13651700	0.75694200
C	0.43149000	-4.39632200	0.21089600
C	0.21411000	-3.29546200	-0.59380100
C	1.95940500	4.76946400	0.46589200
C	0.63734300	5.13656000	0.75698600
C	-0.43147500	4.39638600	0.21097400
C	-0.21414400	3.29553300	-0.59374500
C	3.88452700	1.09660900	-2.25299200
C	5.23229100	1.36338600	-2.08687700
C	5.68013700	2.44429800	-1.30394000
C	4.74852000	3.28224300	-0.67731100
H	-1.44677900	4.70326800	0.43254600
H	5.09253800	4.10361300	-0.05832200
H	-1.04229100	2.73145700	-1.00503300
H	3.54978700	0.26215100	-2.85784400
H	5.96604000	0.72751700	-2.56870900
N	0.00003800	-0.00002900	1.02430600
H	-1.38573000	-1.65221600	-4.22126900
H	-0.00017400	0.00010000	-5.50126700
H	1.38547300	1.65236200	-4.22129200
H	-3.54996100	-0.26211400	-2.85771700
H	-5.96619300	-0.72752800	-2.56850100
H	-5.09253700	-4.10364000	-0.05818700
H	-2.78283200	-5.33444300	0.88805900
H	1.44680600	-4.70319100	0.43242400
H	1.04223200	-2.73136800	-1.00511400
H	2.78288800	5.33444800	0.88802300
N	-7.06342400	-2.67965100	-1.14755100
N	7.06335900	2.67960300	-1.14777600
N	-0.37596200	-6.23889200	1.59222600
N	0.37605400	6.23892900	1.59229600
C	0.70545400	-6.20224300	2.51051700
C	1.51500900	-7.32741800	2.68797000
C	0.96888800	-5.04569900	3.24973200
C	2.56476700	-7.29504600	3.59596800
H	1.31680500	-8.22385500	2.11052900
C	2.03127000	-5.01748300	4.14310000
H	0.34026400	-4.17158900	3.11974000
C	2.83197400	-6.14064300	4.32517100
H	3.18566100	-8.17644600	3.72362000
H	2.22465100	-4.11163200	4.70902500
H	3.65740100	-6.11638800	5.02921700
C	-0.70532800	6.20228000	2.51062500
C	-1.51486600	7.32746200	2.68811800
C	-0.96874800	5.04573200	3.24983800
C	-2.56459300	7.29509200	3.59615200
H	-1.31667300	8.22390200	2.11067700

C	-2.03109900	5.01751800	4.14324200
H	-0.34013800	4.17161700	3.11981400
C	-2.83178600	6.14068500	4.32535300
H	-3.18547300	8.17649700	3.72383500
H	-2.22447100	4.11166200	4.70916500
H	-3.65718800	6.11643000	5.02942700
C	-1.21125000	-7.38454700	1.54506400
C	-1.63902600	-7.99621400	2.72631600
C	-1.61069600	-7.91701900	0.31610300
C	-2.44713700	-9.12399900	2.67469700
H	-1.33538900	-7.58167300	3.68135800
C	-2.43210100	-9.03556200	0.27406300
H	-1.27113000	-7.45036500	-0.60223500
C	-2.85182800	-9.64767300	1.45082400
H	-2.77268300	-9.58840600	3.60037800
H	-2.73406800	-9.43861900	-0.68766600
H	-3.48843500	-10.52570400	1.41450000
C	1.21136000	7.38457000	1.54513000
C	1.63919100	7.99620200	2.72638000
C	1.61076500	7.91706900	0.31616700
C	2.44731600	9.12397700	2.67475800
H	1.33558500	7.58164100	3.68142400
C	2.43218400	9.03560100	0.27412200
H	1.27115500	7.45044300	-0.60217000
C	2.85196700	9.64767500	1.45088300
H	2.77290500	9.58835600	3.60043800
H	2.73412000	9.43867800	-0.68760900
H	3.48858500	10.52569800	1.41455600
C	7.95618500	1.59088200	-0.97794900
C	9.18778200	1.57834800	-1.63843500
C	7.61645700	0.51885600	-0.14804400
C	10.06378900	0.51550000	-1.46300600
H	9.45250100	2.40516200	-2.28855500
C	8.49133000	-0.54802800	0.00779300
H	6.66522400	0.52775700	0.37291500
C	9.72052400	-0.55532700	-0.64380400
H	11.01705300	0.52029200	-1.98265100
H	8.21284100	-1.37352300	0.65558200
H	10.40455100	-1.38775100	-0.51434900
C	-7.95626800	-1.59094500	-0.97770400
C	-9.18787300	-1.57842800	-1.63817400
C	-7.61654500	-0.51892000	-0.14779600
C	-10.06389500	-0.51559500	-1.46272500
H	-9.45258600	-2.40524200	-2.28829600
C	-8.49143400	0.54794800	0.00806200
H	-6.66530500	-0.52781100	0.37315000
C	-9.72063700	0.55523100	-0.64352000
H	-11.01716700	-0.52039900	-1.98235800
H	-8.21295100	1.37344300	0.65585300
H	-10.40467600	1.38764200	-0.51404900
C	7.56266000	4.00611800	-1.14145600
C	8.54050300	4.39034000	-0.21954500
C	7.08482300	4.94653400	-2.05888900
C	9.03343600	5.68829700	-0.22377800
H	8.90976100	3.66639000	0.49857500

C	7.57122500	6.24685600	-2.04468500
H	6.33295400	4.65064000	-2.78238700
C	8.55016300	6.62538500	-1.13149600
H	9.79270300	5.97111900	0.49889100
H	7.19011600	6.96523300	-2.76402400
H	8.93309000	7.64070900	-1.12748400
C	-7.56270300	-4.00617400	-1.14120600
C	-8.54051400	-4.39040300	-0.21926300
C	-7.08487600	-4.94659000	-2.05864400
C	-9.03342700	-5.68836800	-0.22347200
H	-8.90976300	-3.66645200	0.49886000
C	-7.57125800	-6.24692000	-2.04441400
H	-6.33303100	-4.65069100	-2.78216400
C	-8.55016400	-6.62545600	-1.13119500
H	-9.79266900	-5.97119600	0.49922000
H	-7.19015700	-6.96529700	-2.76375800
H	-8.93307500	-7.64078600	-1.12716400

Atom coordinates for optimized S0 structure of Mb at B3LYP/6-31G(d) level of theory (energy=-3697.1912 a.u.)

C	-1.17458900	0.86249100	-2.01662400
C	-1.13693900	1.42155000	-3.29296500
C	0.07828600	1.72994000	-3.92431300
C	1.26966800	1.45242800	-3.23585900
C	1.26142300	0.88227100	-1.96365300
C	0.03132700	0.58181000	-1.33190200
C	0.00648600	0.00528300	-0.02327000
N	-0.01421400	-0.46297600	1.04129500
C	4.48361300	3.71634000	-0.65041800
C	5.61928800	3.09450900	-0.08561900
C	5.66040000	1.70167200	0.03412600
C	4.58010700	0.94187200	-0.42238900
C	3.44723800	1.58815300	-0.97389800
C	3.38658600	2.97868900	-1.08293100
C	4.30452800	-0.48146900	-0.44236300
C	3.01352000	-0.64435800	-0.99905200
N	2.48964100	0.62061900	-1.31083500
C	5.03450300	-1.60194600	-0.03538400
C	4.49057600	-2.87659300	-0.21823100
C	3.21517100	-3.01589500	-0.80972300
C	2.46327900	-1.91198600	-1.19455100
N	5.21308500	-4.03821400	0.18305300
N	6.71443100	3.89245800	0.35780600
C	4.56093400	-5.03710600	0.95363700
C	6.58868400	-4.15958100	-0.14711100
C	6.46904700	5.02504500	1.17840400
C	8.04091100	3.52368200	0.00960200
C	4.83576300	-6.39871200	0.73933200
C	4.19091000	-7.37448100	1.49632500
C	3.24879100	-7.01831800	2.46397900
C	2.96545900	-5.66701900	2.67155600
C	3.61850400	-4.68182800	1.93314000
C	7.51156900	-4.65775100	0.78790600
C	8.85877300	-4.77771900	0.45246200

C	9.31648400	-4.38808200	-0.80798800
C	8.40380800	-3.88205100	-1.73603700
C	7.05191300	-3.77463600	-1.41656400
C	5.47637400	4.98531900	2.17170900
C	5.22443400	6.10608300	2.96087500
C	5.96391100	7.27801600	2.78983100
C	6.95724500	7.31823600	1.80866600
C	7.20475400	6.20944200	1.00220400
C	9.08260800	3.62007500	0.94743500
C	10.38209900	3.26017000	0.59583300
C	10.66670700	2.78090800	-0.68450000
C	9.63162000	2.67354400	-1.61578300
C	8.33225400	3.04765200	-1.27978500
C	-3.23488900	2.68555500	1.55835700
C	-4.52792000	2.17474500	1.80977300
C	-5.05236400	1.17820700	0.98139000
C	-4.28816400	0.70513500	-0.08903200
C	-2.98253900	1.20865800	-0.30093600
C	-2.44954200	2.20663200	0.51620600
C	-4.53817600	-0.27351600	-1.12922200
C	-3.37603200	-0.32136800	-1.93693000
N	-2.42572600	0.57168600	-1.42159900
C	-5.61940100	-1.11083500	-1.41637700
C	-5.54951300	-1.96850400	-2.51883300
C	-4.38439400	-1.99058900	-3.31711900
C	-3.28662800	-1.18645000	-3.02911000
N	-6.64429600	-2.82209200	-2.84371100
N	-5.28878700	2.68622000	2.90119700
C	-6.40724900	-4.19869900	-3.09864900
C	-7.96508900	-2.30068300	-2.85258700
C	-6.65676500	3.01673400	2.71361300
C	-4.68211900	2.81390100	4.17930900
C	-7.11606500	-4.87161400	-4.10861600
C	-6.87842700	-6.22201000	-4.35547500
C	-5.92084000	-6.92326800	-3.61907600
C	-5.20769400	-6.25529100	-2.62181700
C	-5.45070800	-4.90920000	-2.35441200
C	-9.03409000	-3.04173200	-2.32135300
C	-10.32725600	-2.52267800	-2.33675100
C	-10.57907800	-1.25346100	-2.86153100
C	-9.51720000	-0.50990300	-3.38100800
C	-8.22354500	-1.02713500	-3.38684300
C	-7.07856000	3.66375000	1.53974300
C	-8.42334100	3.97486600	1.35041400
C	-9.37032300	3.66589000	2.32922700
C	-8.95380600	3.02991200	3.50053000
C	-7.61392600	2.69801600	3.69163000
C	-4.96602400	3.92119800	4.99675100
C	-4.36790200	4.04314200	6.24910600
C	-3.46367400	3.08021400	6.70297500
C	-3.17078100	1.98475500	5.88830700
C	-3.77798300	1.84328600	4.64173500
H	-2.07795500	1.60744800	-3.79902000
H	2.22780500	1.68933800	-3.68539100
H	4.47023000	4.79780800	-0.73839300

H	6.52816800	1.22334600	0.47736200
H	2.51854500	3.47762600	-1.50200000
H	6.01746900	-1.49241700	0.41186800
H	2.81427300	-4.01343100	-0.95636000
H	1.48322000	-2.04502400	-1.64059900
H	5.55449900	-6.68464100	-0.02193900
H	4.41731400	-8.42224400	1.31536800
H	2.74218900	-7.78268000	3.04632400
H	2.23844700	-5.37088900	3.42329500
H	3.39968400	-3.63373700	2.10951600
H	7.16592700	-4.94900900	1.77452200
H	9.55701800	-5.16495500	1.19014600
H	10.36879500	-4.47612000	-1.06269900
H	8.74205700	-3.57933400	-2.72381300
H	6.34592800	-3.39212300	-2.14688000
H	4.90732200	4.07325600	2.32003100
H	4.45261200	6.05483200	3.72457100
H	5.76924900	8.14722200	3.41156100
H	7.53699400	8.22518700	1.65686000
H	7.96775000	6.25326300	0.23159700
H	8.86646900	3.97714600	1.94916600
H	11.17399400	3.34109300	1.33607700
H	11.67957100	2.49369800	-0.95197300
H	9.83656400	2.30747400	-2.61861700
H	7.53490100	2.97319100	-2.01230000
H	-2.84783000	3.46762800	2.20318100
H	-6.04805200	0.78854400	1.16822200
H	-1.45720800	2.61152600	0.34699000
H	-6.51026500	-1.10056800	-0.79623200
H	-4.34870200	-2.66030800	-4.17020700
H	-2.39610800	-1.22834300	-3.64828100
H	-7.85132200	-4.33030600	-4.69554600
H	-7.43746800	-6.72437400	-5.14086900
H	-5.73341500	-7.97422800	-3.81981500
H	-4.46396300	-6.78702000	-2.03384800
H	-4.90259500	-4.40170700	-1.56712600
H	-8.84437400	-4.02243700	-1.89720700
H	-11.14040100	-3.11139600	-1.91984200
H	-11.58726400	-0.84914600	-2.86433300
H	-9.69633100	0.47777900	-3.79826600
H	-7.40520400	-0.44859000	-3.80346300
H	-6.34620900	3.91831200	0.78024000
H	-8.72903300	4.47538100	0.43510300
H	-10.41698900	3.91579900	2.18090000
H	-9.67869000	2.77372500	4.26902800
H	-7.30099000	2.18992700	4.59804700
H	-5.65568900	4.68137600	4.64398300
H	-4.60036900	4.90689600	6.86690700
H	-2.99320700	3.18305000	7.67669600
H	-2.47282500	1.22358300	6.22714900
H	-3.55352900	0.98245700	4.02019800
C	0.10277900	2.33262100	-5.27863500
C	1.10948400	2.00304200	-6.20099300
C	-0.88336600	3.24842100	-5.68200000
C	1.12586700	2.56726200	-7.47382100

H	1.86826700	1.27306300	-5.93341200
C	-0.85899100	3.81144200	-6.95473300
H	-1.66312900	3.54263400	-4.98511600
C	0.14601300	3.48466900	-7.87517800
H	1.90933300	2.28237500	-8.17209600
H	-1.63173300	4.52281100	-7.23679800
C	0.18402800	4.11908400	-9.24480600
H	0.72577700	5.07421100	-9.22363200
H	0.68984600	3.47461700	-9.97113200
H	-0.82405500	4.32708200	-9.61882600

Atom coordinates for optimized T1 strcuture of Mb at UCAM-B3LYP/6-31G(d) level of theory

C	-1.10346500	1.05996400	-2.33605500
C	-1.02795100	1.54263200	-3.61469700
C	0.21322300	1.77693800	-4.26099500
C	1.37824800	1.46544600	-3.49460100
C	1.31981800	0.97944300	-2.21991000
C	0.06380700	0.74781000	-1.54868100
C	-0.02020800	0.23144700	-0.25290900
N	-0.12093100	-0.18520100	0.83641300
C	4.29554900	3.72194500	-0.31724600
C	5.36125400	3.07326100	0.33255000
C	5.43589100	1.68601400	0.33513900
C	4.45037000	0.95118200	-0.32125700
C	3.38287500	1.61940600	-0.95676400
C	3.29523700	3.01025200	-0.95622300
C	4.22150200	-0.46490200	-0.51416500
C	3.02751700	-0.58022600	-1.25418400
N	2.52741600	0.68607100	-1.52357200
C	4.90736300	-1.61265100	-0.12037200
C	4.41252500	-2.85653200	-0.49054100
C	3.22842900	-2.94979500	-1.24485400
C	2.52035700	-1.82390600	-1.62503600
N	5.10239300	-4.04796400	-0.11328300
N	6.36665700	3.85049100	0.98369300
C	4.40614700	-5.05274400	0.59327600
C	6.47270500	-4.18166000	-0.43076500
C	5.98279900	4.77486200	1.97887400
C	7.72174300	3.66116900	0.63149100
C	4.68771900	-6.40799200	0.38231700
C	3.99022600	-7.38738600	1.07601300
C	2.98721000	-7.04261100	1.97651800
C	2.69546400	-5.69784700	2.17811800
C	3.39888800	-4.70968800	1.50207700
C	7.36467600	-4.78640800	0.46199800
C	8.70965600	-4.90696100	0.13860700
C	9.19740900	-4.41243000	-1.06657400
C	8.31597500	-3.79873100	-1.95058900
C	6.96653700	-3.68875300	-1.64349600
C	4.90209000	4.49591000	2.82293500
C	4.50563400	5.41488200	3.78554700
C	5.18137200	6.62080500	3.93799800
C	6.25861500	6.90025600	3.10289200
C	6.65271300	5.99548500	2.12673700

C	8.73258800	3.71483300	1.59785200
C	10.05971700	3.52120700	1.23847500
C	10.40609600	3.25140300	-0.08143200
C	9.40250500	3.18407400	-1.04219200
C	8.07444500	3.39293800	-0.69557100
C	-2.93435100	3.00907700	1.19096600
C	-4.20859300	2.48703600	1.56992600
C	-4.81727700	1.47149100	0.78362900
C	-4.14952400	0.98793700	-0.30911700
C	-2.86349000	1.50331200	-0.65145200
C	-2.26628500	2.53675400	0.09690500
C	-4.44708100	-0.04089600	-1.29651800
C	-3.33890700	-0.08723600	-2.15845500
N	-2.39158600	0.86419600	-1.74521700
C	-5.51507500	-0.90194500	-1.48152000
C	-5.47779500	-1.80867400	-2.55002300
C	-4.35763400	-1.83281100	-3.40213800
C	-3.27719500	-0.98541100	-3.21318000
N	-6.55037900	-2.69381700	-2.76573400
N	-4.84060900	2.96216300	2.69296300
C	-6.30746700	-4.01807400	-3.22281700
C	-7.88435100	-2.28147800	-2.50988500
C	-6.25815500	2.85704200	2.84684800
C	-4.10337000	3.55658600	3.76498000
C	-7.09507200	-4.56494300	-4.23786900
C	-6.86710300	-5.86356600	-4.67429200
C	-5.84349000	-6.62473200	-4.11931400
C	-5.05350500	-6.07770300	-3.11334100
C	-5.28721200	-4.78659500	-2.65802900
C	-8.76580800	-3.12820700	-1.83358100
C	-10.07536700	-2.72985500	-1.59907600
C	-10.51927100	-1.47980500	-2.01822700
C	-9.64051200	-0.63260800	-2.68568200
C	-8.33451500	-1.03046600	-2.94005800
C	-7.10413900	3.32159200	1.83995400
C	-8.48025900	3.22752400	2.00252800
C	-9.01270500	2.68309900	3.16660700
C	-8.16344600	2.23053800	4.17231400
C	-6.78672300	2.31497400	4.01759400
C	-4.52739900	4.77247600	4.29976100
C	-3.82477100	5.33855600	5.35438400
C	-2.70377300	4.69853600	5.87504300
C	-2.28774200	3.48363600	5.34008900
C	-2.98682400	2.90484300	4.28902000
H	-1.95663200	1.79377000	-4.11655600
H	2.36172000	1.57705300	-3.93807300
H	4.26555700	4.80659000	-0.30812800
H	6.25944200	1.19157900	0.84063800
H	2.47736500	3.51657600	-1.45674700
H	5.82149600	-1.54677300	0.46110500
H	2.86750800	-3.93409900	-1.52400900
H	1.60485900	-1.90449600	-2.20017000
H	5.45540500	-6.68923900	-0.32994500
H	4.22593100	-8.43241600	0.89705000
H	2.43924000	-7.81169800	2.51138300

H	1.91709400	-5.40756700	2.87753100
H	3.16812200	-3.66419600	1.67257500
H	6.99786100	-5.16032100	1.41145400
H	9.38440600	-5.37977200	0.84619800
H	10.25071000	-4.50156000	-1.31222800
H	8.67764400	-3.40839600	-2.89727000
H	6.28435300	-3.21659700	-2.34167300
H	4.37560300	3.55385200	2.71851000
H	3.66462500	5.17637100	4.43004800
H	4.87262300	7.33396200	4.69555600
H	6.79304100	7.84077500	3.19980200
H	7.48312900	6.23130100	1.47058400
H	8.47208200	3.90700900	2.63275200
H	10.82806700	3.56693300	2.00466100
H	11.44369600	3.09271800	-0.35689900
H	9.65336700	2.97624500	-2.07815100
H	7.29922500	3.34651100	-1.45223500
H	-2.50403000	3.81154800	1.77539200
H	-5.77687700	1.06469300	1.07704700
H	-1.30506200	2.94181700	-0.19425400
H	-6.36626600	-0.89128300	-0.81023500
H	-4.34323500	-2.53505400	-4.22713500
H	-2.41987400	-1.01386900	-3.87533300
H	-7.88512000	-3.96759200	-4.68018300
H	-7.48718900	-6.27704600	-5.46363200
H	-5.66266900	-7.63629300	-4.46791500
H	-4.25554400	-6.66315900	-2.66741700
H	-4.67891800	-4.36774900	-1.86346300
H	-8.41875600	-4.09895100	-1.49659500
H	-10.74953700	-3.39954600	-1.07410300
H	-11.54192200	-1.16991700	-1.82926500
H	-9.97671200	0.34131800	-3.02806300
H	-7.65706500	-0.37566800	-3.47775800
H	-6.68184200	3.76180200	0.94291600
H	-9.13707800	3.59217800	1.21978300
H	-10.08816900	2.61463500	3.29211100
H	-8.57377200	1.80300700	5.08109900
H	-6.11886100	1.95910200	4.79437000
H	-5.39810100	5.26856700	3.88506300
H	-4.15159400	6.28753000	5.76642400
H	-2.15664400	5.14529400	6.69853000
H	-1.41980100	2.97532800	5.74637500
H	-2.67382300	1.95118600	3.87769100
C	0.29230600	2.30712200	-5.61671300
C	1.45606400	2.93452600	-6.10423500
C	-0.78831500	2.22084100	-6.51691200
C	1.52785300	3.43666300	-7.39387500
H	2.31565600	3.05316800	-5.45270100
C	-0.70987100	2.73270800	-7.80250900
H	-1.69926200	1.71266800	-6.21644400
C	0.44737300	3.35483700	-8.27451400
H	2.44773200	3.91450100	-7.72351200
H	-1.56766400	2.63326900	-8.46406900
C	0.51934900	3.93367200	-9.66322500
H	0.22646900	4.99103700	-9.67665500

H	1.53405800	3.87579100	-10.06899100
H	-0.14799300	3.40541200	-10.35106600

Atom coordinates for optimized SI strcuture of Mb at CAM-B3LYP/6-31G(d) level of theory

C	-1.14125700	1.34267400	-2.30188000
C	-1.04287800	2.00728100	-3.49993900
C	0.20072000	2.29990100	-4.08756000
C	1.35341700	1.84291600	-3.37232900
C	1.27224200	1.18435900	-2.17944800
C	0.00674900	0.90262200	-1.55109400
C	-0.12310000	0.29023300	-0.30458100
N	-0.28304400	-0.22213500	0.73747400
C	4.44892100	3.55063900	-0.09780700
C	5.48826400	2.78028200	0.45443500
C	5.47590600	1.39731500	0.32374300
C	4.43034500	0.78968100	-0.36876500
C	3.39158100	1.57796200	-0.90615900
C	3.39084200	2.96496700	-0.77064600
C	4.10922200	-0.58536800	-0.68624200
C	2.89242800	-0.55869300	-1.39703200
N	2.46525000	0.75495300	-1.53053200
C	4.73334900	-1.80344700	-0.42324300
C	4.15499700	-2.97509900	-0.89418400
C	2.94994600	-2.92623500	-1.61837000
C	2.30206700	-1.72973000	-1.86812400
N	4.77900600	-4.23581300	-0.65104900
N	6.55537900	3.43000800	1.14546500
C	4.04237500	-5.25756000	-0.01349900
C	6.13220600	-4.41694600	-1.01558600
C	6.25358000	4.27525300	2.23540200
C	7.88770900	3.18857500	0.74274300
C	4.23840200	-6.60272700	-0.34943700
C	3.50289300	-7.59870500	0.27817800
C	2.54547200	-7.27882600	1.23577300
C	2.33814600	-5.94274800	1.56149600
C	3.08035100	-4.93984100	0.95182400
C	7.00704100	-5.14765700	-0.20387900
C	8.33558200	-5.31274400	-0.57248200
C	8.82448800	-4.74004000	-1.74204700
C	7.96084100	-4.00168300	-2.54451300
C	6.62689500	-3.84547300	-2.19294000
C	5.17957900	3.97997500	3.08218200
C	4.86453300	4.82371800	4.13918400
C	5.61671900	5.96760500	4.38373900
C	6.68762600	6.26270800	3.54585600
C	7.00067600	5.43448200	2.47678600
C	8.91893500	3.08771500	1.68349700
C	10.22309500	2.84442100	1.27373900
C	10.52494800	2.67766800	-0.07384400
C	9.50021300	2.76395900	-1.01050000
C	8.19588000	3.02358800	-0.61205100
C	-3.40263600	3.62077900	0.76392200
C	-4.59982900	3.00576500	1.20059100
C	-5.01423500	1.78195300	0.61437200

C	-4.23511700	1.21438500	-0.36147400
C	-3.03734000	1.84644400	-0.77643000
C	-2.61738700	3.05432700	-0.21656100
C	-4.32895500	-0.02154800	-1.13953100
C	-3.18375800	-0.04966800	-1.96486200
N	-2.42735900	1.08481300	-1.73981700
C	-5.23499000	-1.05484000	-1.17453600
C	-5.00162800	-2.14239100	-2.04928700
C	-3.85221700	-2.14387700	-2.86758600
C	-2.93758100	-1.10841500	-2.83348300
N	-5.89752700	-3.20655300	-2.08877600
N	-5.36084800	3.58348000	2.20265900
C	-5.46195700	-4.51807600	-2.44235400
C	-7.27402000	-3.01758300	-1.77611000
C	-6.76008300	3.32637100	2.30723400
C	-4.77129500	4.45299700	3.17019900
C	-6.17120800	-5.25300400	-3.39222100
C	-5.76161000	-6.53899200	-3.71999500
C	-4.63962100	-7.09526500	-3.11424000
C	-3.93165000	-6.35954400	-2.16899300
C	-4.34288900	-5.07861300	-1.82484000
C	-7.91511000	-3.89239100	-0.89800700
C	-9.26247500	-3.72150800	-0.60965700
C	-9.97815600	-2.67474300	-1.18271600
C	-9.33792100	-1.80202900	-2.05654800
C	-7.99393800	-1.97445200	-2.36161200
C	-7.58758600	3.47698000	1.19370600
C	-8.95059100	3.23497600	1.30709400
C	-9.49748600	2.85884400	2.52955400
C	-8.67173500	2.72132200	3.64123500
C	-7.30645600	2.94954500	3.53398900
C	-5.36064700	5.68735800	3.44069100
C	-4.80356900	6.52296400	4.39979200
C	-3.65601100	6.13787800	5.08566700
C	-3.06991000	4.90580300	4.81309700
C	-3.62701500	4.05857900	3.86427700
H	-1.96198500	2.33278200	-3.97615100
H	2.34047400	1.98084000	-3.79959900
H	4.48565900	4.62905800	0.01606200
H	6.27861900	0.80773700	0.75525200
H	2.59296800	3.56523800	-1.19320800
H	5.66348900	-1.84679000	0.13443600
H	2.52332800	-3.85660800	-1.97822200
H	1.36868200	-1.70204000	-2.41873300
H	4.97013600	-6.86277800	-1.10623300
H	3.67276400	-8.63554700	0.00282900
H	1.96821400	-8.06015900	1.71970300
H	1.59714300	-5.67182100	2.30770700
H	2.91592500	-3.90224400	1.21956900
H	6.64021500	-5.58376600	0.71864900
H	8.99741000	-5.88332100	0.07243400
H	9.86539700	-4.86466100	-2.02258500
H	8.32379100	-3.54840300	-3.46220700
H	5.95800400	-3.27518000	-2.82787800
H	4.59352300	3.08505800	2.90551200

H	4.02690900	4.57409900	4.78379700
H	5.37136900	6.62142500	5.21447600
H	7.28092200	7.15661200	3.71472900
H	7.82721300	5.68298300	1.82033300
H	8.69216400	3.19875400	2.73800900
H	11.00775800	2.76955300	2.02086900
H	11.54426700	2.47987200	-0.38936200
H	9.71637000	2.63831000	-2.06731600
H	7.40451600	3.09741000	-1.34959700
H	-3.10497500	4.56261400	1.20581800
H	-5.91602200	1.29495800	0.96417900
H	-1.70616000	3.53374000	-0.55241200
H	-6.10336200	-1.06042000	-0.52694900
H	-3.68972600	-2.97414400	-3.54287200
H	-2.06242600	-1.11215300	-3.47207900
H	-7.04026900	-4.81247900	-3.86900200
H	-6.31805700	-7.10432400	-4.46072500
H	-4.31890100	-8.09818400	-3.37615400
H	-3.05963500	-6.78754600	-1.68521400
H	-3.80038300	-4.50894500	-1.07783300
H	-7.35261200	-4.70219600	-0.44616800
H	-9.75264400	-4.40622800	0.07499400
H	-11.03018300	-2.54242000	-0.95236800
H	-9.89009900	-0.98944800	-2.51793100
H	-7.49781500	-1.30751000	-3.05880300
H	-7.15986600	3.78987900	0.24701200
H	-9.58883200	3.35585700	0.43773700
H	-10.56361300	2.67722800	2.61688300
H	-9.09035000	2.42628400	4.59794800
H	-6.65772000	2.83653400	4.39579200
H	-6.25105800	5.98588600	2.89787300
H	-5.26497600	7.48353300	4.60488700
H	-3.22083500	6.79476100	5.83155300
H	-2.17951300	4.59396000	5.34908500
H	-3.18008600	3.09161200	3.65921600
C	0.31130200	3.02047400	-5.35567600
C	1.48105600	3.71603400	-5.71124600
C	-0.74101400	3.05405800	-6.28903300
C	1.58569500	4.39749800	-6.91422600
H	2.31902800	3.74363100	-5.02222000
C	-0.63178900	3.74548500	-7.48550900
H	-1.65310100	2.50018000	-6.08988200
C	0.53219800	4.43527300	-7.82859700
H	2.50964400	4.92270300	-7.14494100
H	-1.46851300	3.73555400	-8.18034800
C	0.63768600	5.20571500	-9.11865900
H	0.28991300	6.23964200	-9.00144500
H	1.67173200	5.25155400	-9.47339900
H	0.03172600	4.74937200	-9.90742300