

Role of the Isopropyl Group in Asymmetric Autocatalytic Zinc Alkylations

Jürgen Klankermayer*, Ilya D. Gridnev*, John M. Brown*

- 1) Full author listing for Gaussian03
- 2) Table of computed enthalpies; Cartesian coordinates of the structures (in Ångstroms).
- 3) Further calculations on favoured conformers of the homo- and heterochiral dimer

1) Full author listing for Gaussian03

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; J. A. Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J.W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M.W.; Johnson, B.; Chen, W.; Wong, M.W.; Gonzalez, C.; Pople, J. A. "Gaussian03, Revision C.02", 2004 Gaussian, Inc., Wallingford CT.

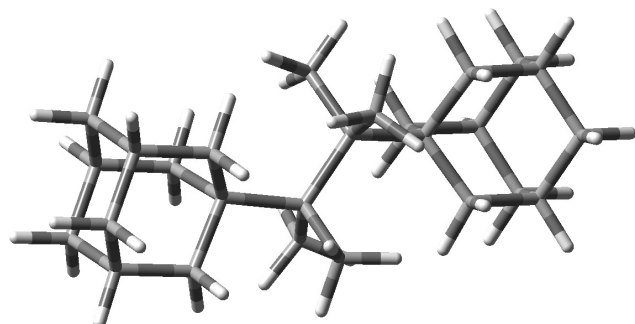
2) Cartesian coordinates of the structures (in Ångstroms)

In the present case computation the geometry of the starting structure was optimized initially at the B3LYP¹/6-31 G(d) level of theory. Where indicated by (*) the derived structures were then subjected to a conformational minimization search (MMFF, Spartan04) with frozen atomic coordinates for the [Zn-O] core. The identified lower energy conformers then served as starting geometries for further full geometry optimizations and energy calculations at the B3LYP/6-31 G(d) level of theory.

Preliminary calculation:

Ad(Me₂C)₄Ad (Ad = 1-adamantyl) is the most crowded hydrocarbon for which X-ray data is available, and considerably distorted. DFT computation closely reproduced the X-ray structure, with core bond angles and torsion angles within 1° of the experimental values, whilst core bond lengths averaged 0.01 Å longer than the X-ray derived average of 1.643 Å. This gives us confidence that the observed enhanced steric strain represents a real effect, one that will inhibit the formation of simple cubic tetramers in the *iso*-propylzincate case, as is observed.

Ad(Me₂C)₄Ad HF energy -1016.0522326



C	0.20303500	-1.64834700	0.78872300
C	0.54641700	-0.61618400	-0.31250300
C	-0.54640900	0.61621300	-0.31248800
C	-0.45662500	1.35485600	-1.67831500
C	0.45670600	-1.35476300	-1.67836100
C	-0.20307900	1.64831800	0.78880400
C	2.14025300	-0.22808800	-0.08667600
C	3.03586500	-1.44967000	-0.50726600
C	4.54313500	-1.19992800	-0.28003200
C	4.81831700	-0.90156700	1.20299000
C	4.00590700	0.33800400	1.61220900
C	4.43598600	1.54520900	0.75974800
C	4.17476800	1.22973800	-0.72442900
C	2.66665100	0.96428600	-0.94364700
C	2.49976100	0.06270900	1.40711300
C	4.99317000	-0.00478600	-1.13774800
C	-2.14025400	0.22810200	-0.08668300
C	-3.03588200	1.44969500	-0.50722400
C	-4.54314900	1.19992800	-0.28001100
C	-4.99315800	0.00480500	-1.13776900
C	-4.17475800	-1.22972900	-0.72446900
C	-4.43599700	-1.54523700	0.75969500

Supplementary Material (ESI) for Chemical Communications

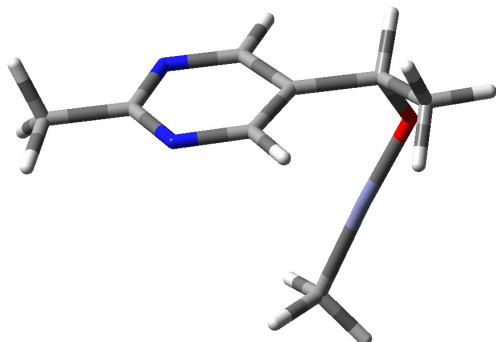
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H	-0.99674300	0.83069700	-2.47248800
H	0.56999700	1.46755700	-2.01652000
H	-0.87558900	2.36250600	-1.60765200
H	0.99681700	-0.83053700	-2.47249400
H	-0.56990200	-1.46751800	-2.01658500
H	0.87573600	-2.36238800	-1.60773300
H	-0.11113700	1.19453100	1.77797200
H	-0.97418900	2.42053700	0.85895400
H	0.73047900	2.16931300	0.57492700
H	2.89715100	-1.67144600	-1.56942100
H	2.74589900	-2.35237600	0.04270800
H	5.09077000	-2.10221600	-0.58541100
H	4.53305100	-1.76215200	1.82427100
H	5.89183400	-0.73082600	1.36591000
H	4.17522400	0.55772800	2.67527700
H	3.87631700	2.44169100	1.06209500
H	5.50077700	1.76596500	0.91939100
H	4.46545500	2.09071600	-1.34187800
H	2.13076400	1.88849000	-0.71385500
H	2.50347900	0.75995900	-2.00987300
H	2.22288500	-0.79287800	2.03251300
H	1.94269100	0.91999300	1.78754900
H	6.06723000	0.18395200	-1.00133800
H	4.83871200	-0.22321000	-2.20372300
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H	-4.53308000	1.76209100	1.82430800
H	-5.89185300	0.73076800	1.36591100

Comparison of the energies of the various oligomers in Hartrees, for computation at the B3LYP/6-31 G(d) level of theory. All tetramer calculations were carried out for homochiral species. Detailed parameters included for entries in bold.

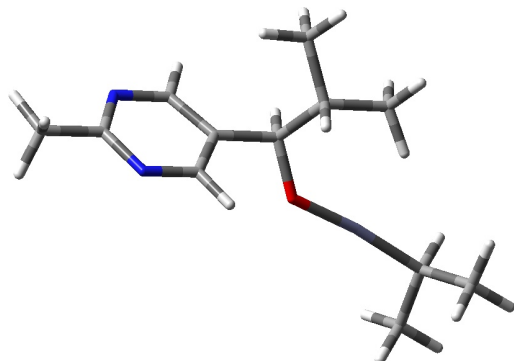
Entry	Structure	HF energy
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2	<i>i</i> -Pr monomer	-2433.1949
3	<i>t</i> -Bu monomer	-2511.8223
4	Me dimer <i>RR</i>	-4551.9631
5	Me dimer <i>RS</i>	-4551.9621
6a	<i>i</i> -Pr dimer <i>RR</i> (syn)	-4866.4569
6b	<i>i</i> -Pr dimer <i>RR</i> (anti)	-4866.4556
7a	<u><i>i</i></u> -Pr dimer <i>RS</i> (anti)	-4866.4576
7b	<i>i</i> -Pr dimer <i>RS</i> (syn)	-4866.4552
8	<i>i</i> -Pr Macrodimer <i>RR</i>	-4866.4447
9	<i>t</i> -Bu dimer <i>RR</i> (syn)	-5023.6997
10	<i>t</i> -Bu dimer <i>RS</i> (anti)	-5023.6996
11	Me tetramer Cube	-9103.9892
12	<i>i</i> -Pr tetramer Cube	-9732.9172
13	Me tetramer Ladder	-9103.9594
14	<i>i</i> -Pr tetramer Ladder	-9732.9085
15	Me tetramer Barrel	-9103.9883
16	<i>i</i> -Pr tetramer Barrel	-9732.9466
17	<i>i</i> -Pr tetramer SMS 1	-9732.9359
18	<i>i</i> -Pr tetramer SMS 2	-9732.9406
19	<i>i</i> -Pr tetramer SMS 3	-9732.9357
20	<i>i</i> -Pr tetramer SMS 4	-9732.9354
21	Me tetramer Macro 1	-9103.9677
22	Me tetramer Macro2	-9103.9661

1 Me monomer



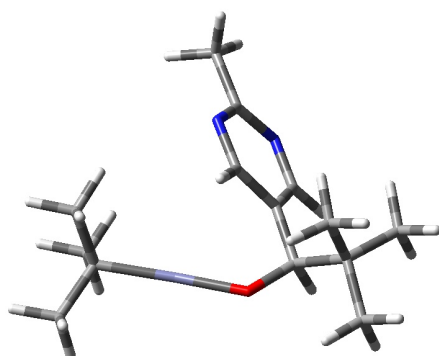
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N	2.32431200	0.31012900	-1.11131900
H	0.83955000	1.52586800	-1.85941700
C	-0.86094200	1.78164000	0.43467200
C	1.06618600	0.37641800	1.29519500
C	2.78320300	-0.32835300	-0.02598400
O	-1.88602400	0.83693900	0.67569700
C	-1.25350300	2.72262500	-0.70705400
N	2.19772100	-0.31811700	1.18759600
C	4.06604500	-1.10313900	-0.15964700
H	-0.76081700	2.39235000	1.34749500
H	0.59408700	0.38579400	2.27843400
Zn	-1.80491500	-0.81158200	0.02094600
H	-1.37977200	2.17258600	-1.64774400
H	-0.51189600	3.51554800	-0.86154300
H	-2.21330900	3.18732000	-0.46435800
H	3.98922700	-2.06263300	0.36036300
H	4.89127000	-0.54865600	0.30458700
H	4.30581400	-1.26381300	-1.21254300
C	-1.87736200	-2.62256800	-0.55909000
H	-1.14122700	-2.82061600	-1.34619100
H	-2.86399700	-2.87651300	-0.96231600
H	-1.66838400	-3.31173900	0.26658900

2 Prⁱ monomer



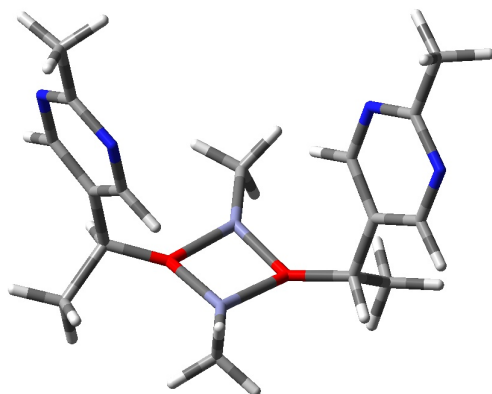
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C	-1.86836700	0.06628800	-0.21672000
C	-2.25860200	-0.59678800	0.95293900
N	-3.48461800	-1.08704000	1.14097600
H	-2.64587300	0.62994700	-2.15265600
H	-1.54367000	-0.74801700	1.75952500
C	-5.74681500	-1.47779000	0.33984600
H	-5.70858000	-2.56564900	0.47007800
H	-6.18921100	-1.06331100	1.25242800
H	-6.38175600	-1.24063100	-0.51577800
C	-0.46498100	0.61709700	-0.39832000
H	-0.34087100	0.84786600	-1.47401000
O	0.44231400	-0.38010200	0.01279500
C	-0.25915100	1.95635200	0.37126700
H	-0.40627700	1.73266200	1.43801800
C	1.16414900	2.50076500	0.18611700
H	1.30207200	3.43744800	0.73692900
H	1.92922300	1.80757000	0.55731000
H	1.37553100	2.70606600	-0.87277700
C	-1.27850600	3.02587400	-0.05034900
H	-1.19154600	3.25382800	-1.12111300
H	-2.30735200	2.70800900	0.14086000
H	-1.10906200	3.95914400	0.49846200
Zn	2.20740100	-0.38195100	-0.15565300
C	4.11842800	-0.57443000	-0.24524500
H	4.45740100	0.07518400	-1.06554900
C	4.78946800	-0.07961700	1.04660900
H	5.88521000	-0.15447700	0.97356000
H	4.55044200	0.96840100	1.26557100
H	4.48967300	-0.67385400	1.91951900
C	4.54478300	-2.01209300	-0.58266600
H	4.12999400	-2.35575500	-1.53784400
H	5.64053200	-2.08794300	-0.65600900
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3 (S)- Bu^t Monomer



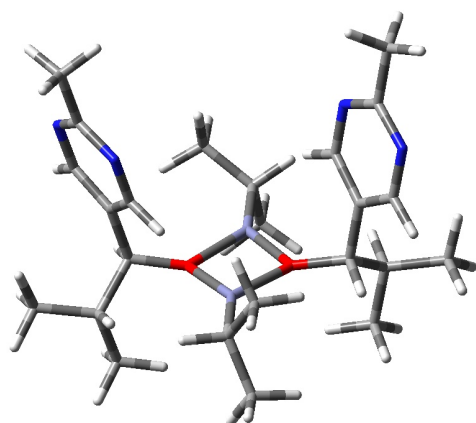
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H	-3.38488	2.66295	-1.40795
H	-3.97605	0.16085	-1.36495
H	3.74051	3.08119	-1.22544
H	4.73404	0.12629	-1.03325
C	3.65015	0.30584	-1.13290
C	-1.03296	-1.53579	-1.18539
H	3.15337	-0.66763	-1.04275
N	-0.49643	-2.74604	-0.99230
H	0.51239	-4.97470	-0.39163
C	-1.43759	0.92483	-0.56810
H	4.99758	2.49261	-0.12848
C	-3.25429	2.63198	-0.31828
C	3.90892	2.63841	-0.23556
C	-3.85703	0.19609	-0.27424
C	-0.87727	-0.46782	-0.29730
O	-0.48760	1.91627	-0.24390
H	-2.51798	3.39144	-0.04581
Zn	1.26492	1.55360	-0.21942
H	-4.21457	2.89350	0.14093
C	3.17260	1.30077	-0.06084
H	-4.83267	0.45761	0.15308
H	-3.60531	-0.81295	0.07185
C	0.22680	-2.91383	0.12605
C	-2.79921	1.23381	0.14443
H	1.94518	-4.18593	0.31617
C	0.85267	-4.26131	0.36264
H	3.61019	3.38092	0.51608
C	-0.10346	-0.77014	0.83180
N	0.44783	-1.96442	1.05353
H	0.59983	-4.63010	1.36253
H	4.54890	0.55144	1.45682
C	3.46643	0.72477	1.33525
H	2.96408	-0.23602	1.50326
C	-2.64447	1.23297	1.67451
H	0.07693	-0.01415	1.59561
H	-1.85708	1.92671	1.98564
H	-3.58168	1.54727	2.15071
H	3.16096	1.40810	2.13889
H	-2.40366	0.23655	2.06249

4 (RR)-Me dimer *



C	3.65320600	2.76046300	-0.05117400
N	2.76186100	2.25308800	-0.91893000
C	4.02823300	4.20984600	-0.20103000
N	4.23179100	2.07975000	0.95315300
C	2.44327800	0.96597700	-0.76229800
C	3.89194900	0.79566500	1.08058400
H	3.69381900	4.77990600	0.67381200
H	3.56896700	4.62978300	-1.09758900
H	5.11654500	4.31876800	-0.25625500
C	2.98595700	0.15293700	0.23342600
H	1.71224800	0.56192000	-1.46197900
H	4.36149700	0.25216200	1.90219700
C	2.63436800	-1.31922800	0.36834900
O	1.24646500	-1.53685400	0.16597100
C	3.44914000	-2.18468300	-0.60047500
H	2.88445600	-1.62937200	1.39427300
Zn	-0.18094600	-1.43094900	1.48842000
Zn	0.17451300	-1.48679800	-1.45751500
H	3.19471400	-3.24074500	-0.46042200
H	4.52488600	-2.05867200	-0.43511400
H	3.23003200	-1.90741000	-1.63843700
O	-1.25257000	-1.53837500	-0.13267000
C	-0.32517200	-1.30516400	3.41209300
C	0.33691400	-1.46077000	-3.38332100
C	-2.63955400	-1.32313300	-0.34719900
H	-1.23633900	-1.78522200	3.78733600
H	0.52227900	-1.79096900	3.90994100
H	-0.34364500	-0.26248000	3.74983200
H	1.03696300	-0.69141200	-3.72818700
H	0.69594200	-2.42296000	-3.76721600
H	-0.62603300	-1.25929500	-3.86685000
C	-2.98944800	0.15171300	-0.24150900
C	-3.46139900	-2.16986000	0.63189400
H	-2.88335200	-1.65163400	-1.36880900
C	-2.45506800	0.98014300	0.74958700
C	-3.88093700	0.78283100	-1.10831000
H	-3.20418100	-3.22812900	0.51581900
H	-4.53569600	-2.04870600	0.45410300
H	-3.25243600	-1.87100500	1.66582000
H	-1.73318500	0.58348800	1.46325100
N	-2.76988600	2.26775400	0.88135000
N	-4.21872600	2.07283400	-1.00506300
H	-4.34346300	0.22940400	-1.92704400
C	-3.65044300	2.76577900	-0.00664300
C	-4.00761400	4.22092700	0.12915300
H	-4.30481300	4.44648500	1.15853900
H	-4.81703000	4.47869300	-0.55610200
H	-3.13605800	4.84701800	-0.09680800

6a (RR)-Prⁱ dimer *



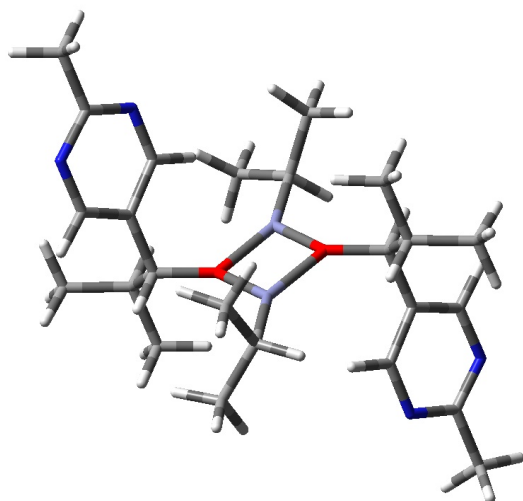
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C	1.50738100	-0.02598200	-0.93358300
C	0.63118600	4.15130000	-2.11793200
C	-1.05437200	0.10360900	-0.87509500
C	2.76103800	3.73170500	-3.42364400
C	-2.19860000	0.10943400	1.09744200
C	5.92664300	5.62830200	1.69685200
C	6.33469500	3.74450700	0.06970000
C	4.43366900	3.54519300	1.73931700
C	3.38176000	4.25425600	2.57536500
C	3.53033300	4.50754000	3.93891600
C	2.17121600	4.69674200	2.03214900
C	1.49749100	5.53637800	4.03938100
C	5.13101700	-1.37690800	2.41394500
C	0.44694600	6.25458300	4.84190700
C	-3.50986100	0.15287300	1.83384100
C	2.16320400	4.04393800	-2.04193100
C	3.85968600	-0.58672900	2.76804500
C	5.27176900	4.51531500	0.86549900
H	4.42768600	4.18338800	4.46739700
H	1.94465900	4.51513500	0.98126800
H	0.97975800	0.00704300	1.79224600
H	-1.09336600	0.13484200	-1.96475500
H	5.13181200	3.04653600	2.43097500
H	6.59884000	5.20874900	2.45692800
H	6.52720000	6.28027200	1.05296100
H	4.57179300	4.98185800	0.15448200
H	2.54596200	5.02933000	-1.73634200
H	6.00889300	-0.72282400	2.32224300
H	5.03319900	-1.92557400	1.46853400
H	5.37011800	-2.11682900	3.19434200
H	7.06115100	3.27586800	0.74696400
H	6.88702500	4.41981600	-0.59330200
H	5.89055100	2.95383100	-0.54137700
H	0.79786400	6.42335000	5.86141800
H	0.19836700	7.21291000	4.37323800
H	-0.47669000	5.66478800	4.87165200
H	-4.34057900	0.01775400	1.13886900
H	-3.53912100	-0.62093900	2.60750800
H	-3.62663100	1.11839800	2.34112300
H	0.32023600	4.90204600	-2.86169800
H	0.16780700	3.20105800	-2.41607000
H	0.18298200	4.44198400	-1.15951100
H	2.43446400	2.75335800	-3.80187500
H	2.44778600	4.47825000	-4.17088700
H	3.85837900	3.72681200	-3.41307700
H	5.18826600	6.25258000	2.20893600
N	-1.07960800	0.06055500	1.84426200
N	1.23488400	5.33158000	2.73479200
N	2.60992700	5.14044200	4.67539400

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N	-2.23278900	0.14067900	-0.24308800
O	3.82350400	2.55127500	0.92669300
O	2.43182600	0.86325700	-0.32286800
Zn	3.39324300	0.69100600	1.36323200
Zn	2.74161500	2.76601300	-0.67919900
C	2.09705100	-1.45971400	-1.00039700
C	1.12291500	-2.45839000	-1.64287300
H	0.86977300	-2.15743500	-2.66805400
H	0.18970400	-2.54962400	-1.07902900
H	1.57913200	-3.45291500	-1.69709300
H	1.34271600	0.30430200	-1.97213400
C	3.99233500	0.07111500	4.15078800
H	4.80625000	0.80860900	4.17689300
H	3.07432100	0.58801800	4.45642500
H	4.21894600	-0.67555400	4.92855400
H	3.03204200	-1.30917200	2.82817200
C	3.43647900	-1.46090300	-1.75132400
H	3.29596200	-1.15357400	-2.79619800
H	4.15933100	-0.77729200	-1.29739500
H	3.87480500	-2.46523000	-1.75756200
H	2.27848400	-1.77541300	0.03915700

7a (RS)-Prⁱ dimer *



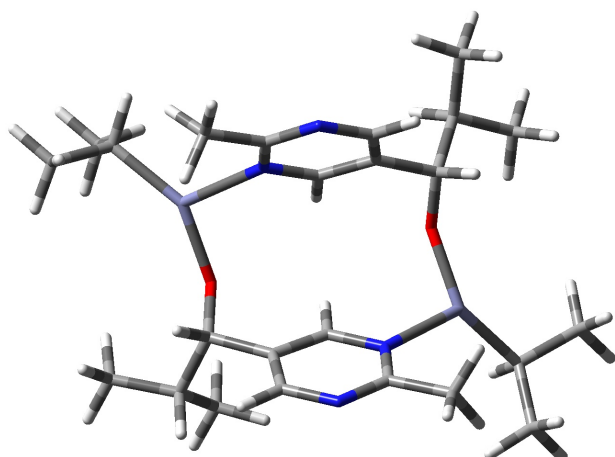
C	0.77945800	-0.24073900	-0.13132300
C	1.49952300	-0.94562200	0.83657100
C	0.90191500	-0.50399500	-1.62289300
C	4.88487200	-0.05869400	-3.38275400
C	-0.06612200	0.74481800	0.38164500
C	5.17089500	1.31635300	-1.27430600
C	0.52330900	0.24060000	2.52270100
C	-0.43911600	-2.67793100	-1.44820200
C	-0.09836200	-1.58121200	-3.69343700
C	2.96599200	6.46463000	-3.93787300
C	2.63830500	5.40162100	-1.67460600
C	1.52552600	4.35878800	-3.70482100
C	1.57891800	4.09670100	-5.20057900
C	0.82241900	4.80790300	-6.13183400
C	2.39354000	3.10288000	-5.75331200
C	-3.14449000	1.53325400	-2.35808700
C	1.70521100	3.61443800	-7.86334400
C	-2.39112900	3.81297000	-1.56214400
C	1.78356000	3.33981700	-9.34058600
C	0.38938600	0.50573700	3.99768600
C	-0.27531800	-1.34103200	-2.18726500
C	4.58584200	1.28383100	-2.69618400
C	-2.15319100	2.68457700	-2.58138200
C	2.75785200	5.14304000	-3.18337800
H	0.13999000	5.59399300	-5.80607900
H	3.00293500	2.47209300	-5.10501800
H	2.20394200	-1.72514000	0.54290100
H	-0.64727700	1.37303700	-0.29390600
H	1.82187800	-1.08789700	-1.78724900
H	0.63645900	4.97855700	-3.50427300
H	2.09161500	7.12027900	-3.83192600
H	3.82900900	7.00227200	-3.53020800
H	-2.35498300	3.09628000	-3.58197800
H	-0.95826400	-2.12515100	-4.10042200
H	0.79791800	-2.18515300	-3.88740800
H	3.63607800	4.50207900	-3.36004600
H	0.00495000	-0.64386500	-4.24689400
H	-1.26273400	-3.25371300	-1.88427800
H	-1.18959700	-0.74793200	-2.03207700
H	-0.65447300	-2.54152700	-0.38404100
H	0.46907600	-3.28913500	-1.53358200
H	5.09422600	2.06810500	-3.27694700
H	-1.76195200	4.69129200	-1.75571200
H	-2.18739000	3.48939700	-0.53250100
H	-3.43859700	4.15319500	-1.58268500
H	1.77889100	6.05036600	-1.45970300
H	3.53564800	5.90478700	-1.29722300
H	2.50506000	4.47438200	-1.11059800

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H	-4.18576300	1.89266700	-2.38257300
H	-3.00432600	1.05121400	-1.38095000
H	-3.05411600	0.75238000	-3.12342800
H	1.21208500	4.08554900	-9.89594300
H	2.82628200	3.34609700	-9.67491400
H	1.38265000	2.34367900	-9.56315400
H	0.29834600	-0.43530900	4.54852300
H	1.28682400	1.01301200	4.37329000
H	-0.47723400	1.14014000	4.19285400
H	5.96661900	-0.26629600	-3.40129100
H	4.41193700	-0.90098900	-2.85945800
H	4.53317300	-0.08365500	-4.42183800
H	4.70302100	0.56877800	-0.61939300
H	6.25035300	1.09645100	-1.28259400
H	5.04466500	2.29432700	-0.79284500
H	3.14302800	6.31014600	-5.00656200
N	1.38361800	-0.72064300	2.14771700
N	2.47087700	2.85267200	-7.05904100
N	0.87410200	4.58225600	-7.44984500
N	-0.20848600	0.99488700	1.68459400
O	1.38172400	3.13299900	-3.00098100
O	1.02663400	0.72552400	-2.32572400
Zn	-0.27284100	2.14593400	-2.60755400
Zn	2.67962900	1.71838600	-2.70576700

8 (RR)-Prⁱ macrocycle *



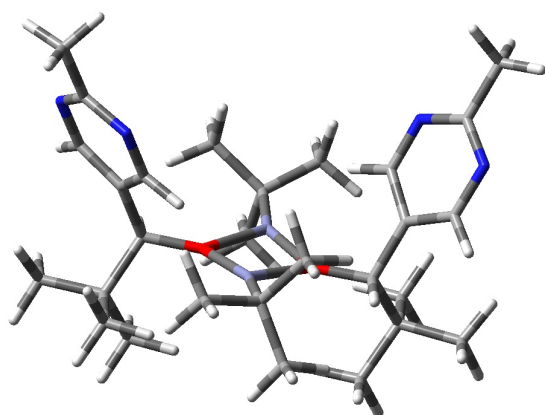
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C	1.93743400	-2.10734300	1.92104500
C	0.53417400	-1.56007800	0.17354300
C	-0.21453700	-2.86846300	1.97045400
N	0.98892900	-2.79976500	2.55526700
N	1.75301000	-1.49053000	0.73325800
Zn	3.14575700	-0.34022500	-0.40624500
C	3.28842300	-1.99895700	2.57106500
C	-2.15336800	-3.61315200	-0.64511900
O	-2.10048600	-1.17355400	-0.70368000
C	-3.62956400	-3.73015500	-1.04683600
C	-1.24059000	-3.74836100	-1.87018300
C	4.71497600	-1.17162100	-1.25123100
C	5.31966100	-2.37977500	-0.52461700
C	5.80404200	-0.13963800	-1.58443100
C	1.89665600	2.37159000	-0.03497300
C	0.53296800	2.32115100	0.65121800
C	-1.91208600	2.12461900	1.84045500
C	-0.53321100	1.65140000	0.05402900
C	0.24708000	2.86397200	1.90407500
N	-0.95283700	2.77658700	2.49740500
N	-1.73972700	1.54724900	0.62983000
Zn	-3.15654400	0.32152600	-0.40538800
C	-3.26101500	1.99370800	2.49141200
C	1.98990300	3.57081500	-1.02546500
O	2.12485400	1.17250600	-0.70031500
C	1.73796500	4.92633900	-0.34822400
C	3.35067500	3.56277100	-1.73265300
C	-4.88383800	1.09101100	-0.93037800
C	-6.07588300	0.46178300	-0.19349000
C	-5.07316000	0.98477900	-2.45297500
H	-2.62775800	-2.29375400	0.97164400
H	0.38403600	-1.02774300	-0.75866400
H	-0.97255200	-3.43476300	2.51221300
H	3.59412900	-0.95083100	2.67224300
H	4.05135100	-2.50667900	1.97114800
H	3.25516800	-2.45516300	3.56145000
H	-1.92339200	-4.43214600	0.05511600
H	-3.89984400	-2.93454900	-1.74868200
H	-4.29019500	-3.65202300	-0.17366900
H	-3.82840100	-4.69344900	-1.53076900
H	-1.41060500	-2.91731700	-2.56158100
H	-1.44315600	-4.68551100	-2.40132100
H	-0.17917500	-3.75006700	-1.59436100
H	4.31781200	-1.54311300	-2.21077500
H	4.57622900	-3.16270700	-0.32586600
H	5.76517900	-2.09562700	0.43899800
H	6.12770800	-2.84571200	-1.11261300

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H	6.25186400	0.28679300	-0.67605300
H	5.41481200	0.69843800	-2.17509800
H	6.62980900	-0.59028800	-2.15990700
H	2.64510000	2.56975000	0.75996500
H	-0.39659500	1.15986400	-0.90336200
H	1.01790400	3.38744100	2.46914800
H	-3.43330400	0.96161300	2.82385400
H	-4.06292600	2.25276300	1.79256600
H	-3.31254600	2.64497600	3.36524600
H	1.20941900	3.40574800	-1.78366700
H	2.46667400	5.10862300	0.45333600
H	0.73526800	4.99856700	0.08721700
H	1.84128600	5.74249700	-1.07215400
H	4.16623500	3.71514200	-1.01217800
H	3.40883200	4.36956600	-2.47281500
H	3.51865000	2.61031900	-2.23979100
H	-4.86585700	2.16267400	-0.67796000
H	-6.00823600	0.58356700	0.89604400
H	-6.15563100	-0.61533600	-0.39351600
H	-7.03158700	0.91272300	-0.50818600
H	-5.08051800	-0.06022400	-2.79054700
H	-4.27788100	1.49790500	-3.00954600
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9 (R,R)-tBu Dimer syn



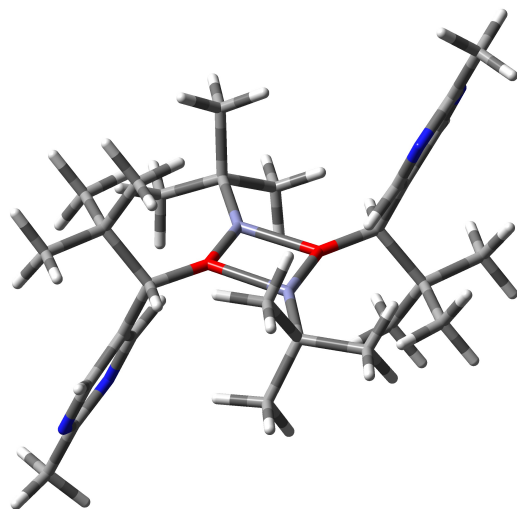
H	-0.47564	1.29468	-5.21634
H	0.22302	-0.24089	-4.68913
H	1.53089	2.55784	-4.47071
C	-0.37582	0.61595	-4.35255
H	-1.38271	0.24442	-4.12178
H	2.31713	1.06752	-3.93621
H	-0.69729	3.25276	-3.62318
C	1.64668	1.87260	-3.61329
H	-2.49276	-2.02672	-3.22956
H	4.01178	-1.76739	-3.01761
C	0.27397	1.34833	-3.16382
H	-4.69877	-0.76626	-2.76122
H	2.16177	2.43821	-2.82637
C	-0.60049	2.55498	-2.77321
H	2.47702	-0.95911	-2.69606
H	-3.18041	-3.48100	-2.49080
H	-1.61726	2.26673	-2.47990
H	-5.30901	-2.28598	-2.09735
C	-2.62625	-2.55825	-2.27930
C	3.46727	-1.17064	-2.27674
H	3.99612	-0.21758	-2.16282
H	3.11702	-3.87776	-1.90342
C	-4.78003	-1.36186	-1.84274
H	-2.55533	0.12049	-2.01948
H	-0.16762	3.12611	-1.94107
H	-1.63604	-2.83710	-1.90719
H	-4.49950	1.61116	-1.51018
H	1.58296	-3.06676	-1.54417
Zn	0.34230	0.12402	-1.61623
H	5.28086	-2.93793	-1.15682
H	-5.40558	-0.81025	-1.13338
C	-3.39286	-1.69465	-1.25874
C	2.59595	-3.25046	-1.17113
C	3.36323	-1.93276	-0.94685
C	-2.57766	-0.36860	-1.03424
H	2.14946	1.50822	-0.75448
C	4.78087	-2.27022	-0.44452
H	5.40442	-1.37729	-0.33680
C	-4.17836	1.55575	-0.47001
O	-1.23260	-0.63107	-0.66341
H	2.51467	-3.82556	-0.24010
H	-4.14180	-3.40387	-0.14208
O	1.24001	-0.88148	-0.22127
C	-3.21803	0.62179	-0.07106
C	-3.57502	-2.48460	0.04699
C	2.93620	1.43899	-0.00658
N	-4.74972	2.43072	0.36376
C	2.59444	-1.10313	0.14400
N	3.51995	2.58808	0.33539
H	4.75355	-2.78527	0.52370
H	5.56378	4.29882	0.78238
H	-2.61246	-2.78138	0.47669

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C	3.26641	0.20121	0.54937
H	-4.12005	-1.90630	0.80024
Zn	-0.33311	-1.40910	0.87327
H	2.59231	-1.74377	1.03764

10 (R,S)-tBu Dimer trans



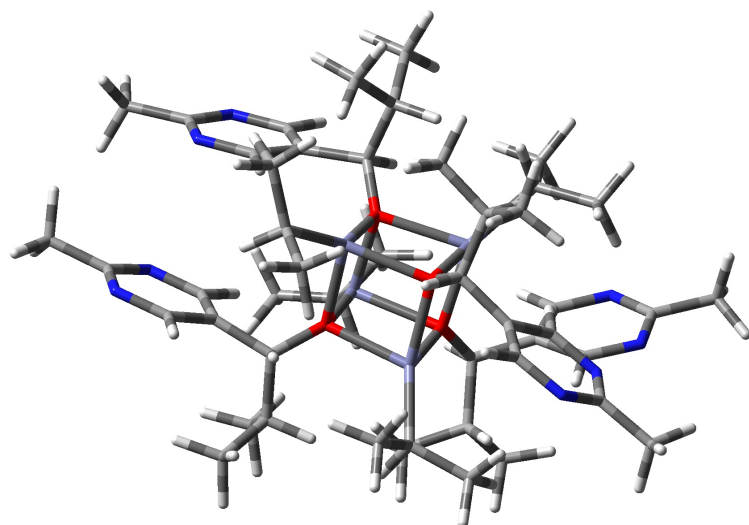
H	0.69440	-3.99031	-6.31873
H	1.23837	-5.38588	-5.35012
C	0.61399	-4.49124	-5.34703
H	-0.43621	-4.77789	-5.22328
H	-1.16112	2.70203	-4.53733
C	1.03757	-3.56069	-4.24349
H	-0.40008	1.11891	-4.35240
N	0.31843	-2.43479	-4.08221
C	-0.56957	2.07690	-3.84497
H	0.40305	2.56644	-3.72633
H	2.59298	0.51119	-3.65449
N	2.08988	-3.91692	-3.49199
H	-3.25558	1.92810	-3.51059
H	-2.61417	0.30073	-3.25469
H	4.43433	-1.16486	-3.01228
H	3.62772	1.79731	-3.02042
C	0.71533	-1.60845	-3.11540
H	0.10971	-0.71530	-2.97496
C	-2.69351	1.29686	-2.80181
C	2.85100	1.07334	-2.74966
H	-2.07559	3.96439	-2.57906
C	2.46060	-3.06260	-2.53278
H	5.40956	0.13367	-2.31688
C	-1.31337	1.91609	-2.51022
H	1.96977	1.64447	-2.44353
C	1.81830	-1.84507	-2.29069
C	4.61325	-0.58774	-2.09931
H	3.30717	-3.37327	-1.91953
C	-1.50732	3.31363	-1.89233
H	-3.31261	1.20162	-1.90059
H	-0.55198	3.81643	-1.69470
C	3.34874	0.15450	-1.62391
H	4.99190	-1.27193	-1.33099
C	2.26039	-0.89084	-1.18948
Zn	-0.37739	0.77661	-1.19484
H	-2.06453	3.28666	-0.94688
H	4.50712	1.72079	-0.64612
O	1.13490	-0.27727	-0.57385
C	3.71342	1.00799	-0.39327
H	-3.93896	-0.67080	-0.36416
H	2.75249	-1.50866	-0.42451
H	2.85238	1.57779	-0.03047
H	-2.63733	-1.74754	0.16643
H	4.07765	0.38279	0.43145
H	-2.74807	1.36131	0.38585
C	-3.53663	-1.21867	0.49627
H	-4.28070	-1.96792	0.79093

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O	-1.05405	0.24597	0.59744
H	-4.96805	1.02531	1.29742
C	-2.21704	0.81814	1.18216
H	1.07167	-3.71473	1.36457
Zn	0.48402	-0.75918	1.24077
H	3.18968	-2.24662	1.52361
C	-3.23621	-0.27194	1.67457
H	-3.45501	3.23624	1.84878
C	-4.55058	0.40972	2.10353
H	-5.29973	-0.34912	2.35823
C	-1.83468	1.85176	2.23195
C	0.81168	-3.35412	2.36871
C	-2.56977	3.01991	2.44774
H	-0.27506	-3.45240	2.48486
C	2.83705	-1.88882	2.49914
H	-1.76634	-1.61597	2.58593
H	3.24968	-0.88464	2.65565
C	1.30315	-1.91578	2.62172
H	-4.41725	1.04684	2.98409
C	-2.68644	-1.08701	2.85561
H	1.27281	-4.05297	3.08858
H	-0.02140	0.89388	2.90575
C	-0.69399	1.73953	3.03170
H	-3.41623	-1.84378	3.16565
H	3.29397	-2.54578	3.25927
N	-2.24761	3.93737	3.36564
H	-2.47466	-0.45492	3.72522
N	-0.34284	2.63309	3.95612
C	-1.14893	3.69944	4.09827
C	0.94011	-1.51000	4.05923
H	-0.13874	-1.53115	4.24823
H	1.30127	-0.50493	4.31389
H	0.16515	5.21030	4.87139
H	1.40525	-2.20572	4.77931
H	-1.55757	5.46010	5.25177
C	-0.77188	4.71028	5.14665
H	-0.59868	4.21559	6.10813

12 (SSSS)-Prⁱ cube *



C	3.07754100	3.42079100	-1.87487900
C	1.96748800	-0.96636600	3.51491100
C	7.10080800	-2.94178400	0.36345300
C	6.45545600	4.42233500	-0.91795400
C	1.75299900	-3.19971600	-1.67096700
C	2.24705100	2.46443600	1.98862700
C	1.80399900	-1.70890200	2.15586700
C	1.89785900	1.20987900	-2.23073700
C	5.25776400	3.57225100	-1.24067100
C	3.99714700	-1.12442800	0.98645800
C	4.32663100	1.48901600	-1.38224700
C	3.09056700	2.02738900	-1.76772700
C	2.30646900	0.24430000	-3.37513600
C	3.16889400	-2.06399300	1.60165000
C	5.70125600	-2.62853600	0.81494600
C	3.75122500	-3.32240200	1.77539200
C	0.62624400	-0.65495600	4.18007300
C	2.84705400	-1.75070600	4.50502800
C	1.09435700	-0.44047400	-4.01097100
C	3.09922000	0.96894800	-4.47970800
C	3.26243900	-3.29471500	-1.93611900
C	1.28244000	-4.44772200	-0.90316500
C	3.75796300	2.29864400	2.21744600
C	1.95876500	3.91365500	1.55912400
N	5.39792700	2.24027700	-1.11732600
N	5.00079400	-3.61272600	1.40250500
N	4.13212400	4.19881200	-1.61514600
N	5.23866700	-1.38847500	0.57767900
O	1.02805600	-0.94130800	1.19999600
O	1.20223400	0.53083200	-1.14045200
Zn	1.05372800	-1.52339100	-0.84654700
Zn	1.30754800	1.11011600	0.86103800
O	-0.89899000	1.06665000	0.86376100
O	-1.08385100	-1.14904500	-0.80303300
Zn	-1.00685700	0.84574100	-1.22091800
Zn	-1.08598700	-0.93149700	1.35315100
C	-1.95799700	-2.21214400	-1.26614300
C	-1.59516400	2.25012700	1.34236400
C	-1.32419500	2.55044600	2.84821900
C	-1.57073900	4.03628100	3.16216800
C	-2.10928600	1.68477400	3.84223200
C	-1.67055000	-2.63110100	-2.73893800
C	-2.20758400	-4.04240200	-3.02764400
C	-2.17194800	-1.64851000	-3.80630500
C	-3.43469500	-1.93284400	-1.06559500
C	-4.07376400	-0.74782200	-1.43675500

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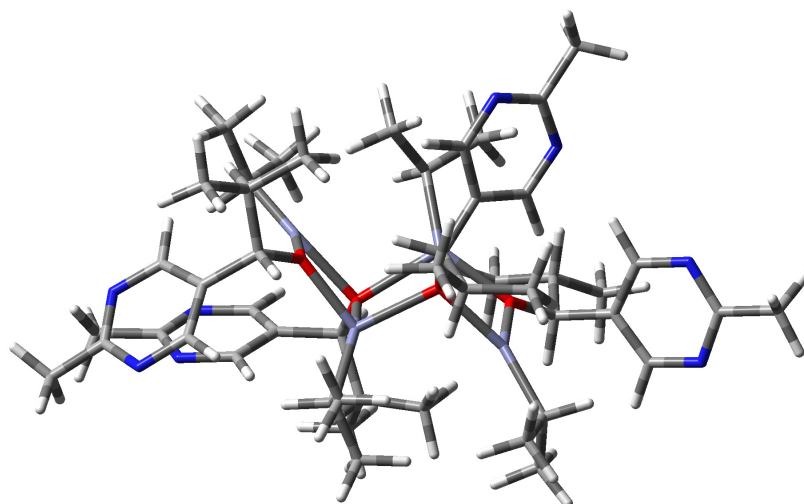
C	-4.29836600	-2.93296900	-0.60604400
N	-5.39633100	-0.57714500	-1.38583100
N	-5.62315700	-2.78976800	-0.52967600
C	-6.12394200	-1.61070900	-0.93213300
C	-3.08132800	2.23123900	1.04060200
C	-3.73613500	3.37234000	0.56714400
C	-3.93226700	1.15526800	1.32078400
N	-5.05687300	3.44738300	0.38278800
N	-5.25551100	1.20585000	1.16683600
C	-5.76987900	2.35430900	0.69485500
C	-7.61208200	-1.42040900	-0.84052700
C	-7.25490600	2.40317300	0.47154600
C	-2.19985400	-2.28759500	2.30209100
C	-2.88551800	-1.93952100	3.63069500
C	-1.43814500	-3.61872000	2.45261200
C	-1.50420200	2.19229400	-2.60200000
C	-2.94980000	2.24090700	-3.12001800
C	-1.07663400	3.60992600	-2.17741800
H	2.17465300	3.93602200	-2.20311600
H	2.47118600	-0.01772300	3.29213100
H	7.73821800	-2.05864900	0.45400200
H	7.09508800	-3.23814900	-0.69349500
H	7.51179100	-3.77095900	0.94340700
H	6.37569300	5.39632500	-1.40538800
H	6.51356000	4.58766400	0.16571900
H	7.37596600	3.91689800	-1.22123000
H	1.27548300	-3.24406000	-2.66051600
H	1.77845500	2.32953900	2.97708800
H	1.26173500	-2.64506400	2.34378900
H	1.18314000	1.92252200	-2.65912800
H	3.64170500	-0.11185800	0.81336700
H	4.48094100	0.41453200	-1.29763900
H	2.95437700	-0.52758600	-2.93850400
H	3.19133700	-4.13113300	2.24589100
H	0.77711300	-0.03951600	5.07391100
H	-0.04366100	-0.10641600	3.51774700
H	0.11621000	-1.57374500	4.48980000
H	3.87405600	-1.87659400	4.15313300
H	2.43096000	-2.74751400	4.70179200
H	2.88750300	-1.22043900	5.46270200
H	0.48019000	-0.94864500	-3.26931900
H	0.46286700	0.28535500	-4.53660400
H	1.41749900	-1.19308400	-4.73863500
H	2.52819900	1.81692600	-4.87957400
H	4.06429100	1.34700800	-4.13420100
H	3.28878900	0.28066000	-5.31062200
H	3.84525300	-3.30612400	-1.01163200
H	3.50677800	-4.22599300	-2.47234100
H	3.63863400	-2.46702900	-2.54899000
H	0.19093600	-4.49038900	-0.79598400
H	1.59243900	-5.37563100	-1.41019000
H	1.70666500	-4.49000900	0.10837200
H	4.33550100	2.38143400	1.29130100
H	4.13386400	3.08004000	2.89744600
H	4.02121400	1.33579500	2.67139400
H	2.32692400	4.63169100	2.30949500
H	2.45849200	4.16574500	0.61768400
H	0.89041000	4.11649700	1.42039200
H	-1.71771600	-3.08805100	-0.64914100
H	-1.16874800	3.09478400	0.78637100
H	-0.25661300	2.35446600	2.99075200
H	-0.99070600	4.69910900	2.51126100
H	-2.63035500	4.29810300	3.05660500
H	-1.28281300	4.25358600	4.19666100
H	-1.71025600	1.82713900	4.85295500
H	-3.16886600	1.96168800	3.86629700
H	-2.05067600	0.61813700	3.61826400
H	-0.58146800	-2.68150500	-2.80645400
H	-3.30232900	-4.07520800	-2.98323300
H	-1.91031700	-4.35919100	-4.03353100
H	-1.81629300	-4.78133900	-2.31889400
H	-1.76700000	-1.92777500	-4.78567400
H	-3.26413900	-1.66403300	-3.88701000
H	-1.86330900	-0.61798200	-3.60895400
H	-3.49905600	0.10267500	-1.79151200
H	-3.90218900	-3.89640400	-0.28400900
H	-3.17082500	4.27262700	0.32789700
H	-3.53442700	0.21053200	1.68364800

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H	-7.98577500	-0.88015500	-1.71538700
H	-8.11609900	-2.38454900	-0.74868200
H	-7.84840400	-0.81790700	0.04531600
H	-7.59014600	3.43480000	0.34852400
H	-7.50200400	1.84251800	-0.43842400
H	-7.78522400	1.92990000	1.30340500
H	-3.01171100	-2.47552300	1.58750900
H	-3.47739100	-2.79307400	3.99788900
H	-2.16914200	-1.69082800	4.42370700
H	-3.57711700	-1.09410000	3.54023200
H	-0.64582100	-3.55345200	3.21025200
H	-2.10993500	-4.42904400	2.77857900
H	-0.96302200	-3.95142200	1.51979000
H	-0.87800500	1.92475000	-3.46773800
H	-3.06750100	3.03677100	-3.87275900
H	-3.25749000	1.30592100	-3.60144400
H	-3.67242800	2.45539000	-2.32302200
H	-0.05102900	3.65930100	-1.78971800
H	-1.13950000	4.31821400	-3.01871200
H	-1.73055100	4.00751900	-1.39274000

14 (SSSS)-Prⁱ ladder *



C	7.43277000	-0.85316400	0.40690500
N	6.77204300	-0.07615500	-0.47102800
C	5.55793500	-0.48345600	-0.84520300
C	4.96166400	-1.65780400	-0.36152600
C	5.74984600	-2.38186100	0.53374200
N	6.97059700	-1.99996700	0.92575500
C	3.57651500	-2.12745700	-0.78062100
O	2.60056200	-1.14916600	-0.40132000
Zn	2.45290100	-0.60363900	1.47962400
Zn	1.02851700	-0.20752200	-1.20870200
O	1.05322900	0.67483300	0.74682500
Zn	-0.92936300	0.03811300	1.34485000
O	-0.93902300	-1.01693700	-0.45804300
Zn	-2.30018400	0.30460300	-1.38422400
O	-2.11219300	1.29212600	0.27073200
C	-3.05629300	2.20058100	0.85748200
C	-4.37997100	1.50909300	1.15563600
C	-5.33391200	1.19302900	0.17957800
N	-6.48977300	0.58515500	0.44960300
C	-6.71704700	0.25998100	1.73434000
N	-5.89724900	0.54084600	2.75831500
C	-4.75325300	1.16239700	2.45601300
C	-7.97766300	-0.49910600	2.03822000
N	-5.10350600	-2.29862000	-0.01661700
C	-3.78700000	-2.15411900	0.12401400
C	-2.86556200	-2.46772400	-0.88672200
C	-1.36157800	-2.38767700	-0.67466500
C	-0.97336700	-3.36784400	0.46548800
C	-3.43724000	-3.00454300	-2.04268000
N	-4.75410900	-3.14583600	-2.21847500
C	-5.54225900	-2.76778600	-1.19975600
C	-7.03043100	-2.86665600	-1.37990500
C	-3.24545500	3.48852800	0.01625000
C	-3.35485600	0.31357000	-3.05764200
C	-1.47015400	-0.39681600	3.21769900
C	1.16489200	2.11040700	0.95123600
C	1.99629200	2.77998500	-0.12599400
C	3.09651300	2.16909100	-0.73223900

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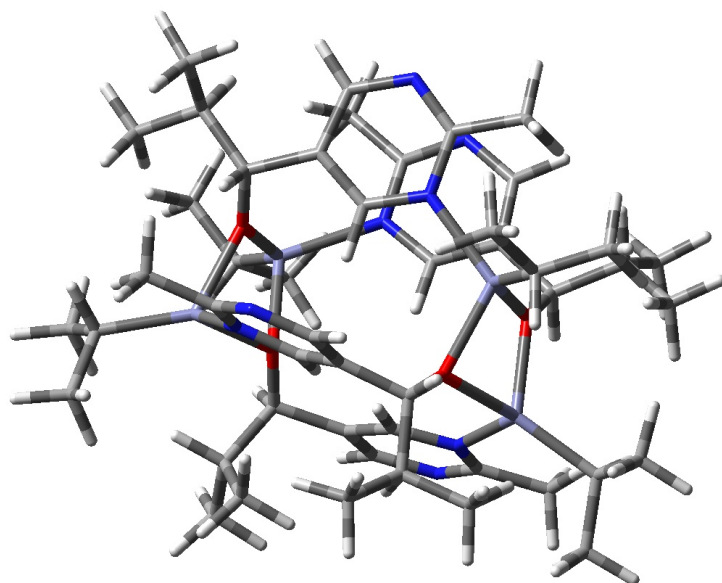
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C	1.76407300	4.09391500	-0.54382900
C	4.40422400	4.71627800	-2.99713200
C	1.69595800	2.44194100	2.38223700
C	0.72853900	0.49354400	-3.05089900
C	3.33349500	-1.25034900	3.12368800
C	3.52760100	-2.48435500	-2.28793100
C	8.79837600	-0.38877200	0.83535600
H	5.04637200	0.15814000	-1.56173000
H	5.38301900	-3.31629600	0.95893300
H	3.36971000	-3.05899100	-0.22638300
H	-2.63637700	2.51403500	1.82613700
H	-5.17150500	1.44616500	-0.86645900
H	-4.10226600	1.40228900	3.29644400
H	-8.80626100	-0.13414900	1.42483500
H	-8.22674400	-0.42178200	3.09849300
H	-7.82491600	-1.55795000	1.79346400
H	-3.45072800	-1.77179100	1.08710300
H	-0.87197600	-2.73576400	-1.59660500
H	-1.57768300	-3.09750400	1.34056000
H	-2.80492500	-3.33798600	-2.86527900
H	-7.48172700	-1.87930200	-1.23004900
H	-7.46213700	-3.53690000	-0.62755700
H	-7.27066300	-3.23807700	-2.37748100
H	-3.69304300	3.20096300	-0.94458700
H	-4.25186200	-0.27127100	-2.80568100
H	-2.56058100	-0.52627500	3.12229100
H	0.14693200	2.50790300	0.87838500
H	3.36278000	1.14614600	-0.48615900
H	0.92780200	4.66489100	-0.14471900
H	5.45917700	4.47238100	-2.84318800
H	4.25567400	5.79723700	-2.96116400
H	4.13166300	4.36314000	-3.99984000
H	1.30643700	1.64473800	3.02707300
H	0.04428100	-0.23317200	-3.51296200
H	4.39951500	-1.05800900	2.92562100
H	3.72492600	-1.55942100	-2.84514800
H	8.72560500	0.57127100	1.35957500
H	9.43678200	-0.22576200	-0.03972100
H	9.26000100	-1.12512900	1.49550000
C	4.61529300	-3.50859800	-2.65554600
H	4.54028200	-3.77473700	-3.71564600
H	5.62442700	-3.12634600	-2.47860600
H	4.49944400	-4.43364700	-2.07530400
C	2.15565800	-3.02352400	-2.71240100
H	1.35104600	-2.31629900	-2.49453600
H	2.13550700	-3.21593500	-3.79079000
H	1.92931800	-3.96911400	-2.20301000
C	1.97923600	0.53236200	-3.94372400
H	2.40624500	-0.46371400	-4.10113300
H	1.73432400	0.93251100	-4.94137300
H	2.77152000	1.16979200	-3.53270900
C	0.02623600	1.85810300	-3.09971700
H	-0.18431400	2.16889900	-4.13568500
H	-0.94028900	1.84879600	-2.57798300
H	0.62702300	2.65427700	-2.64712600
C	3.17651600	-2.77251000	3.29293100
H	3.44916100	-3.33478700	2.39130900
H	3.81360000	-3.14367900	4.11052900
H	2.14539500	-3.04777000	3.54615400
C	2.98969100	-0.54811000	4.44527800
H	3.57867800	-0.97107800	5.27460300
H	3.20110900	0.52535200	4.42201800
H	1.93433800	-0.66871900	4.71648300
C	3.22729300	2.45682700	2.49955200
H	3.66774900	3.27987800	1.92821100
H	3.52310100	2.58258400	3.54590500
H	3.68662900	1.52510300	2.14800500
C	1.12163800	3.77245600	2.89234300
H	1.44621100	3.95690500	3.92216100
H	1.46613200	4.61860900	2.28565300
H	0.02582300	3.77006500	2.88428200
C	-2.68376800	-0.37301900	-4.25748000
H	-2.30892100	-1.37718100	-4.02797900
H	-3.38965300	-0.47692700	-5.09611200
H	-1.83491700	0.21314200	-4.62720100

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C	-3.83056400	1.70991800	-3.49343400
H	-4.43161400	1.64953500	-4.41434200
H	-4.45688900	2.20613500	-2.74250700
H	-2.98936800	2.38121600	-3.70839400
C	-1.90854200	4.17352000	-0.28194700
H	-1.22520000	3.50842500	-0.81363000
H	-2.06323900	5.06460300	-0.90098700
H	-1.42447600	4.49941400	0.64895100
C	-4.19775000	4.47356400	0.71550200
H	-5.19815400	4.05624600	0.86227600
H	-3.80779700	4.76227700	1.70061800
H	-4.30051600	5.38868500	0.12199600
C	-0.93868600	-1.68087300	3.87060500
H	-1.35127400	-1.81069300	4.88452500
H	-1.19931600	-2.58447900	3.30858000
H	0.15285200	-1.66990100	3.97571500
C	-1.26050600	0.77850400	4.19027300
H	-0.19680100	0.93811400	4.40974200
H	-1.65353300	1.73081200	3.80967400
H	-1.75185500	0.59188700	5.15902900
C	0.49606900	-3.30076600	0.87334100
H	0.76844000	-2.31718700	1.26360900
H	0.69970700	-4.02702500	1.66649600
H	1.15541400	-3.52426400	0.03020200
C	-1.32331900	-4.81642200	0.07617200
H	-2.38800200	-4.95111300	-0.13268000
H	-0.76289200	-5.12983700	-0.81431500
H	-1.05596900	-5.49877900	0.89004200

16 (RRR)-Pr^I barrel -4B-*



Zn	3.34066000	-1.20630100	-0.42230600
O	2.06576800	-0.99825000	1.17313400
O	2.90673700	0.78195100	-0.55942500
N	1.93789000	-1.89959000	-2.05590600
C	5.21206100	-1.85562000	-0.73299300
Zn	2.53877800	1.03812200	1.38340200
C	2.92021900	1.53235100	-1.75212800
C	1.83311500	-1.73149400	2.36413000
C	0.67105300	-1.97077500	-1.61035700
C	2.13139000	-2.06315900	-3.38411800
C	3.71500100	1.26984500	2.98403300
N	0.74725800	2.36101300	1.40589300
H	5.51191600	-1.29937900	-1.63800900
C	1.55782600	2.21804100	-1.94348600
C	0.40530200	-1.51484100	2.84636000
C	-0.42900200	-2.17495800	-2.43880200
N	1.14262700	-2.27742400	-4.26074000
C	4.12213100	2.51029900	-1.88990100
C	-0.48019800	1.82535700	1.38213000
C	0.82282600	3.71293300	1.48557800
C	3.52212500	-2.00754900	-3.94918400
H	3.01857500	0.82009800	-2.59172400
H	2.49417400	-1.36483600	3.16817500
H	0.55809600	-1.80827400	-0.54698600
H	4.07953900	0.24393000	3.15861600
C	1.33773200	3.55806400	-2.26586600
C	0.38605200	1.48205500	-1.74976400
C	-1.86305400	-2.15233400	-1.92049500
C	-0.10676800	-2.32276600	-3.79125800
C	0.06215700	-1.33449100	4.19090700
C	-0.67516300	-1.49287200	1.97515000
C	-1.66106900	2.56957700	1.45554300
N	-0.24075700	4.51423100	1.53037900
C	2.17808600	4.35632600	1.51215200
H	3.89169900	3.42644700	-1.32454400
H	-0.52683300	0.75117000	1.27029300
H	3.50614900	-1.48048100	-4.90681100
H	4.22280400	-1.52891200	-3.26601400
H	3.88368500	-3.02411400	-4.14621700
N	0.11756600	4.09890600	-2.39220400
N	-0.84517200	1.99582300	-1.87386900
O	-1.98482200	-1.17925800	-0.89861800
N	-1.19546500	-1.19716700	4.61926400

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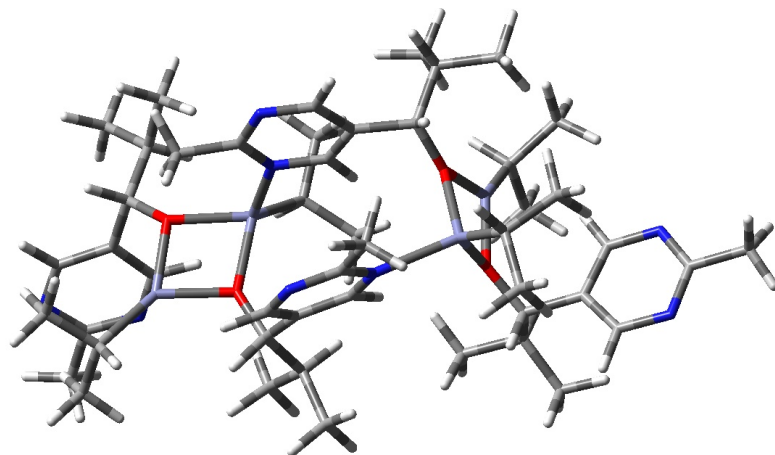
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C	-3.00943600	1.83219800	1.42573800
C	-1.45632300	3.94784200	1.51908200
H	2.16153800	4.24807900	-2.42203400
H	0.43645800	0.44276100	-1.45235700
H	-0.89025400	-2.46436700	-4.53495600
H	0.83475800	-1.29570500	4.95830100
H	-0.54496200	-1.56055800	0.90339500
H	2.71368700	4.09130300	2.42875500
H	2.79297500	4.01888500	0.67117100
H	2.06493700	5.44030900	1.46468000
C	-0.93698400	3.30811800	-2.20128800
Zn	-2.59355200	0.70885100	-1.55309100
C	-2.17106900	-1.22077800	3.70241900
Zn	-3.31044400	-1.12300200	0.65851400
O	-2.99466400	0.86551900	0.40302600
C	-4.24442300	2.77500000	1.39453200
H	-3.07407700	1.29546500	2.38998700
H	-2.28772500	4.64598500	1.55010200
C	-5.08814400	-2.00593400	0.85420900
C	-3.82045100	0.57104500	-3.12876200
C	-2.29972200	3.91725200	-2.35469400
C	-3.58060400	-1.07322300	4.20212400
H	-4.06770700	3.56022100	0.64297900
H	-5.63169700	-1.39688300	1.59689300
H	-4.19558300	-0.46394400	-3.06543500
H	-2.19867100	4.98988300	-2.52582300
H	-2.83039400	3.46694900	-3.19930600
H	-2.91251200	3.74972700	-1.46255500
H	-4.30961200	-1.31008700	3.42687600
H	-3.73499400	-1.72707400	5.06545400
H	-3.75077900	-0.04584300	4.54689900
H	-2.49336500	-1.86210800	-2.77613000
C	-2.37619200	-3.56015900	-1.49810400
H	-3.37303400	-3.36476600	-1.08404400
C	6.23460100	-1.45661400	0.34517900
H	6.23328600	-0.37774500	0.54016300
H	6.04615300	-1.95417800	1.30508800
H	7.26084400	-1.73197900	0.04922100
C	5.36732200	-3.34523500	-1.08054000
H	4.70339200	-3.65862200	-1.89601100
H	6.39827200	-3.58511300	-1.39027300
H	5.14252400	-3.99325900	-0.22487800
C	2.95112200	1.67752100	4.25466700
H	2.10337100	1.01143400	4.46588900
H	3.59897800	1.66873200	5.14762100
H	2.53646200	2.69338500	4.18602600
C	4.97410200	2.13525700	2.82375200
H	4.74237600	3.18796100	2.61029100
H	5.58737500	2.13435200	3.74105300
H	5.61813600	1.78076000	2.00973900
C	4.36359100	2.88083500	-3.36600800
H	3.47030600	3.25428000	-3.87686300
H	5.14059900	3.64883400	-3.44988300
H	4.71091000	2.00095800	-3.92224200
C	5.40747200	1.92241000	-1.29851900
H	6.22963000	2.64098100	-1.39582900
H	5.28663400	1.67783800	-0.24243900
H	5.70136800	1.00631800	-1.82343000
C	-1.54116300	-4.25004800	-0.41271400
H	-1.45634900	-3.63937400	0.49039200
H	-2.01022900	-5.19642200	-0.12089600
H	-0.52876900	-4.48303600	-0.76576300
C	-2.54820200	-4.48491300	-2.71316100
H	-3.17262600	-4.02471100	-3.48830000
H	-1.58258800	-4.74410100	-3.16559400
H	-3.02899900	-5.42294800	-2.41415600
C	-3.08955100	0.68503200	-4.47745300
H	-3.76378400	0.49978100	-5.33093000
H	-2.65897800	1.68428000	-4.63610600
H	-2.25740100	-0.02718000	-4.56605300
C	-5.07126400	1.46255400	-3.12898900
H	-5.71115000	1.26396700	-4.00549100
H	-5.69080100	1.30286400	-2.23812200
H	-4.82991100	2.53394900	-3.16009900
C	-5.93616800	-1.96177500	-0.42773700
H	-6.94067400	-2.38961200	-0.26943400
H	-6.07385400	-0.93858700	-0.79858800

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H	-5.48000000	-2.53698500	-1.24579000
C	-5.04572900	-3.43760700	1.41220100
H	-6.05721000	-3.84579700	1.57689900
H	-4.54065600	-4.13125900	0.72604700
H	-4.51264000	-3.50051400	2.37047700
C	-4.47157000	3.43928700	2.76630600
H	-5.28483700	4.17143700	2.71051000
H	-4.76235200	2.68396600	3.50767800
H	-3.58840400	3.95385000	3.15802000
C	-5.51343900	2.01835700	0.98211700
H	-5.73073800	1.20211100	1.68209800
H	-6.37457300	2.69672100	0.98427000
H	-5.41749400	1.58633900	-0.01499600
C	2.13505400	-3.25442800	2.20226100
H	1.69165600	-3.55251000	1.23985700
C	1.52916500	-4.14067400	3.30322400
H	1.86834700	-3.82728500	4.29941900
H	0.43492900	-4.13459800	3.30285600
H	1.85394600	-5.17793400	3.16376600
C	3.64872200	-3.47313800	2.14532100
H	4.10518100	-3.25743900	3.12021200
H	3.89146600	-4.50876800	1.88302500
H	4.10629900	-2.81668600	1.40575900

18 (SSSS)-Prⁱ SMS *



C	-1.62261900	3.20914000	1.16113600
N	-1.27572600	2.21902200	0.30878300
C	-3.03480900	3.29460600	1.66244600
N	-0.76422400	4.12799700	1.62227700
C	0.02000000	2.13804100	-0.05054800
C	0.51096000	4.02856100	1.24469100
Zn	-2.40666900	0.59637900	-0.61411200
C	0.99157700	3.02112600	0.40322300
O	-2.61432900	-0.67690000	0.96182300
Zn	-4.51610200	-0.40278600	1.30607000
O	-4.37637100	0.86933200	-0.15169500
C	-1.78190000	0.14879800	-2.46041000
C	2.46736100	2.88808800	0.03935500
C	-1.84982300	-1.58400100	1.73314000
C	-5.66512600	-0.99450500	2.77739300
C	-5.54845600	1.16405100	-0.90506300
O	2.80746700	1.53932400	-0.17905800
C	2.86396300	3.86637400	-1.10492000
C	-0.70070400	-0.82554000	2.39122300
C	-1.42701200	-2.84816300	0.95332700
C	-6.30368400	-0.12283300	-1.19852100
C	-5.22886100	1.97988000	-2.18231400
Zn	3.14737300	0.21066600	-1.58676100
Zn	3.44561300	0.42336500	1.41309100
C	0.57839500	-0.64552300	1.86473000
C	-0.92486600	-0.16930100	3.60419700
C	-7.63387500	-0.31736100	-0.82198600
C	-5.72402900	-1.20924500	-1.86840900
O	3.37099400	-0.97989900	-0.04648500
C	3.16708500	0.16665900	-3.55875600
C	5.02854100	0.93037200	2.51231200
N	1.51141400	0.12344200	2.46063100
N	-0.02125900	0.59827200	4.21299300
N	-8.31455700	-1.44294900	-1.06420900
N	-6.37597800	-2.34480800	-2.12442500
C	4.08779500	-2.20721200	0.03027600
C	1.16994800	0.73441100	3.61886200
C	-7.65413400	-2.41686300	-1.70893000
C	5.57727000	-1.99494700	-0.19290300
C	3.51727800	-3.27119600	-0.94771300
C	2.16276200	1.63053300	4.30117900
C	-8.38951300	-3.70267300	-1.97201800
C	6.07043400	-1.19515600	-1.22543700

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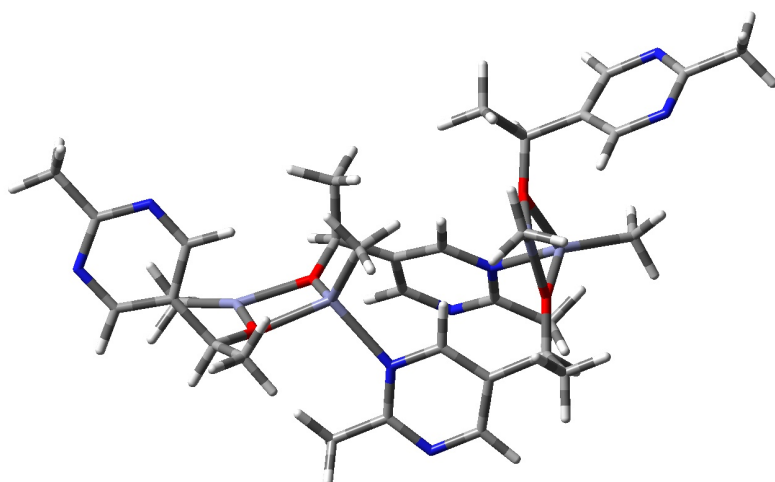
C	6.56378600	-2.60005800	0.58778800
N	7.36859000	-1.01912800	-1.47315500
N	7.87385800	-2.44534500	0.37089200
C	8.22631500	-1.66093200	-0.65958100
C	9.69590000	-1.45958100	-0.91180100
H	-3.05332600	3.04049800	2.72989100
H	-3.69707500	2.61789100	1.12106300
H	-3.39551400	4.32419900	1.57752300
H	0.28171900	1.32710600	-0.72037300
H	1.18755400	4.78434700	1.64543200
H	-2.66184000	-0.32499300	-2.92745700
C	-1.43175300	1.36182300	-3.33801500
C	-0.65640000	-0.89437100	-2.53935500
H	3.03170900	3.24414900	0.91989500
H	-2.48841800	-1.93713800	2.56243900
C	-6.43397100	-2.29435200	2.49385200
H	-4.98623300	-1.19850500	3.62182900
C	-6.62581200	0.11670400	3.23169600
H	-6.21015500	1.79371500	-0.28439600
C	2.09372600	3.64114300	-2.41180300
C	4.38232700	3.85021800	-1.32516300
H	2.59670200	4.86691300	-0.73067600
C	-2.63341200	-3.47331000	0.24000200
C	-0.76897500	-3.87254900	1.89231600
H	-0.69849200	-2.55642600	0.18530400
C	-4.53706100	3.30505800	-1.83346300
C	-6.49424800	2.25151900	-3.01181000
H	-4.53900100	1.37682200	-2.78945300
H	0.89621900	-1.12149700	0.94157300
H	-1.88654000	-0.26876200	4.10832000
H	-8.17750800	0.46881200	-0.29644500
H	-4.69007600	-1.16227700	-2.20862000
H	2.25132500	0.69605700	-3.86192800
C	4.35814100	0.91802100	-4.17782800
C	3.07267400	-1.24466900	-4.15872100
C	5.48790300	-0.15950100	3.49457200
C	6.21368900	1.39772100	1.65126300
H	4.73269600	1.80020100	3.11822000
H	3.95968600	-2.61296700	1.04812000
H	3.68740500	-2.89736900	-1.96652000
C	2.00889800	-3.45518800	-0.75064700
C	4.23519300	-4.62330400	-0.80831100
H	3.07665900	1.08737900	4.55588300
H	1.71187900	2.03047100	5.21029800
H	2.45486100	2.46186700	3.65098600
H	-9.46775000	-3.54677000	-1.89956100
H	-8.10143400	-4.45853500	-1.23009400
H	-8.12780800	-4.09838800	-2.95724700
H	5.38280900	-0.65830200	-1.87776300
H	6.28904800	-3.23924400	1.42758600
H	9.89260900	-1.38033100	-1.98429600
H	10.27294600	-2.27955600	-0.47896700
H	10.03217000	-0.52411900	-0.44628600
H	-7.23511500	2.81424000	-2.42829000
H	-6.97036900	1.32867500	-3.35647700
H	-6.24858900	2.85128000	-3.89515400
H	-5.18685400	3.93012300	-1.20670800
H	-4.31012900	3.87114800	-2.74397400
H	-3.59911500	3.15026900	-1.29461100
H	-7.03203100	-2.60298600	3.36662800
H	-5.76432200	-3.12932700	2.25026800
H	-7.13404100	-2.18313200	1.65607700
H	-7.22282300	-0.19649100	4.10365900
H	-7.34129100	0.38376300	2.44237300
H	-6.09791500	1.03623300	3.51653700
H	-0.55078000	1.90156100	-2.96376600
H	-2.24917300	2.09148300	-3.39260800
H	-1.19482900	1.06417000	-4.37306400
H	0.28750100	-0.52435500	-2.10773800
H	-0.42319200	-1.16995200	-3.58125700
H	-0.90996000	-1.82035500	-2.00922700
H	-1.47128300	-4.19316500	2.67289000
H	0.12102400	-3.47352700	2.39119500
H	-0.46544100	-4.76584800	1.33608200
H	-3.06416800	-2.79232300	-0.49819900
H	-3.42012200	-3.73797400	0.95956400
H	-2.33977300	-4.39228700	-0.27945800
H	1.61729700	-4.20367900	-1.44907900

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H	1.46432000	-2.52345800	-0.92012100
H	1.78895400	-3.80360900	0.26694800
H	3.79632900	-5.35684800	-1.49365600
H	4.13161400	-5.02261500	0.20957000
H	5.30307900	-4.55511000	-1.03553700
H	5.94131000	2.23338700	0.99415400
H	6.59811400	0.59809500	1.00663800
H	7.06023300	1.73547000	2.27262400
H	4.69200500	-0.47291500	4.18510900
H	6.33816400	0.17426800	4.11273100
H	5.82404800	-1.06305900	2.96918700
H	4.92242100	4.06817400	-0.39623300
H	4.67225700	4.60209000	-2.06766400
H	4.72483500	2.87575200	-1.68665400
H	1.01594200	3.78729200	-2.28099400
H	2.25181600	2.63231100	-2.80246600
H	2.43011900	4.34779300	-3.17859600
H	2.98991600	-1.20146100	-5.25643200
H	2.20297300	-1.80111200	-3.78987400
H	3.96641600	-1.84392500	-3.93889900
H	4.41006300	1.96618600	-3.86163100
H	4.29580800	0.91485800	-5.27763500
H	5.31928700	0.45348900	-3.91965800

21 (SSSS)-Me SMS *



C	-1.58693700	-3.18273800	1.45184700
N	-1.17954300	-1.90339000	1.30637300
C	-3.02170200	-3.52831100	1.17678800
N	-0.77548900	-4.18547700	1.81327900
C	0.12050600	-1.64176900	1.53013000
C	0.51203700	-3.89881500	2.01966100
Zn	-2.15947600	-0.08962600	0.59535600
C	1.04474000	-2.61374700	1.88700600
O	-2.45799800	-0.48860600	-1.36632700
Zn	-4.40083200	-0.58598100	-1.34140300
O	-4.14365200	-0.41257300	0.56832700
C	-1.18755300	1.47164800	1.31776500
C	2.51884100	-2.27407300	2.09666400
C	-1.65615600	-0.21832800	-2.49988900
C	-5.77140200	-0.87149400	-2.67683100
C	-5.16573100	0.01686100	1.45758400
O	2.88055200	-1.14510600	1.34474500
C	2.83153800	-2.08155900	3.58823700
C	-0.41863000	-1.10516800	-2.45651600
C	-1.33996300	1.27518900	-2.62738900
C	-5.87142400	1.25128100	0.92170500
C	-4.58852900	0.25267000	2.85749200
Zn	2.83885600	0.76483300	1.74389700
Zn	3.52801000	-1.01689300	-0.57824800
C	0.75816600	-0.79245000	-1.77922000
C	-0.42602000	-2.36517100	-3.05971300
C	-5.18396600	2.41305600	0.54645200
C	-7.25592800	1.31933000	0.77062600
O	2.98469100	0.90067000	-0.18433500
C	2.76261400	1.84753300	3.34973300
C	5.30177900	-1.57059700	-1.22259700
N	1.79322400	-1.64776000	-1.69464400
N	0.59049400	-3.22808800	-2.99285800
N	-5.79230000	3.50319600	0.07746600
N	-7.89636300	2.39940700	0.30816600
C	3.40977500	2.02940500	-0.93211300
C	1.67087600	-2.84959300	-2.30217300
C	-7.13428800	3.45265500	-0.02078200
C	4.89885200	2.29485500	-0.77687900
C	2.58656300	3.26614100	-0.54653000
C	2.80621300	-3.82734400	-2.19808800
C	-7.82490000	4.67961500	-0.55186100
C	5.54478000	2.25276400	0.46160300
C	5.72441500	2.62682700	-1.84984600
N	6.84006200	2.51662000	0.62723000
N	7.02770200	2.89960000	-1.72066400
C	7.53439000	2.83705700	-0.48034600
C	8.99878900	3.13576900	-0.30420000
H	-3.09280900	-4.06484400	0.22190700

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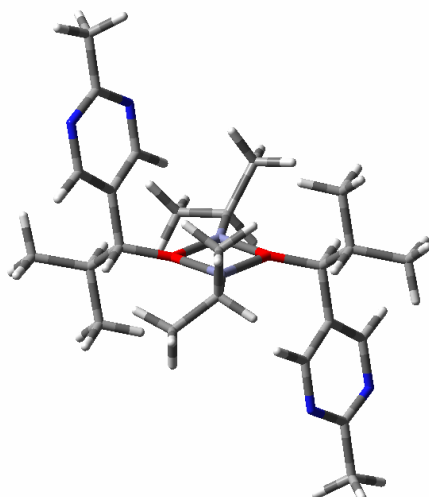
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H	-3.64297600	-2.63288600	1.12084700
H	-3.39371500	-4.20579500	1.95077900
H	0.42584900	-0.61031100	1.40517600
H	1.14890800	-4.73960800	2.29698000
H	-0.18608000	1.60575500	0.88257700
H	-1.71848600	2.41270700	1.12086400
H	-1.04696300	1.42037800	2.40613700
H	3.10317800	-3.14123600	1.74533000
H	-2.21872700	-0.51914700	-3.39833600
H	-6.17810500	0.07368700	-3.05462600
H	-5.39098200	-1.42949800	-3.54111400
H	-6.61381400	-1.44451100	-2.27153700
H	-5.92094600	-0.78218200	1.53464400
H	3.89974600	-1.87763800	3.71395500
H	2.57713900	-2.97523800	4.17009500
H	2.26640200	-1.23503200	3.99394200
H	-2.27499500	1.83552100	-2.72953500
H	-0.71883700	1.48056600	-3.50727900
H	-0.82657500	1.65185000	-1.73656000
H	-4.11569700	-0.66461500	3.22602000
H	-5.37400600	0.54344400	3.56384100
H	-3.83336800	1.04606900	2.83723200
H	0.90815500	0.15891800	-1.27577700
H	-1.29691100	-2.69489200	-3.62644800
H	-4.09831000	2.46215400	0.62371400
H	-7.88207800	0.46436300	1.02993500
H	2.74483400	2.92010000	3.12414500
H	1.86609300	1.63397200	3.94407500
H	3.63048600	1.66610800	3.99553300
H	6.08663500	-0.95045700	-0.77202100
H	5.55017400	-2.61206800	-0.98011500
H	5.41159500	-1.46583800	-2.31080100
H	3.22417400	1.82227700	-1.99841600
H	1.51838300	3.06568700	-0.68378900
H	2.86218400	4.13180000	-1.15924700
H	2.75361900	3.52706600	0.50478000
H	3.73896000	-3.38902300	-2.56425600
H	2.56554900	-4.72153200	-2.77459800
H	2.97843100	-4.11364900	-1.15393400
H	-7.53366100	5.56202500	0.02796600
H	-8.90813800	4.55288500	-0.51141100
H	-7.52306900	4.86585000	-1.58933900
H	4.98976600	1.98470500	1.36041000
H	5.32297800	2.67326300	-2.86336900
H	9.52731000	2.24425800	0.05344500
H	9.14097800	3.91582300	0.45149800
H	9.43728400	3.45592900	-1.25100800

3) Further calculations on favoured conformers of the hetero- and homochiral dimer

The many potentially significant conformations of the dimers make a thorough theoretical investigation using DFT methods time-consuming and computationally demanding. The investigation of a very large number of conformations is readily achievable with Molecular Mechanics methods. The unbiased conformational search for all low-energy conformations was performed with Spartan04 (MMFF). The input structures were the initially optimized structures at the B3LYP/6-31G(d) level of theory with frozen atomic coordinates for the [Zn-O] core. Not to bias the conformational search, each input structure was subjected to a combination of systematic and Monte-Carlo conformational search. The identified low energy conformers then served as starting geometries for further full geometry optimizations and energy calculations at the B3LYP/6-31G(d)-B3LYP/LANL2DZ(Zn) (ONIOM calculations) and B3LYP/6-31G(d) level of theory.

Heterochiral Dimer –trans-



B3LYP/6-31G(d)-B3LYP/LANL2DZ(Zn)

Zero-point correction = 0.612092 (Hartree/Particle)
Thermal correction to Energy = 0.652543
Thermal correction to Enthalpy = 0.653488
Thermal correction to Gibbs Free Energy = 0.530871
Sum of electronic and zero-point Energies = -1438.794694
Sum of electronic and thermal Energies = -1438.754242
Sum of electronic and thermal Enthalpies = -1438.753298
Sum of electronic and thermal Free Energies = -1438.875914

B3LYP/6-31G(d)

0.1722 Debye

Supplementary Material (ESI) for Chemical Communications

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E = -4866.4576041

Zero-point correction = 0.612523 (Hartree/Particle)

Thermal correction to Energy = 0.652760

Thermal correction to Enthalpy = 0.653704

Thermal correction to Gibbs Free Energy = 0.532549

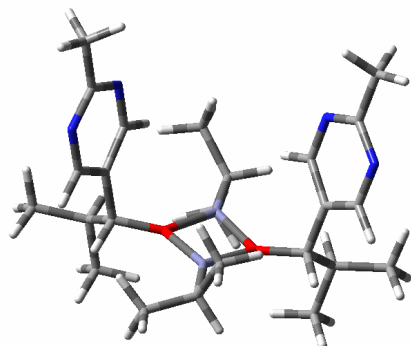
Sum of electronic and zero-point Energies = -4865.845081

Sum of electronic and thermal Energies = -4865.804845

Sum of electronic and thermal Enthalpies = -4865.803900

Sum of electronic and thermal Free Energies = -4865.925055

Heterochiral Dimer –cis-



B3LYP/6-31G(d)-B3LYP/LANL2DZ(Zn)

Zero-point correction = 0.611420 (Hartree/Particle)
Thermal correction to Energy = 0.652185
Thermal correction to Enthalpy = 0.653129
Thermal correction to Gibbs Free Energy = 0.527910
Sum of electronic and zero-point Energies = -1438.792495
Sum of electronic and thermal Energies = -1438.751730
Sum of electronic and thermal Enthalpies = -1438.750785
Sum of electronic and thermal Free Energies = -1438.876005

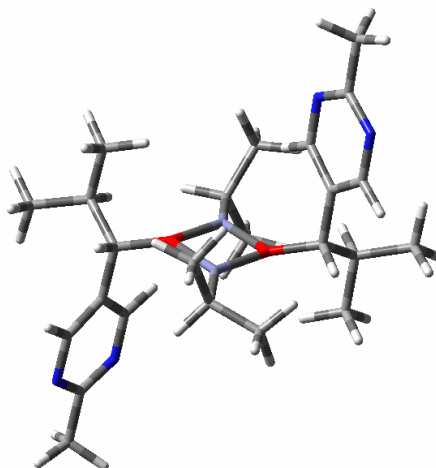
B3LYP/6-31G(d)

3.2393 Debye

E = -4866.4552496

Zero-point correction = 0.611973 (Hartree/Particle)
Thermal correction to Energy = 0.652538
Thermal correction to Enthalpy = 0.653482
Thermal correction to Gibbs Free Energy = 0.530019
Sum of electronic and zero-point Energies = -4865.843277
Sum of electronic and thermal Energies = -4865.802712
Sum of electronic and thermal Enthalpies = -4865.801767
Sum of electronic and thermal Free Energies = -4865.925230

Homochiral Dimer –trans-



B3LYP/6-31G(d)-B3LYP/LANL2DZ(Zn)

Zero-point correction = 0.611433 (Hartree/Particle)
Thermal correction to Energy = 0.651271
Thermal correction to Enthalpy = 0.652215
Thermal correction to Gibbs Free Energy = 0.528661
Sum of electronic and zero-point Energies = -1438.793127
Sum of electronic and thermal Energies = -1438.753289
Sum of electronic and thermal Enthalpies = -1438.752345
Sum of electronic and thermal Free Energies = -1438.875899

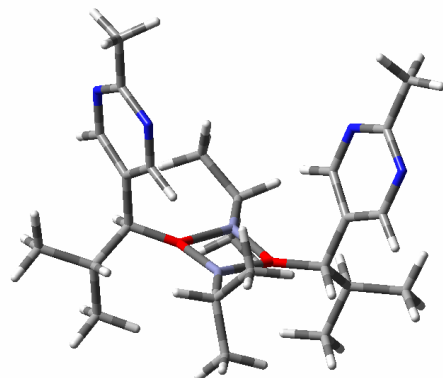
B3LYP/6-31G(d)

0.3104 Debye

E = -4866.4556108

Zero-point correction = 0.611756 (Hartree/Particle)
Thermal correction to Energy = 0.652398
Thermal correction to Enthalpy = 0.653342
Thermal correction to Gibbs Free Energy = 0.528902
Sum of electronic and zero-point Energies = -4865.843855
Sum of electronic and thermal Energies = -4865.803213
Sum of electronic and thermal Enthalpies = -4865.802269
Sum of electronic and thermal Free Energies = -4865.926709

Homochiral Dimer –cis–



B3LYP/6-31G(d)-B3LYP/LANL2DZ(Zn)

Zero-point correction = 0.611451 (Hartree/Particle)
Thermal correction to Energy = 0.652167
Thermal correction to Enthalpy = 0.653111
Thermal correction to Gibbs Free Energy = 0.528758
Sum of electronic and zero-point Energies = -1438.794505
Sum of electronic and thermal Energies = -1438.753789
Sum of electronic and thermal Enthalpies = -1438.752844
Sum of electronic and thermal Free Energies = -1438.877197

B3LYP/6-31G(d)

3.1070 Debye

E = -4866.4569100

Zero-point correction = 0.611995 (Hartree/Particle)
Thermal correction to Energy = 0.652510
Thermal correction to Enthalpy = 0.653454
Thermal correction to Gibbs Free Energy = 0.530073
Sum of electronic and zero-point Energies = -4865.844915
Sum of electronic and thermal Energies = -4865.804400
Sum of electronic and thermal Enthalpies = -4865.803456
Sum of electronic and thermal Free Energies = -4865.926837

¹ (a) C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B* **1988**, *37*, 785-789; (b) A. D. Becke, *J. Chem. Phys.* **1993**, *98*, 5648-5652.