

## A covalently linked dimer of $[\text{Ag}_{25}(\text{DMBT})_{18}]^{-}$

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### A Isomer

Ag	15.164230000	16.096740000	22.226480000
Ag	12.727850000	15.021010000	23.176390000
Ag	13.483520000	14.759360000	20.392940000
Ag	13.834040000	17.460790000	24.322190000
Ag	12.766070000	17.373320000	21.492310000
Ag	16.816960000	17.464530000	24.029390000
Ag	17.510780000	17.225240000	21.104580000
Ag	16.532310000	14.680470000	20.223010000
Ag	15.017160000	17.277320000	19.645320000
Ag	15.301200000	15.054980000	24.849740000
Ag	17.504840000	14.742200000	22.992020000
Ag	15.306640000	18.922330000	22.024170000
Ag	15.072930000	13.262430000	22.312620000
Ag	12.937960000	19.730660000	19.771280000
Ag	12.237750000	15.193050000	26.082070000
Ag	17.749090000	16.317370000	18.039410000
Ag	18.246000000	15.368660000	25.935960000
Ag	12.330530000	12.185950000	21.789460000

Ag	10.885850000	17.583970000	23.941020000
Ag	19.719310000	15.282100000	20.485830000
Ag	16.649170000	12.439860000	24.821290000
Ag	18.169040000	19.808590000	22.894040000
Ag	15.279850000	20.080140000	24.765440000
Ag	14.751890000	12.228000000	19.326800000
Ag	12.620650000	16.731030000	18.007390000
S	17.431570000	21.220870000	24.745850000
S	11.231740000	13.081360000	23.764470000
S	18.293530000	17.796590000	26.105620000
S	15.594190000	17.105950000	17.199110000
S	12.595820000	14.299940000	18.092730000
S	14.176100000	13.876870000	26.764140000
S	12.949990000	19.617570000	25.324230000
S	14.077450000	21.050910000	21.517980000
S	10.054550000	16.236190000	25.790180000
S	15.085490000	11.060560000	23.549490000
S	10.833360000	18.957060000	21.910190000
S	16.615970000	13.287750000	18.142030000
S	20.006530000	14.562790000	22.809970000
S	19.580710000	18.671870000	21.244060000
S	12.247420000	19.085840000	17.514690000
S	20.044840000	15.481990000	18.080870000
S	18.480420000	12.981760000	26.344100000
S	12.823560000	10.825250000	19.841590000
C	17.072770000	22.819540000	24.011830000
C	18.127400000	23.617700000	23.481190000

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C	16.492670000	25.387990000	22.903470000
C	15.467940000	24.592680000	23.463070000
C	15.753200000	23.331390000	24.008260000
C	19.550890000	23.118810000	23.440030000
C	16.181850000	26.707320000	22.234680000
C	9.557960000	13.426240000	23.211260000
C	8.570610000	12.401930000	23.321360000
C	7.237510000	12.723900000	22.986290000
C	6.842970000	14.008560000	22.550890000
C	7.840670000	15.000140000	22.432030000
C	9.175260000	14.705680000	22.749750000
C	8.928510000	11.005490000	23.769850000
C	5.403610000	14.303260000	22.189850000
C	15.871290000	18.740260000	16.518820000
C	16.248000000	18.850850000	15.146650000
C	16.410390000	20.143030000	14.601390000
C	16.192640000	21.323090000	15.347770000
C	15.800370000	21.187190000	16.697640000
C	15.652490000	19.914690000	17.273690000
C	16.431170000	17.627290000	14.280000000
C	16.390540000	22.687780000	14.723710000
C	10.853590000	13.874950000	18.166660000
C	10.117850000	13.764200000	16.947240000
C	8.771640000	13.348670000	17.016790000
C	8.127760000	13.025960000	18.233450000
C	8.873290000	13.148920000	19.424630000

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C	10.754370000	14.064970000	15.611740000
C	6.688600000	12.557300000	18.250720000
C	14.635660000	14.632090000	28.324360000
C	14.057480000	14.123470000	29.527680000
C	14.475790000	14.676960000	30.756120000
C	15.440890000	15.705460000	30.845830000
C	15.991230000	16.198150000	29.642490000
C	15.594240000	15.667070000	28.403460000
C	13.041070000	13.007670000	29.499830000
C	15.889870000	16.232600000	32.191490000
C	13.027510000	19.494750000	27.112760000
C	12.891700000	20.675970000	27.899510000
C	12.855460000	20.539680000	29.304630000
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C	13.088050000	18.137920000	29.153680000
C	13.135680000	18.242010000	27.756720000
C	12.800700000	22.043150000	27.265170000
C	12.846410000	19.176220000	31.460680000
C	15.150910000	22.124750000	20.569080000
C	14.605360000	23.289190000	19.946140000
C	15.482090000	24.147490000	19.246930000
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C	9.340680000	17.815380000	29.496030000
C	9.127350000	19.188480000	29.255960000
C	9.232960000	19.645660000	27.922860000
C	9.551580000	18.757990000	26.883640000
C	9.903990000	15.446890000	28.807170000
C	8.836860000	20.142950000	30.393020000
C	16.248680000	9.931440000	22.773570000
C	16.601240000	8.722360000	23.447230000
C	17.477750000	7.824360000	22.798620000
C	18.010180000	8.066280000	21.512760000
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C	16.074080000	8.405610000	24.826250000
C	18.921000000	7.068850000	20.830490000
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C	8.152750000	18.919870000	21.174020000
C	7.070820000	18.436190000	20.406220000
C	7.202360000	17.379170000	19.478870000
C	8.477120000	16.792560000	19.323750000
C	9.569550000	17.248120000	20.076360000
C	7.948410000	20.051880000	22.151810000
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C	18.222910000	11.246830000	17.169910000
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C	22.464120000	11.319350000	22.404900000
C	21.658900000	10.223140000	22.790840000
C	20.313850000	10.483420000	23.129680000
C	19.803610000	11.791320000	23.087900000
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C	22.229960000	8.823740000	22.852770000
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C	20.816700000	20.766650000	19.908970000
C	21.011300000	21.582400000	18.775260000
C	20.234060000	21.457570000	17.600960000
C	19.200870000	20.496260000	17.589470000
C	18.967030000	19.684960000	18.712120000
C	21.732450000	20.894880000	21.105530000
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C	17.772100000	12.592480000	27.946710000
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H	12.652660000	22.829990000	28.037950000
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H	9.252040000	17.432770000	30.533990000
H	9.066600000	20.717040000	27.691280000
H	9.644540000	19.137280000	25.845810000
H	9.243670000	14.767040000	28.220290000
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H	10.953290000	15.157040000	28.549220000
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H	8.031990000	20.867190000	30.130790000
H	9.742840000	20.742420000	30.651840000
H	17.758690000	6.892420000	23.333270000
H	18.059170000	9.505990000	19.868230000
H	16.528590000	11.135610000	20.975890000
H	16.444880000	9.145840000	25.576160000
H	16.397660000	7.392220000	25.152370000
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H	19.634220000	7.577740000	20.143490000
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H	5.257920000	17.656740000	18.517420000
H	19.544930000	9.721410000	16.379060000
H	20.757760000	11.440490000	20.188760000
H	18.723170000	12.884510000	20.167900000
H	16.227140000	10.907110000	16.363540000
H	17.578940000	10.346080000	15.303910000
H	17.182150000	12.103550000	15.453840000
H	21.798170000	9.243760000	19.281490000
H	22.445350000	10.212470000	17.922780000
H	21.452430000	8.753810000	17.578230000
H	23.521550000	11.138490000	22.118180000
H	19.641260000	9.651980000	23.418350000
H	18.739620000	11.974560000	23.343820000
H	22.445130000	14.344720000	21.097900000
H	23.886290000	13.380100000	21.618800000
H	23.052100000	14.497720000	22.775710000
H	22.796590000	8.564680000	21.928230000
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H	22.939920000	8.712490000	23.707250000
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H	22.414530000	20.013090000	21.185300000
H	20.669350000	23.377060000	16.647000000
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H	21.476430000	21.964220000	15.889150000
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H	8.225490000	17.441150000	15.202110000
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H	6.237480000	20.047290000	14.969360000
H	22.155820000	18.873050000	15.143330000
H	23.682900000	18.674970000	19.202600000
H	21.965220000	16.903670000	19.729610000
H	20.248140000	15.907130000	15.171610000
H	20.397730000	17.539150000	14.398270000
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H	23.848180000	20.906940000	17.392320000
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H	19.536010000	14.647640000	30.137970000
H	18.949050000	15.164620000	28.508200000
H	16.593890000	10.344430000	32.137890000
H	15.093480000	11.269200000	31.813780000
H	16.483660000	12.070260000	32.629000000
H	15.228840000	6.482760000	19.772840000
H	12.756590000	7.249250000	23.268060000
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H	14.010000000	9.065260000	17.725660000
H	15.438310000	7.995830000	18.034270000
H	15.447460000	9.721690000	18.561180000
H	14.760320000	4.652710000	21.362740000
H	13.647820000	4.903050000	22.758300000
H	15.343980000	5.482560000	22.843450000
C	20.000260000	18.468200000	26.308200000
H	20.326790000	18.191370000	27.338910000
H	19.852950000	19.577360000	26.304580000
C	21.117790000	18.138540000	25.335380000
C	20.916670000	17.563030000	24.068740000
C	22.450870000	18.449910000	25.689190000
C	22.006540000	17.381920000	23.200910000
N	23.515610000	18.276230000	24.866470000
C	23.303030000	17.759820000	23.598160000
H	22.682110000	18.862270000	26.690690000

H	21.823340000	16.931650000	22.208870000
C	24.501090000	17.626790000	22.736490000
N	25.703090000	18.047040000	23.275440000
C	26.858790000	17.839930000	22.561320000
H	27.796300000	18.179750000	23.044390000
C	26.912310000	17.211020000	21.293130000
C	25.659680000	16.867940000	20.724190000
H	25.622140000	16.407890000	19.715640000
C	24.472780000	17.066300000	21.442070000
H	23.512890000	16.761170000	20.992990000
H	26.250950000	13.498990000	25.387160000
C	26.101900000	14.396620000	26.015350000
C	26.078850000	14.324020000	27.427150000
C	25.937710000	15.643290000	25.401910000
C	25.878480000	15.501690000	28.155800000
N	25.757700000	16.802270000	26.097350000
C	25.711640000	16.737460000	27.483280000
H	26.214390000	13.357560000	27.948810000
H	25.960730000	15.742080000	24.300800000
H	25.849880000	15.469290000	29.260430000
C	25.468750000	18.015270000	28.153160000
N	25.289980000	19.103300000	27.306910000
C	25.018880000	20.317180000	27.868090000
H	24.873050000	21.149520000	27.154450000
C	24.926860000	20.526040000	29.247690000
C	25.117610000	19.425310000	30.116210000
H	25.051630000	19.551350000	31.213350000

C	25.386890000	18.171960000	29.558020000
H	25.540040000	17.297850000	30.217610000
C	29.900500000	18.976290000	25.614290000
C	30.157150000	20.293070000	25.169820000
C	28.575180000	18.532660000	25.674360000
C	29.073320000	21.108550000	24.825090000
N	27.510400000	19.312570000	25.332770000
C	27.749570000	20.616620000	24.922270000
H	31.195370000	20.667820000	25.081120000
H	28.328980000	17.502840000	25.994460000
H	29.253810000	22.138940000	24.468150000
C	26.552190000	21.392970000	24.575410000
N	25.353400000	20.698030000	24.657830000
C	24.202010000	21.342730000	24.313570000
H	23.275930000	20.740500000	24.372680000
C	24.165820000	22.681540000	23.908630000
C	25.378220000	23.404910000	23.841990000
H	25.388160000	24.468020000	23.534500000
C	26.571150000	22.749830000	24.172960000
H	27.532500000	23.294020000	24.125890000
H	24.712300000	21.539670000	29.633480000
H	30.719740000	18.291080000	25.898480000
H	23.193460000	23.141290000	23.649870000
Ru	25.522380000	18.713800000	25.270720000
C	28.182100000	16.740650000	20.580190000
H	28.542250000	15.827850000	21.117860000
H	27.890930000	16.407750000	19.558860000

H	19.893830000	17.258220000	23.771460000
Ag	32.840440000	16.752110000	15.970260000
Ag	34.895910000	18.642900000	15.502530000
Ag	34.301290000	16.642870000	13.496670000
Ag	34.320630000	17.645650000	18.180980000
Ag	35.532050000	15.868060000	16.018640000
Ag	31.428230000	16.951820000	18.515340000
Ag	30.901930000	14.761910000	16.350460000
Ag	31.306220000	15.923930000	13.753730000
Ag	33.427820000	14.148680000	15.003580000
Ag	32.298860000	19.309420000	17.004480000
Ag	30.188540000	17.661600000	15.870640000
Ag	33.356790000	14.727390000	17.852220000
Ag	32.266400000	18.649310000	13.966440000
Ag	36.082450000	13.035960000	16.497400000
Ag	35.184250000	20.726010000	17.553470000
Ag	30.659590000	13.028350000	13.516430000
Ag	29.379710000	19.181180000	18.446460000
Ag	34.732570000	19.616540000	12.531040000
Ag	37.251590000	17.832330000	17.623040000
Ag	28.383620000	15.074710000	14.900840000
Ag	30.368920000	20.644270000	15.255490000
Ag	30.700420000	14.208950000	19.325220000
Ag	33.500720000	15.871230000	20.542320000
Ag	32.655100000	17.352290000	11.086870000
Ag	35.816810000	13.870070000	13.187530000
S	31.645150000	14.646470000	21.531510000



S	35.873330000	20.696950000	14.399400000
S	29.678120000	17.836460000	20.464630000
S	33.013800000	12.448700000	13.196620000
S	35.303000000	15.520740000	11.468150000
S	32.967170000	21.725090000	17.276530000
S	35.591300000	17.102930000	20.300960000
S	35.075720000	13.137430000	18.752720000
S	37.551690000	20.234520000	17.889490000
S	31.704700000	20.995590000	13.246780000
S	37.765930000	15.477310000	17.159770000
S	31.201340000	15.401520000	11.302530000
S	27.734700000	17.126160000	16.070560000
S	29.065070000	13.552400000	17.622440000
S	36.793150000	11.992330000	14.400390000
S	28.244360000	13.231740000	13.317470000
S	28.616600000	20.937500000	16.924420000
S	34.175000000	19.055790000	10.226880000
C	32.359000000	13.078240000	22.041340000
C	31.512900000	11.962680000	22.309820000
C	32.104460000	10.766250000	22.767320000
C	33.493000000	10.628740000	22.977130000
C	34.309260000	11.751840000	22.715580000
C	33.752180000	12.954120000	22.253680000
C	30.024060000	12.026140000	22.078970000
C	34.094430000	9.314820000	23.422410000
C	37.619200000	20.413510000	14.082190000
C	38.359040000	21.385670000	13.346480000

C	39.754260000	21.202240000	13.218220000
C	40.443040000	20.108850000	13.788600000
C	39.685130000	19.147740000	14.492970000
C	38.296570000	19.296910000	14.621190000
C	37.682850000	22.577180000	12.712610000
C	41.936570000	19.940790000	13.618820000
C	33.188110000	10.797940000	13.871560000
C	32.882060000	9.679050000	13.039290000
C	33.092170000	8.385690000	13.563210000
C	33.614250000	8.155580000	14.856130000
C	33.916160000	9.279360000	15.656050000
C	33.694620000	10.578660000	15.172060000
C	32.371710000	9.861090000	11.629380000
C	33.826700000	6.748920000	15.372450000
C	36.887000000	16.251390000	11.040450000
C	37.689460000	15.621080000	10.040120000
C	38.899590000	16.244340000	9.665570000
C	39.340320000	17.465630000	10.224840000
C	38.525670000	18.073050000	11.204020000
C	37.328260000	17.464110000	11.613640000
C	37.261270000	14.329050000	9.386420000
C	40.637510000	18.107780000	9.783190000
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C	32.978760000	23.554550000	19.368070000
C	32.589800000	23.987350000	20.653840000
C	31.798920000	23.200980000	21.518920000
C	31.406300000	21.919330000	21.074930000

C	31.791550000	21.456960000	19.807150000
C	33.776830000	24.466530000	18.469370000
C	31.342550000	23.742710000	22.856440000
C	35.289300000	18.441610000	21.459020000
C	35.629080000	18.255850000	22.831600000
C	35.473410000	19.348640000	23.711760000
C	35.006670000	20.610800000	23.285970000
C	34.657620000	20.764140000	21.926330000
C	34.798240000	19.694830000	21.029000000
C	36.139080000	16.926630000	23.333060000
C	34.933470000	21.783800000	24.238570000
C	34.316260000	11.527150000	18.936430000
C	35.138780000	10.405260000	19.259570000
C	34.517600000	9.153170000	19.458120000
C	33.121090000	8.967730000	19.364690000
C	32.327490000	10.093590000	19.054880000
C	32.917080000	11.347770000	18.837180000
C	36.635430000	10.547830000	19.384900000
C	32.494530000	7.602480000	19.543000000
C	37.963400000	20.504820000	19.608350000
C	37.841160000	21.805720000	20.180260000
C	38.260330000	21.994060000	21.514080000
C	38.794260000	20.953820000	22.303670000
C	38.925130000	19.678830000	21.708870000
C	38.517420000	19.459710000	20.384860000
C	37.261070000	22.958320000	19.401250000
C	39.171250000	21.185590000	23.749370000

C	30.406980000	20.939460000	12.007870000
C	29.791260000	22.164060000	11.607870000
C	28.810800000	22.118980000	10.595230000
C	28.425850000	20.921760000	9.952330000
C	29.043930000	19.723100000	10.368350000
C	30.013080000	19.732930000	11.385510000
C	30.159250000	23.480170000	12.248990000
C	27.400620000	20.928370000	8.838390000
C	39.046450000	15.582980000	15.905870000
C	40.411580000	15.546420000	16.318380000
C	41.411190000	15.558560000	15.320170000
C	41.111970000	15.590550000	13.939850000
C	39.752470000	15.618470000	13.557240000
C	38.738470000	15.620790000	14.526760000
C	40.790890000	15.477350000	17.778810000
C	42.205340000	15.609420000	12.893940000
C	29.595140000	15.901330000	10.688350000
C	29.305750000	15.753320000	9.299530000
C	27.999390000	16.059620000	8.856710000
C	26.976260000	16.490840000	9.728170000
C	27.289700000	16.632460000	11.098760000
C	28.579860000	16.349080000	11.565300000
C	30.345980000	15.261500000	8.321320000
C	25.582920000	16.798540000	9.224760000
C	26.806010000	17.946000000	14.766820000
C	25.489220000	17.497250000	14.440990000
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C	26.594270000	19.765150000	13.127020000
C	27.342070000	19.059410000	14.084100000
C	24.889990000	16.266660000	15.074470000
C	24.448260000	20.107730000	11.790630000
C	29.296310000	11.786470000	17.402970000
C	28.451180000	10.887690000	18.121670000
C	28.577980000	9.505560000	17.867570000
C	29.482990000	8.979980000	16.917760000
C	30.312230000	9.888120000	16.225610000
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C	27.419490000	11.393080000	19.102080000
C	29.540960000	7.497890000	16.622300000
C	38.539910000	12.072600000	14.003990000
C	39.560480000	11.803040000	14.962650000
C	40.896590000	11.735360000	14.513230000
C	41.268270000	11.908360000	13.162440000
C	40.240520000	12.172300000	12.231100000
C	38.902970000	12.253280000	12.647400000
C	39.248910000	11.577660000	16.422120000
C	42.713280000	11.788440000	12.731050000
C	27.416390000	11.898220000	14.178400000
C	27.601640000	10.545190000	13.766170000
C	26.799240000	9.548760000	14.363420000
C	25.827470000	9.830910000	15.345700000
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C	25.012260000	8.727200000	15.980260000
C	29.031950000	22.526560000	17.634950000
C	28.511210000	22.922780000	18.901970000
C	28.835840000	24.208470000	19.386580000
C	29.642410000	25.120450000	18.670830000
C	30.119570000	24.717310000	17.404500000
C	29.823820000	23.442480000	16.900800000
C	27.669350000	21.986150000	19.732520000
C	29.990420000	26.478560000	19.239170000
C	33.257700000	20.482380000	9.649690000
C	32.297360000	20.353240000	8.603440000
C	31.679860000	21.524130000	8.114690000
C	31.975770000	22.813030000	8.607160000
C	32.943010000	22.919220000	9.632550000
C	33.568490000	21.772250000	10.146340000
C	31.925620000	19.010050000	8.027250000
C	31.251540000	24.030740000	8.078370000
H	31.444270000	9.895520000	22.960590000
H	35.404990000	11.682410000	22.865060000
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H	29.801010000	12.250950000	21.005900000
H	33.347640000	8.672360000	23.940110000
H	34.952900000	9.469070000	24.114980000
H	34.478870000	8.738770000	22.546200000

H	40.329530000	21.962410000	12.650470000
H	40.179540000	18.265260000	14.943950000
H	37.709050000	18.526470000	15.162840000
H	36.934880000	22.253360000	11.949500000
H	38.424710000	23.240350000	12.215340000
H	37.119760000	23.173510000	13.466690000
H	42.166670000	19.182390000	12.831940000
H	42.417230000	19.578500000	14.555850000
H	42.431570000	20.890810000	13.318260000
H	32.853620000	7.516590000	12.916250000
H	34.324050000	9.146660000	16.677410000
H	33.923990000	11.451460000	15.818810000
H	31.493560000	10.547200000	11.597600000
H	32.076150000	8.887050000	11.181520000
H	33.145640000	10.328780000	10.976050000
H	32.885880000	6.320870000	15.796570000
H	34.590000000	6.728110000	16.181880000
H	34.160110000	6.060250000	14.563000000
H	39.528640000	15.746150000	8.898400000
H	38.840390000	19.023040000	11.678510000
H	36.721370000	17.935030000	12.414850000
H	36.991770000	13.557410000	10.145560000
H	38.066420000	13.924100000	8.734310000
H	36.345550000	14.473290000	8.766150000
H	41.443640000	17.351990000	9.637380000
H	40.989320000	18.850700000	10.533670000
H	40.517250000	18.648440000	8.813710000

H	32.914470000	24.994590000	20.988250000
H	30.798340000	21.261270000	21.728890000
H	31.476170000	20.448840000	19.465090000
H	34.671360000	23.951420000	18.050180000
H	34.112280000	25.373620000	19.019030000
H	33.169950000	24.784070000	17.589330000
H	32.038960000	24.515990000	23.252490000
H	31.268320000	22.931910000	23.618430000
H	30.334230000	24.220690000	22.774120000
H	35.746570000	19.207380000	24.778260000
H	34.276940000	21.735950000	21.556190000
H	34.532640000	19.835390000	19.958600000
H	35.362450000	16.131660000	23.212490000
H	36.425310000	16.978880000	24.406750000
H	37.021030000	16.587520000	22.741520000
H	34.838960000	21.452640000	25.297140000
H	34.073870000	22.451530000	23.999390000
H	35.855720000	22.411460000	24.169190000
H	35.159980000	8.281100000	19.700250000
H	31.229740000	9.986900000	18.965680000
H	32.276530000	12.216700000	18.569550000
H	37.079690000	10.926840000	18.433370000
H	37.114230000	9.576090000	19.638460000
H	36.905590000	11.297940000	20.165450000
H	32.339460000	7.101650000	18.556900000
H	31.495720000	7.673860000	20.029450000
H	33.134670000	6.931140000	20.158140000



H	38.159860000	23.007860000	21.956130000
H	39.346200000	18.836530000	22.293490000
H	38.619440000	18.452540000	19.932280000
H	37.837180000	23.157450000	18.467790000
H	37.236340000	23.886030000	20.014310000
H	36.216280000	22.725870000	19.076360000
H	39.349580000	22.264630000	23.956860000
H	40.090280000	20.622660000	24.030670000
H	38.357300000	20.843200000	24.434820000
H	28.330330000	23.071670000	10.290360000
H	28.756270000	18.762320000	9.898920000
H	30.476280000	18.776860000	11.710820000
H	29.913000000	23.483660000	13.338100000
H	29.615310000	24.321270000	11.765050000
H	31.253360000	23.672730000	12.169860000
H	26.564190000	21.634410000	9.051370000
H	26.969260000	19.914030000	8.683590000
H	27.854660000	21.248720000	7.868710000
H	42.472460000	15.527250000	15.645810000
H	39.480350000	15.636580000	12.483950000
H	37.674860000	15.638460000	14.207150000
H	40.419480000	16.366740000	18.341440000
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H	40.334650000	14.587680000	18.273010000
H	42.427150000	16.652910000	12.560860000
H	41.904140000	15.034100000	11.988800000
H	43.153530000	15.173630000	13.281480000

H	27.767900000	15.930260000	7.779300000
H	26.518530000	16.971540000	11.816710000
H	28.815510000	16.476940000	12.643020000
H	31.229530000	15.941710000	8.281610000
H	29.919220000	15.183410000	7.297120000
H	30.739500000	14.263340000	8.622230000
H	25.343070000	17.883510000	9.332900000
H	24.810920000	16.243170000	9.806510000
H	25.463140000	16.531710000	8.151400000
H	23.744580000	17.860340000	13.215290000
H	27.055150000	20.632000000	12.611910000
H	28.378860000	19.379960000	14.314300000
H	25.475990000	15.358950000	14.787590000
H	23.838800000	16.120830000	14.745720000
H	24.908050000	16.325410000	16.186600000
H	24.080930000	19.432820000	10.981620000
H	25.036080000	20.924880000	11.316810000
H	23.544520000	20.564400000	12.259620000
H	27.926020000	8.811040000	18.437040000
H	31.053380000	9.516120000	15.492420000
H	30.900320000	11.967110000	15.935500000
H	27.877400000	12.046450000	19.881020000
H	26.904370000	10.546900000	19.607790000
H	26.652320000	12.015250000	18.583930000
H	29.537620000	6.880010000	17.550060000
H	30.454260000	7.245100000	16.039250000
H	28.658290000	7.179710000	16.016990000

H	41.685840000	11.530980000	15.265400000
H	40.487900000	12.321660000	11.160510000
H	38.106670000	12.455820000	11.904420000
H	38.743890000	12.466570000	16.874420000
H	40.176080000	11.374520000	17.002250000
H	38.555310000	10.714700000	16.556370000
H	43.402740000	12.256170000	13.470500000
H	42.884530000	12.276010000	11.745510000
H	43.020410000	10.719580000	12.631070000
H	26.938860000	8.498700000	14.031550000
H	24.906570000	11.441940000	16.505040000
H	26.311260000	13.243890000	15.489440000
H	28.450880000	10.688350000	11.760240000
H	28.628080000	9.067830000	12.547500000
H	29.653380000	10.462050000	13.063690000
H	25.005530000	7.809620000	15.350510000
H	23.956420000	9.041510000	16.147010000
H	25.431440000	8.444070000	16.975700000
H	28.441840000	24.507060000	20.381490000
H	30.744980000	25.407590000	16.802130000
H	30.249850000	23.132190000	15.924550000
H	26.767300000	21.641190000	19.174230000
H	27.339440000	22.472150000	20.677800000
H	28.240520000	21.059780000	19.995250000
H	29.283100000	27.266500000	18.884750000
H	31.014180000	26.792420000	18.931100000
H	29.954740000	26.471220000	20.351830000

H	30.930130000	21.418940000	7.302820000
H	33.215860000	23.914820000	10.038310000
H	34.322150000	21.868680000	10.953780000
H	32.811210000	18.484670000	7.598900000
H	31.154220000	19.118170000	7.233910000
H	31.514570000	18.337990000	8.821600000
H	30.847550000	23.853980000	7.056720000
H	31.918390000	24.921930000	8.038950000
H	30.386830000	24.293960000	8.734340000

#### B Isomer

Ag	14.331050000	14.747390000	19.909370000
Ag	11.571060000	14.779290000	20.488750000
Ag	13.153430000	12.383280000	20.887310000
Ag	12.663810000	16.381280000	18.314520000
Ag	12.592220000	13.360250000	18.178500000
Ag	15.509750000	17.056570000	18.877750000
Ag	17.076000000	14.517060000	19.264920000
Ag	15.997680000	13.221920000	21.585030000
Ag	15.262100000	12.341130000	18.718170000
Ag	13.378650000	17.193480000	20.970410000
Ag	16.003530000	16.145920000	21.693610000
Ag	15.058140000	14.789060000	17.152790000
Ag	13.702110000	14.624410000	22.678510000
Ag	13.735860000	11.959720000	15.880520000

Ag	10.182870000	17.382490000	20.274690000
Ag	18.058920000	11.601610000	20.208400000
Ag	15.793600000	19.163350000	21.227990000
Ag	11.142820000	13.183340000	23.180810000
Ag	10.087230000	15.066900000	17.591670000
Ag	18.857550000	14.592110000	21.674270000
Ag	14.215230000	17.473380000	23.777670000
Ag	17.521600000	16.621400000	16.773710000
Ag	14.329140000	17.446040000	15.997390000
Ag	14.219050000	11.649460000	23.616270000
Ag	13.532180000	9.948950000	18.716190000
S	16.510330000	18.254520000	15.262980000
S	9.635570000	14.757610000	22.101100000
S	16.203520000	19.497890000	18.851380000
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S	13.081830000	9.888210000	21.106210000
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Ag	34.772380000	11.240360000	16.867530000
Ag	30.054670000	11.805760000	20.458030000
Ag	36.193990000	19.134410000	18.379870000
Ag	37.595680000	13.693520000	20.494940000
Ag	32.469960000	19.235340000	21.606730000

Ag	30.570720000	16.522330000	22.923150000
Ag	35.671550000	13.991910000	15.042140000
Ag	30.873200000	15.162260000	14.947250000
S	31.133160000	18.786290000	23.594640000
S	33.889190000	10.118690000	18.845820000
S	34.767510000	17.637190000	23.368130000
S	32.310290000	17.880920000	15.068340000
S	32.646830000	13.722380000	14.116370000
S	35.490060000	11.794480000	22.262550000
S	29.896380000	14.191850000	22.905770000
S	28.333340000	16.376790000	20.067530000
S	31.037600000	9.957220000	21.675280000
S	37.525500000	12.253560000	18.529070000
S	28.592820000	13.084390000	18.991250000
S	35.655120000	16.417830000	14.714590000
S	37.394680000	18.146580000	20.288140000
S	33.993010000	20.343200000	20.038310000
S	28.762130000	16.368470000	15.227920000
S	36.252730000	20.418590000	16.278950000
S	38.616920000	14.888120000	22.350720000
S	35.750130000	11.577820000	14.670740000
C	29.645640000	19.774650000	23.597530000
C	29.714350000	21.192530000	23.446770000
C	28.522010000	21.938410000	23.576250000
C	27.273810000	21.350810000	23.864320000
C	27.227720000	19.945810000	24.021610000
C	28.393120000	19.175880000	23.890370000

C	31.012050000	21.906130000	23.163320000
C	26.032790000	22.199890000	24.013460000
C	32.579180000	9.082160000	18.194670000
C	32.881490000	7.742120000	17.811090000
C	31.813430000	6.902310000	17.421720000
C	30.469760000	7.334220000	17.396960000
C	30.201390000	8.677490000	17.743120000
C	31.242270000	9.535550000	18.126030000
C	34.300600000	7.226220000	17.808380000
C	29.342170000	6.406990000	16.998940000
C	34.313190000	17.100600000	25.016010000
C	35.059540000	17.594720000	26.128030000
C	34.655550000	17.208890000	27.425090000
C	33.536520000	16.381260000	27.666370000
C	32.812840000	15.908290000	26.549080000
C	33.205580000	16.254510000	25.247270000
C	36.241130000	18.516370000	25.936130000
C	33.103260000	16.034120000	29.074410000
C	31.231210000	19.235720000	14.641350000
C	31.499510000	19.974460000	13.448710000
C	30.642040000	21.046070000	13.118740000
C	29.528940000	21.406080000	13.907990000
C	29.278810000	20.647860000	15.075450000
C	30.118440000	19.583920000	15.440350000
C	32.667480000	19.624740000	12.558870000
C	28.632350000	22.559890000	13.508950000
C	31.860050000	12.136050000	13.825750000

C	31.324280000	11.851040000	12.531660000
C	30.803690000	10.559620000	12.295950000
C	30.809740000	9.540340000	13.275560000
C	31.338850000	9.849090000	14.545730000
C	31.845320000	11.129340000	14.817370000
C	31.333070000	12.880550000	11.423730000
C	30.287000000	8.153550000	12.971230000
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C	35.757530000	12.407530000	26.860290000
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C	35.308150000	13.303770000	24.628510000
C	36.131730000	9.562620000	24.287210000
C	35.929250000	12.607500000	28.350540000
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C	29.677880000	13.859370000	25.665130000
C	30.097210000	13.301510000	26.893370000
C	31.263470000	12.514910000	27.018280000
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C	31.655930000	12.852700000	24.629040000
C	28.430330000	14.705620000	25.598550000
C	31.652930000	11.879470000	28.334380000
C	30.284650000	9.941190000	23.298560000
C	30.889940000	9.186690000	24.345830000
C	30.227870000	9.118210000	25.590870000
C	29.000990000	9.767500000	25.844150000

C	28.415410000	10.499200000	24.786080000
C	29.044480000	10.580540000	23.534750000
C	32.215550000	8.494340000	24.149680000
C	28.351170000	9.719150000	27.208570000
C	38.957800000	12.863930000	17.631730000
C	40.231470000	12.261280000	17.870710000
C	41.330440000	12.693200000	17.098520000
C	41.221600000	13.679380000	16.092420000
C	39.957300000	14.271230000	15.885840000
C	38.847430000	13.873440000	16.650030000
C	40.421660000	11.202270000	18.929500000
C	42.415350000	14.074150000	15.250100000
C	28.143620000	11.879300000	17.739000000
C	27.264540000	10.797440000	18.060860000
C	26.824380000	9.962250000	17.009630000
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C	28.112650000	11.200780000	15.381480000
C	28.564910000	12.054230000	16.401080000
C	26.815000000	10.530160000	19.478240000
C	26.737370000	9.216840000	14.572030000
C	37.373790000	16.912350000	14.619710000
C	38.029120000	16.891570000	13.353000000
C	39.353090000	17.380380000	13.280490000
C	40.042270000	17.895710000	14.399470000
C	39.370620000	17.905180000	15.643850000
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C	37.329150000	16.394170000	12.110560000

C	41.454580000	18.425920000	14.280810000
C	39.020760000	17.872160000	19.580830000
C	39.908380000	18.981620000	19.417080000
C	41.215440000	18.727400000	18.952930000
C	41.683000000	17.428700000	18.645810000
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C	39.473820000	16.575080000	19.252430000
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C	43.096390000	17.212030000	18.152720000
C	32.983930000	21.564790000	19.205370000
C	32.992900000	22.904960000	19.702190000
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C	27.201180000	13.536280000	12.720210000
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C	34.412430000	22.270070000	14.510600000
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C	38.881360000	13.609030000	23.574180000
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C	39.739900000	10.861750000	14.098770000
C	40.043820000	9.837800000	15.021600000
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C	37.719870000	9.947680000	15.782950000
C	38.209880000	12.535260000	12.979150000
C	41.443890000	9.275710000	15.126040000
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H	34.931120000	7.799730000	17.086760000
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H	31.940220000	15.242160000	26.691430000
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H	37.012850000	18.059600000	25.272260000
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H	35.933520000	19.465790000	25.438620000
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H	30.858770000	21.627250000	12.198840000
H	28.433440000	20.904440000	15.742520000
H	29.926740000	19.010620000	16.369780000
H	33.611900000	19.548030000	13.148280000
H	32.802810000	20.381560000	11.756700000

H	32.523680000	18.623210000	12.089010000
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H	27.615820000	22.212380000	13.204200000
H	29.053390000	23.122290000	12.646870000
H	30.387750000	10.341140000	11.289660000
H	31.340800000	9.083670000	15.345340000
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H	30.735560000	12.532830000	10.551760000
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H	30.185630000	7.553920000	13.902540000
H	30.980790000	7.600980000	12.294460000
H	36.220540000	10.278020000	26.907590000
H	35.244730000	14.493180000	26.445830000
H	35.033250000	14.162470000	23.979870000
H	35.289690000	9.212790000	23.644990000
H	36.302920000	8.810720000	25.089230000
H	37.030570000	9.589770000	23.627510000
H	35.552710000	11.735820000	28.933520000
H	35.390870000	13.517560000	28.698730000
H	37.005450000	12.736860000	28.620860000
H	29.478540000	13.492940000	27.795130000
H	32.980760000	11.715890000	25.924100000
H	32.276280000	12.669740000	23.725780000
H	28.677860000	15.743860000	25.267720000
H	27.931300000	14.762330000	26.590710000

H	27.705540000	14.305230000	24.852070000
H	31.178110000	12.393550000	29.200280000
H	32.756730000	11.896230000	28.480150000
H	31.337000000	10.808600000	28.367720000
H	30.703130000	8.528670000	26.402400000
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H	28.785560000	8.914210000	27.841720000
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H	42.320090000	12.230540000	17.298050000
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H	37.863270000	14.360680000	16.484580000
H	40.226950000	11.618230000	19.947110000
H	41.460340000	10.803830000	18.910640000
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H	43.330850000	14.223040000	15.868590000
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H	28.464600000	11.359730000	14.344700000
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H	27.694060000	10.322490000	20.138640000
H	26.136290000	9.649980000	19.522380000

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H	27.282860000	8.242590000	14.588500000
H	26.896260000	9.663710000	13.565400000
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H	39.863390000	17.368620000	12.294670000
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H	37.548620000	17.421090000	16.733530000
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H	42.157700000	17.848390000	14.926780000
H	41.517920000	19.488500000	14.612810000
H	41.830410000	18.369660000	13.235440000
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H	41.107810000	15.320220000	18.556540000
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H	38.672220000	20.697520000	18.953440000
H	40.309750000	21.110790000	19.589320000
H	39.008340000	20.506680000	20.698430000
H	43.310740000	17.829820000	17.249040000
H	43.272690000	16.146250000	17.888160000
H	43.848530000	17.504080000	18.922560000
H	32.299720000	24.929590000	19.372900000
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H	32.257450000	20.226630000	17.642880000
H	33.579520000	22.591450000	21.782570000
H	33.544710000	24.325300000	21.249690000

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H	30.337840000	25.404620000	17.603310000
H	30.316870000	24.317070000	16.157910000
H	31.731960000	25.364600000	16.486330000
H	24.262560000	14.552650000	14.143060000
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H	29.167440000	14.310330000	13.241600000
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H	24.615390000	11.765390000	12.869580000
H	25.280130000	12.287790000	11.286560000
H	23.886780000	13.167320000	12.019470000
H	34.236180000	24.851010000	15.304360000
H	36.562890000	24.561360000	18.964150000
H	36.915060000	22.123940000	18.531970000
H	35.184750000	21.774970000	13.877320000
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H	33.672880000	21.476720000	14.781780000
H	34.748490000	26.879530000	16.527340000
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H	39.669790000	10.252400000	23.737800000
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H	39.362390000	16.071560000	25.001620000
H	38.761070000	15.384450000	26.565700000

H	37.635280000	15.649680000	25.178450000
H	40.917910000	10.268840000	26.531930000
H	39.299960000	9.548640000	26.252540000
H	39.516850000	10.812960000	27.517210000
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H	36.916970000	9.584820000	16.455900000
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H	39.140950000	12.792300000	12.428430000
H	37.836160000	13.461080000	13.482470000
H	41.966730000	9.294290000	14.143150000
H	41.440510000	8.226690000	15.497500000
H	42.061000000	9.875890000	15.837670000

#### C Isomer

Ag	14.642820000	16.559010000	20.590430000
Ag	12.058570000	16.707390000	21.743390000
Ag	12.991500000	14.278890000	20.468650000
Ag	13.293400000	19.045360000	20.537060000
Ag	12.416380000	16.670260000	18.869270000
Ag	16.270650000	18.829340000	20.660790000
Ag	17.137330000	16.294790000	19.267280000
Ag	16.023770000	14.118510000	20.792720000
Ag	14.757260000	15.109270000	18.150040000
Ag	14.499860000	18.105230000	22.954250000
Ag	16.800470000	16.439210000	22.381250000
Ag	15.030200000	18.001810000	18.171070000
Ag	14.303600000	15.017460000	22.956820000

Ag	12.887820000	16.637370000	15.970280000
Ag	11.382020000	19.191960000	23.196600000
Ag	17.417900000	13.250740000	18.315110000
Ag	17.339560000	19.227340000	23.608550000
Ag	11.516180000	13.989720000	23.252120000
Ag	10.397960000	18.805890000	19.873980000
Ag	19.142930000	14.714740000	20.840030000
Ag	15.645140000	16.616000000	25.215360000
Ag	17.885170000	19.236500000	18.238200000
Ag	14.892160000	20.915040000	18.773660000
Ag	14.134840000	11.971420000	22.064640000
Ag	12.432680000	13.463280000	17.377900000
S	17.132620000	21.550650000	18.060060000
S	10.352070000	16.114260000	23.502820000
S	17.579630000	20.749860000	21.727760000
S	15.443460000	13.015650000	16.913060000
S	12.221930000	12.144210000	19.416130000
S	13.149460000	19.005100000	24.876760000
S	12.510560000	21.099060000	19.288550000
S	14.055690000	18.811130000	16.007520000
S	9.324420000	19.553730000	21.928970000
S	14.071910000	14.771830000	25.459290000
S	10.603540000	17.901010000	17.601000000
S	16.175780000	11.614210000	20.751400000
S	19.281410000	16.250070000	22.734010000
S	19.307580000	17.246020000	18.376070000
S	12.279190000	14.421810000	15.143410000



S	19.571710000	12.827450000	19.373390000
S	17.409750000	18.190950000	25.801720000
S	12.051670000	11.619140000	23.285280000
C	16.964820000	21.874760000	16.300530000
C	18.119720000	21.909930000	15.465510000
C	17.953670000	22.206020000	14.096780000
C	16.695310000	22.475090000	13.519560000
C	15.568090000	22.459140000	14.369740000
C	15.699530000	22.163340000	15.735540000
C	19.493120000	21.595170000	16.004070000
C	16.550480000	22.715080000	12.034410000
C	8.755280000	15.828710000	22.729800000
C	7.686050000	15.319420000	23.526100000
C	6.408330000	15.209720000	22.933880000
C	6.145450000	15.581230000	21.596530000
C	7.223730000	16.066150000	20.824090000
C	8.505740000	16.179000000	21.383780000
C	7.903100000	14.896830000	24.959520000
C	4.764110000	15.429410000	20.997390000
C	15.941160000	13.404770000	15.236860000
C	16.433020000	12.353610000	14.406970000
C	16.760510000	12.661900000	13.068720000
C	16.589540000	13.948810000	12.512900000
C	16.081190000	14.967460000	13.349980000
C	15.773410000	14.698440000	14.692810000
C	16.566770000	10.939630000	14.918920000
C	16.955770000	14.231160000	11.072130000

C	10.453530000	11.953570000	19.648160000
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C	36.978110000	13.489780000	27.523750000

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C	39.121560000	14.405120000	29.179020000
C	37.876520000	15.074360000	29.171020000
C	36.825610000	14.623960000	28.357410000
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H	25.076560000	14.888630000	29.591840000
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#### E Isomer

Ag	14.870350000	17.499300000	19.932980000
Ag	12.152760000	16.774370000	20.332600000
Ag	13.933700000	15.069680000	18.810200000
Ag	12.939080000	19.565790000	20.093290000
Ag	13.102630000	17.658230000	17.740170000
Ag	15.771550000	19.936950000	20.996210000
Ag	17.565350000	18.140980000	19.323780000
Ag	16.755300000	15.421300000	19.910540000
Ag	15.867690000	16.888230000	17.343860000

Ag	13.833390000	18.211340000	22.459140000
Ag	16.567420000	17.270210000	22.165090000
Ag	15.345460000	19.641440000	18.130530000
Ag	14.455530000	15.275630000	21.664640000
Ag	14.141690000	18.585580000	15.148920000
Ag	10.573470000	18.503500000	22.140770000
Ag	18.755040000	15.642720000	17.776570000
Ag	16.104980000	19.694360000	24.093930000
Ag	12.048530000	13.653150000	20.896420000
Ag	10.400040000	18.913710000	18.674500000
Ag	19.495060000	16.574240000	21.012260000
Ag	14.838830000	16.354810000	24.510630000
Ag	17.691550000	21.359080000	19.255250000
Ag	14.308010000	22.156140000	19.353460000
Ag	15.210310000	12.643630000	20.042690000
Ag	14.275240000	15.130470000	15.553220000
S	16.392630000	23.421020000	19.445160000
S	10.343490000	15.331750000	21.338580000
S	16.215650000	21.745860000	22.780180000
S	17.275260000	15.421510000	15.843110000
S	14.005870000	13.251400000	17.080590000
S	11.945510000	18.183230000	24.130670000
S	11.911920000	21.703270000	19.200190000
S	14.627760000	20.829410000	16.036580000
S	8.794400000	18.795280000	20.500750000
S	13.780550000	14.250330000	23.874600000
S	11.297170000	18.798920000	16.394440000

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S	18.859650000	17.460790000	23.208050000
S	19.531610000	19.739180000	19.274330000
S	14.322100000	16.663990000	13.656460000
S	20.684500000	15.378160000	19.251910000
S	15.958230000	18.042170000	25.878790000
S	13.103120000	11.502220000	20.498210000
C	16.505820000	24.226060000	17.842070000
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C	21.754040000	20.097670000	15.212380000
C	20.792230000	19.086270000	15.419860000

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