Electronic Supplementary Information

(for the communication **"A Novel Ditopic Zinc-Salophen Macrocycle as Potential Wheel for [2] Pseudorotaxanes with pH driven intra wheel Motion of the Axle"**

submitted by Antonella Dalla Cort,* Luigi Mandolini, Chiara Pasquini, Luca Schiaffino)

A Novel Ditopic Zinc-Salophen Macrocycle as Potential Wheel for [2]-Pseudorotaxanes with pH driven intra wheel Motion of the Axle

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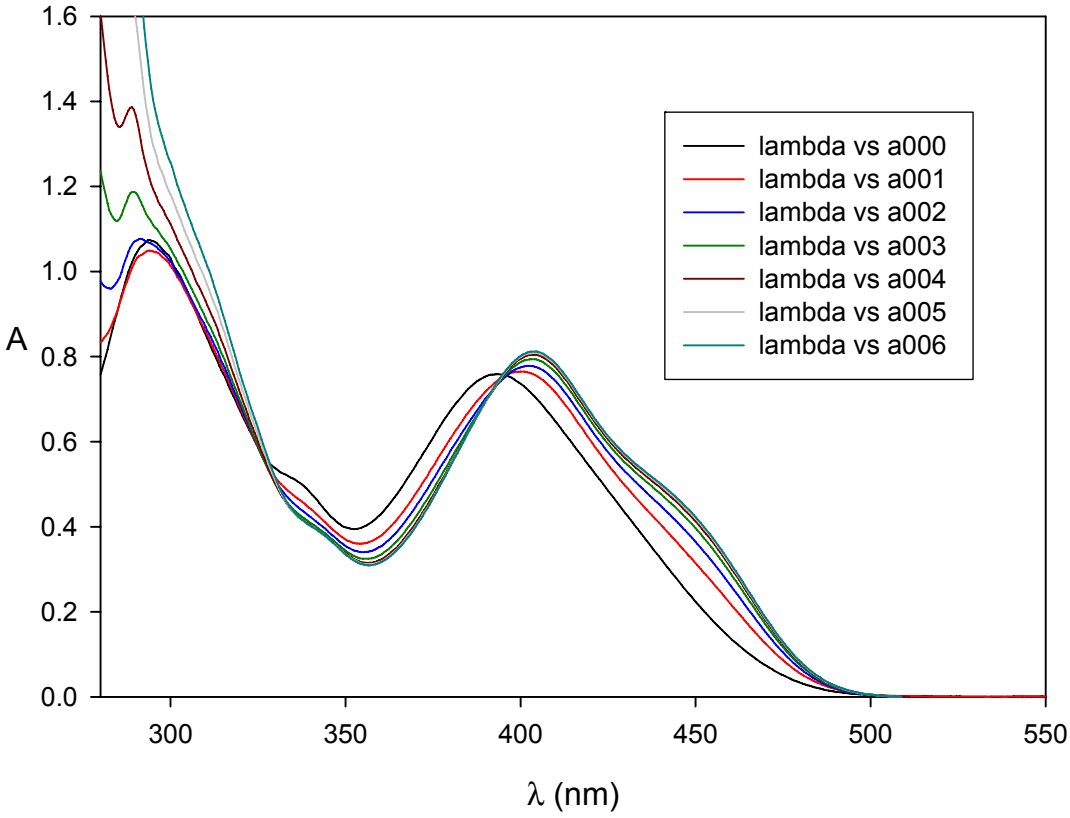
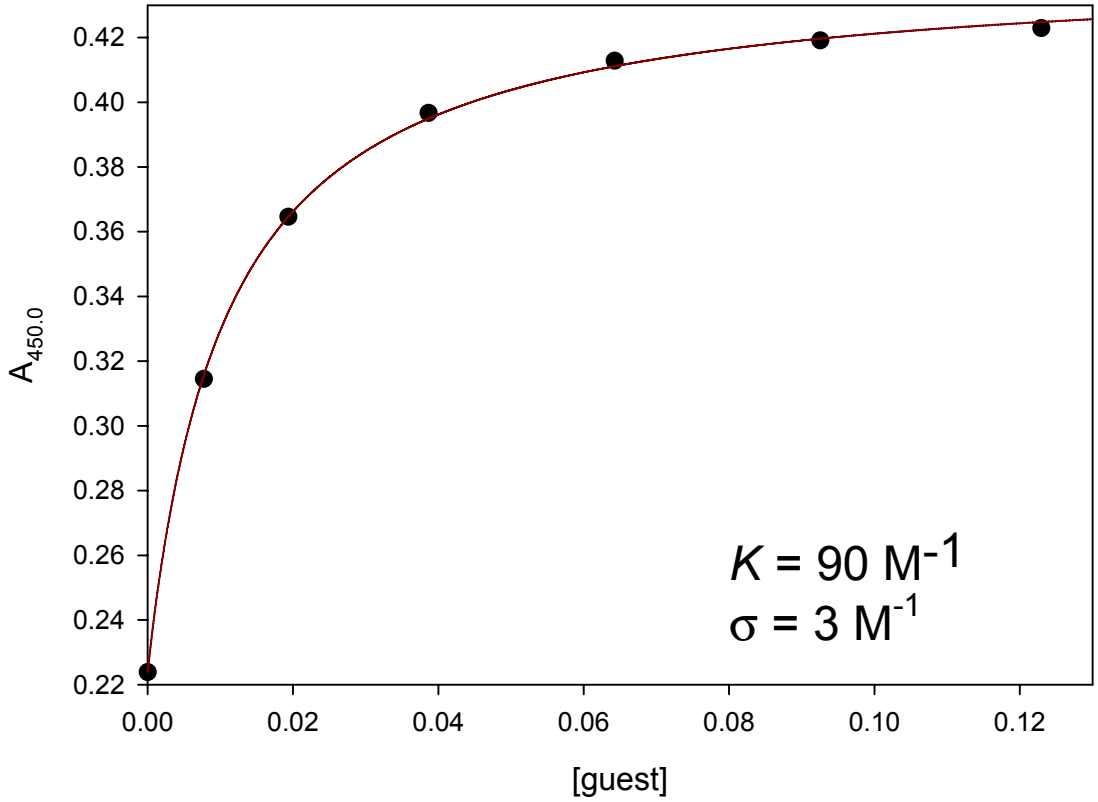
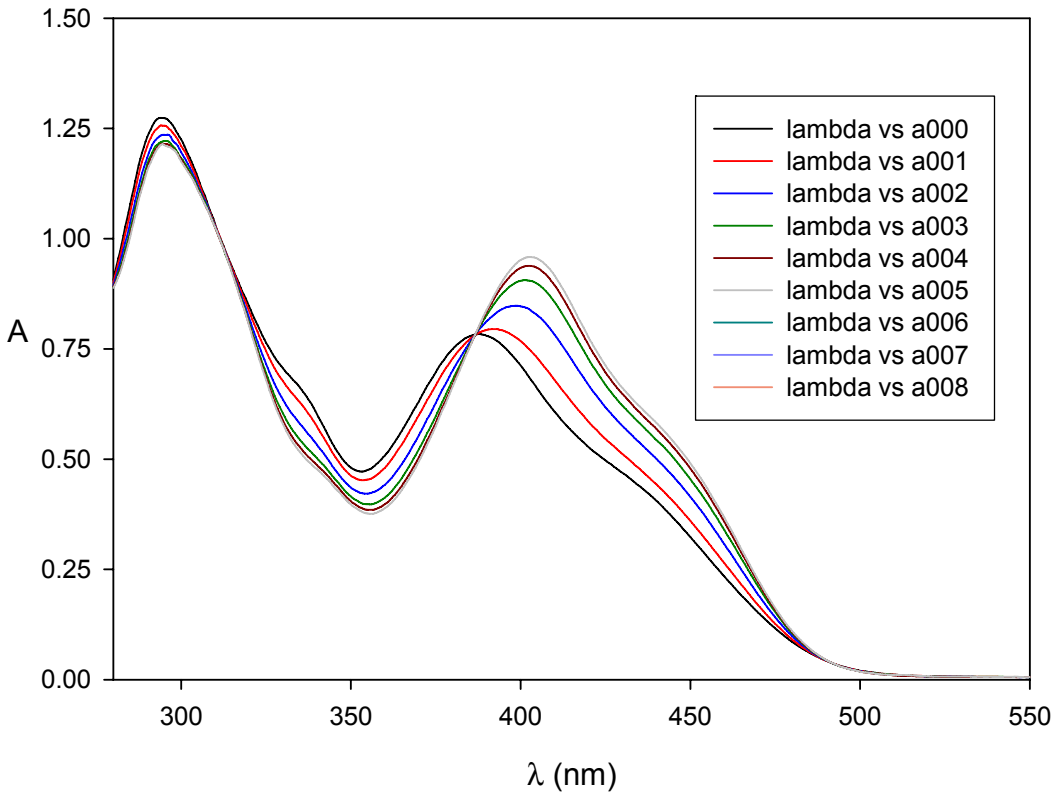
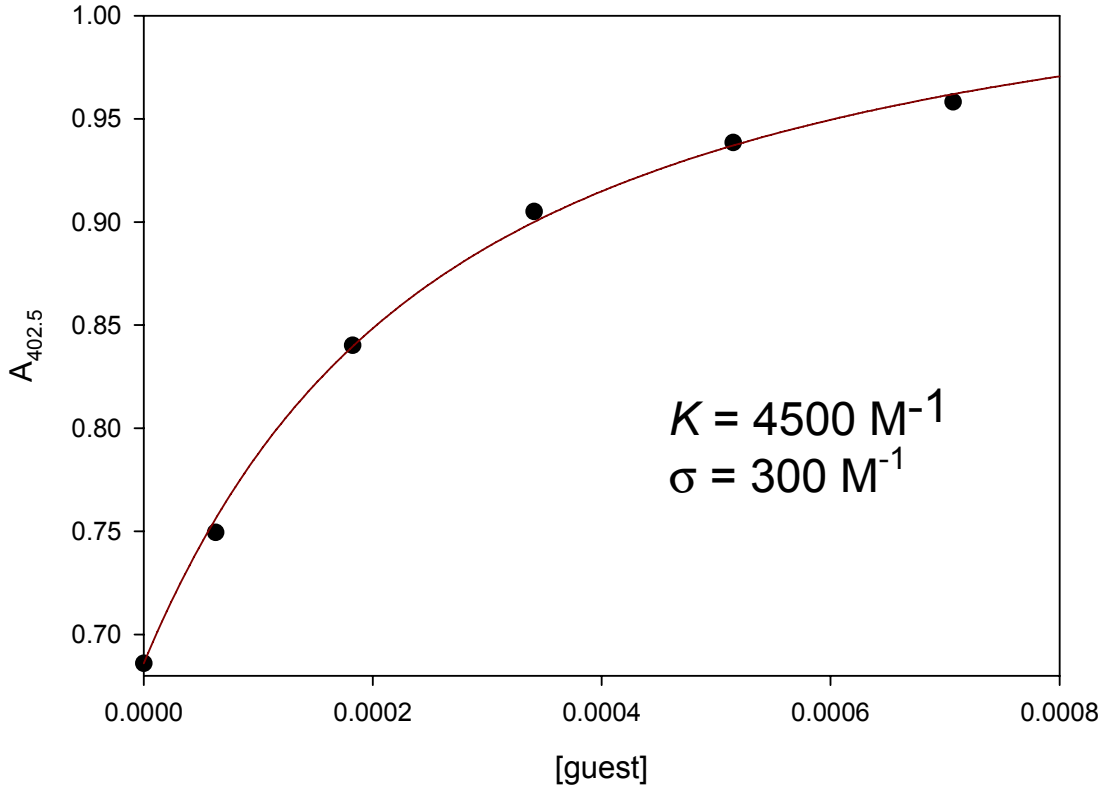
UV-vis titration of 1 with dibenzylamine



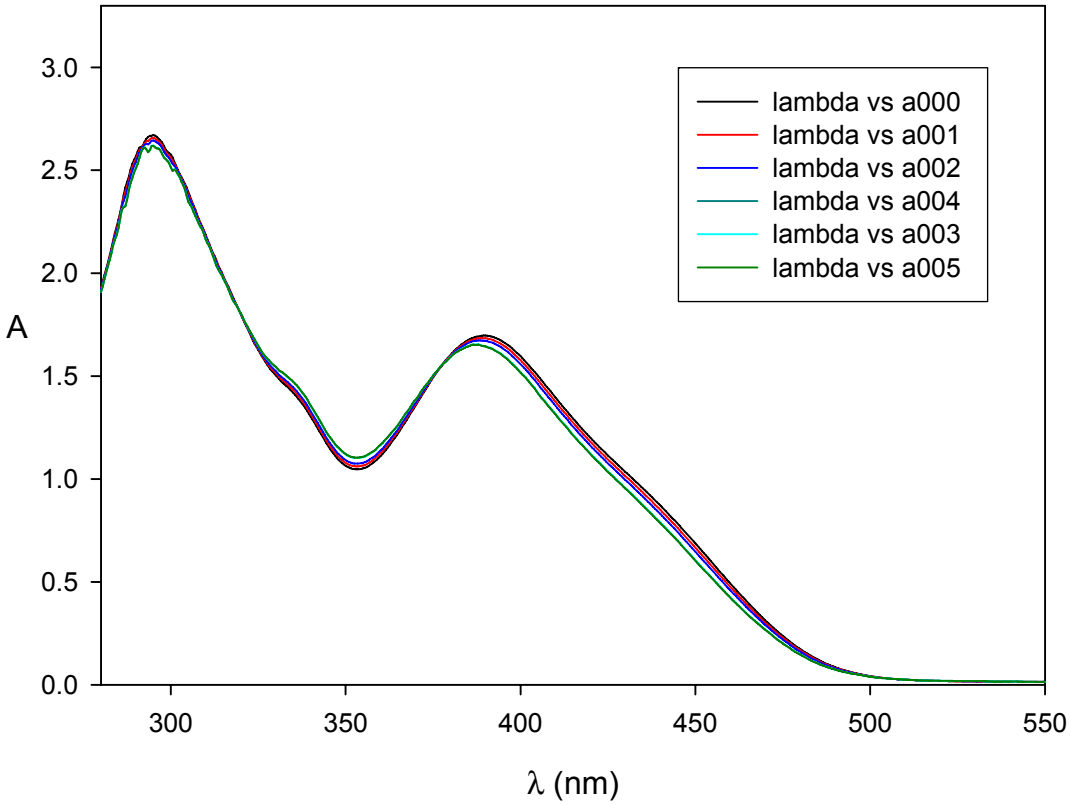

0.42
0.40
0.38
0.36
0.34
0.32
0.30
0.28
0.26
0.24
0.22
A450.0
0.00
0.02
0.04
0.06
0.08
0.10
0.12
[guest]
K = 90 M-1
σ = 3 M-1

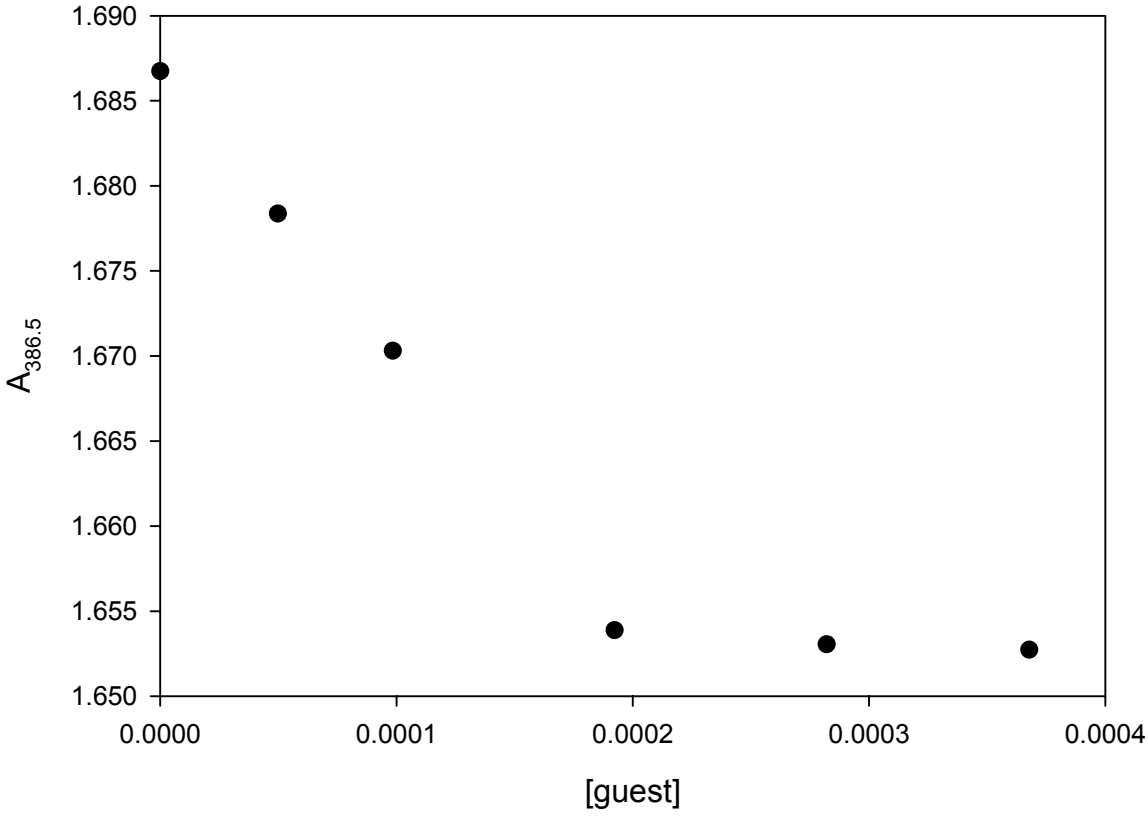
UV-vis titration of 1 with dipropylamine





UV-vis titration of 1 with dipropylammonium methanesulfonate





Calculation details

Molecular mechanics calculation were carried out utilising the force field MM3 as implemented in Macromodel Version 6.0. The parameters introduced for zinc, imine nitrogens, phenoxide oxygens, and imine hydrogens are given below. Partial atomic charges were computed using the electrostatic potential (ESP) from the wavefunction obtained by an AM1 calculation in SPARTAN Version 5.0.1, whilst charge +2 on the zinc was used for the zinc cation.

Lines added in the file atom.typ

at_typ	at_no	at_wt	name	color	vdw_rad	deloc	cat del	1-3 eqv	el_neg	wild	UA root	no_H	pdb_name	1-3 slv	fchg
204	30	65.37000	Z1	15	0.74	F	F	!	1.20	F	!	!	!	!	+2
205	8	15.99940	OZ	16	1.52	T	T	OM	3.50	F	!	!	!	!	0
206	7	14.00670	NZ	4	1.55	T	T	!	3.00	F	N2	0	!	!	0
207	1	1.00797	HI	5	1.20	F	F	!	2.00	F	!	!	!	!	0

Lines added in the file mm3.fld

Stretching Interactions

OZ - C2	1.3550	6.0000	-0.0010 0000 0000	O 3
NZ - C2	1.3300	6.3000	-1.0000 0000 0000	A 2
NZ = C2	1.3450	10.0000	-1.3000 0000 0000	O 3
C2 – HI	1.1010	5.1500	-0.6000 0000 0000	O 1

Bending Interactions

HI - C2 = NZ	120.0000	0.0200	0.3000 0000 0000 0000	O 2
C2 - C2 – HI	117.0000	0.0200	0.3000 0000 0000 0000	O 1

Torsional Interactions

C2 * C2 * C2 = NZ	0.0000	15.0000	0.0000 0000 0000 0000 0000	A 2

Benzenoid

1 OZ	1.2700	8.7800

1 NZ	1.3780	6.3200	-0.6300		
1 2 OZ	120.0000	5.0000		0000 0000 0000	
1 2 C2	126.0000	19.6000		OZ00 0000 0000	
1 2 C3	123.0000	0.9000		OZ00 0000 0000	
1 2 NZ	125.0000	10.0000		H100 0000 0000	
1 NZ C2	117.0000	3.0000			
1 C2 NZ	123.0000	3.0000			
1 C2 HI	120.0000	0.4900		0000 0000 0000	
1 2 NZ 00	0.0000	3.5000	0.0000		
1 2 NZ C2	0.0000	3.6000	2.6000	H100 0000 0000 0000	
1 2 C2 NZ	0.0000	20.0000	0.0000		
1 NZ C2 00	0.0000	65.0000	0.0000		
1 2 C2 HI	0.0000	1.6000	0.0000		

Van der Waals Interactions

Z1	2.0500	0.0500	0.0000	2.0000	0000	A 2
OZ	1.8300	0.0800	0.0000		0000	A 2
NZ	1.2600	0.0800	0.0000		0000	O 2
HI	1.5200	0.0200	-0.0770		0000	O 1

Special Van der Waals Interactions

N3 OZ	5.0000	0.1230	0000	0000	O 1
N3 NZ	5.0000	0.1230	0000	0000	O 1
N3 Z1	2.7000	0.1500	0000	0000	O 1
O3 NZ	4.8900	0.1230	0000	0000	O 1
O3 Z1	2.5900	0.1500	0000	0000	O 1
HI H1	1.8000	0.0230	0000	0000	O 1

Structure of the 1-dibenzylammonium complex in Cartesian coordinates

O	-11.71837	6.23600	-6.70005
C	-5.35625	3.99300	-5.97017
C	-6.19314	3.33127	-6.85859
C	-7.43507	3.86369	-7.14543
C	-7.82304	5.03933	-6.55775
C	-7.01100	5.70375	-5.68055
C	-5.76148	5.18029	-5.37831
O	-8.97335	5.53370	-6.81789
C	-7.33502	6.95377	-5.00278
N	-8.53034	7.55509	-5.21395
C	-8.79098	8.73683	-4.51625
C	-7.83188	9.54248	-3.91498
C	-8.22582	10.70531	-3.25353
C	-9.57425	11.05914	-3.20112
C	-10.53345	10.25077	-3.81031
C	-10.13857	9.09064	-4.46373
N	-10.99421	8.20247	-5.11957
C	-12.31604	8.28214	-4.83551
C	-13.26291	7.37165	-5.47297
C	-14.59053	7.55380	-5.10370
C	-15.57462	6.74283	-5.65474
C	-15.23696	5.75666	-6.57416
C	-13.90987	5.58453	-6.92734
C	-12.94492	6.39407	-6.37746
H	-5.87849	2.38970	-7.33697
H	-5.08649	5.69926	-4.67413
H	-6.60349	7.38696	-4.30373
H	-6.76214	9.27747	-3.95301
H	-7.47200	11.35304	-2.77120
H	-9.87733	11.98382	-2.67798
H	-11.59497	10.54512	-3.76579
H	-12.69477	9.02084	-4.11194
H	-14.87712	8.33675	-4.37818
H	-16.01592	5.11364	-7.01946
O	-4.20824	2.24922	-4.88118
C	-17.00970	6.95988	-5.25064
C	-3.99876	3.42515	-5.65763
H	-13.62963	4.80701	-7.65265
H	-8.10541	3.34820	-7.84724
H	-17.70904	6.25608	-5.74787
H	-17.32240	7.98275	-5.55246
H	-3.43620	3.21324	-6.59107
H	-3.38445	4.13908	-5.06926
C	-17.34270	5.53946	-3.33695
H	-17.61999	5.61985	-2.26292
H	-18.21083	5.07605	-3.85281
C	-3.80846	1.07289	-5.57804
C	-4.05691	-0.14961	-4.69217
H	-2.72295	1.14075	-5.81259

H	-4.35696	0.96489	-6.53796
H	-3.41772	-0.98593	-5.05095
H	-3.73388	0.06220	-3.65056
C	-16.08988	4.67942	-3.46852
H	-15.90634	4.45241	-4.53813
H	-15.22048	5.25161	-3.08225
C	-15.09879	2.64003	-2.70112
C	-14.19907	3.05935	-1.53943
H	-15.42555	1.58842	-2.54911
H	-14.55877	2.66993	-3.67025
H	-14.76866	2.95374	-0.58978
H	-13.89943	4.12451	-1.63148
C	-6.34506	0.31417	-4.15027
C	-7.66451	-0.43344	-3.94379
H	-5.94850	0.69987	-3.18862
H	-6.50202	1.18336	-4.82349
H	-8.13616	-0.61768	-4.93353
H	-7.48029	-1.43538	-3.49783
C	-12.25432	2.50066	-0.34059
H	-11.69917	3.45719	-0.45539
H	-12.91757	2.60506	0.54651
C	-8.13186	0.44233	-1.77534
C	-9.31578	0.30977	-0.82049
H	-7.64597	1.43501	-1.65306
H	-7.37813	-0.33425	-1.51868
H	-8.94769	0.37633	0.22690
H	-9.79800	-0.68494	-0.94413
C	-11.28698	1.34698	-0.08560
H	-11.83386	0.37861	-0.09574
H	-10.83485	1.46678	0.92360
O	-17.10181	6.85527	-3.83242
O	-16.26214	3.46284	-2.74239
O	-13.03406	2.23232	-1.50979
O	-10.25811	1.35121	-1.07208
O	-8.58850	0.28627	-3.12515
O	-5.41287	-0.59893	-4.72610
Zn	-10.05057	6.91735	-6.23102
H	-10.15597	-2.04025	-4.08128
C	-11.03004	-2.05671	-3.40940
C	-13.23145	-2.13630	-1.69947
C	-11.95584	-1.00997	-3.41926
C	-11.20520	-3.13807	-2.54602
C	-12.30514	-3.17782	-1.69077
C	-13.05842	-1.05413	-2.56201
C	-11.76661	0.16076	-4.35349
H	-10.47387	-3.96477	-2.53979
H	-12.44403	-4.03501	-1.00948
H	-13.80084	-0.23972	-2.55966
H	-14.10393	-2.17129	-1.02430
H	-12.75391	0.42225	-4.80147
H	-11.12171	-0.15412	-5.20729

N	-11.16515	1.33744	-3.64445
H	-10.26911	1.05834	-3.21953
C	-10.93779	2.48854	-4.58747
H	-11.86711	2.72024	-5.15850
H	-10.16711	2.22637	-5.35175
C	-10.49812	3.71965	-3.83188
C	-9.67211	5.96901	-2.39388
C	-9.15173	3.88342	-3.49776
C	-11.42928	4.68900	-3.44984
C	-11.01622	5.81145	-2.73100
C	-8.74053	5.00579	-2.77925
H	-8.40282	3.12590	-3.79140
H	-12.49663	4.56977	-3.70481
H	-11.75543	6.57136	-2.42029
H	-7.67499	5.12448	-2.51189
H	-9.34441	6.85325	-1.81847
H	-11.78033	1.62893	-2.87086

Structure of the 1-dipropylamine inner complex in Cartesian coordinates

O	-12.33583	7.43580	-8.42673
C	-5.82990	5.05616	-8.76632
C	-6.80924	4.38853	-9.48788
C	-8.11632	4.83355	-9.42891
C	-8.43192	5.93194	-8.66562
C	-7.47407	6.59994	-7.95105
C	-6.15692	6.16817	-8.00339
O	-9.64266	6.32099	-8.58557
C	-7.70067	7.77116	-7.10600
N	-8.94412	8.25258	-6.89120
C	-9.06479	9.39658	-6.10165
C	-8.01766	10.01815	-5.42371
C	-8.26650	11.15203	-4.65097
C	-9.55943	11.66310	-4.55274
C	-10.61029	11.04204	-5.22627
C	-10.36595	9.91028	-6.00115
N	-11.33198	9.19628	-6.70387
C	-12.60725	9.63266	-6.64047
C	-13.67470	8.95079	-7.37215
C	-14.95037	9.45123	-7.14072
C	-16.04250	8.87566	-7.77787
C	-15.86074	7.81289	-8.65521
C	-14.58384	7.32628	-8.87732
C	-13.50722	7.90227	-8.24060
H	-6.55522	3.50396	-10.09578
H	-5.36683	6.68873	-7.43259
H	-6.82508	8.27051	-6.66184
H	-6.99134	9.62306	-5.49183
H	-7.43979	11.64898	-4.11366
H	-9.74809	12.56102	-3.93845
H	-11.62808	11.45400	-5.13858
H	-12.86907	10.52190	-6.04497

H	-15.10990	10.29745	-6.44844
H	-16.72367	7.35346	-9.16732
O	-4.19845	4.00167	-7.49192
C	-17.41818	9.42304	-7.50461
C	-4.40189	4.58628	-8.77429
H	-14.42479	6.48232	-9.56383
H	-8.90412	4.30977	-9.98778
H	-18.21484	8.87668	-8.05106
H	-17.46537	10.47943	-7.84632
H	-4.18039	3.86269	-9.58610
H	-3.70929	5.44549	-8.90105
C	-18.13151	8.14342	-5.58464
H	-18.49989	8.31748	-4.54993
H	-19.00353	7.78586	-6.17303
C	-4.66868	2.65624	-7.42562
C	-4.95375	2.29276	-5.95512
H	-3.88743	1.98530	-7.84480
H	-5.58665	2.50773	-8.03217
H	-4.53200	1.28636	-5.74374
H	-4.43393	3.00188	-5.27616
C	-17.02194	7.09550	-5.54673
H	-16.76817	6.79260	-6.58257
H	-16.11434	7.53805	-5.08443
C	-16.48541	4.91213	-4.73681
C	-15.60077	5.07958	-3.50047
H	-17.01810	3.93811	-4.67365
H	-15.87588	4.87461	-5.66445
H	-16.20415	4.89032	-2.58594
H	-15.20133	6.11389	-3.43345
C	-6.98268	3.52997	-5.64288
C	-8.51011	3.34862	-5.76393
H	-6.70212	4.05622	-4.70743
H	-6.62340	4.16113	-6.47729
H	-8.81149	3.55398	-6.81283
H	-8.80381	2.29582	-5.56415
C	-13.85291	3.96700	-2.33971
H	-13.50424	4.93616	-1.92198
H	-14.56869	3.52604	-1.61112
C	-9.18702	3.75305	-3.53583
C	-10.40824	2.88741	-3.21265
H	-9.15115	4.61666	-2.83874
H	-8.25661	3.17519	-3.34807
H	-10.21300	2.32156	-2.27516
H	-10.59828	2.14584	-4.01804
C	-12.66846	3.01232	-2.52452
H	-12.94703	2.18216	-3.20984
H	-12.40302	2.56374	-1.54190
O	-17.65347	9.38682	-6.09838
O	-17.45916	5.95538	-4.80576
O	-14.51465	4.15817	-3.58831
O	-11.54423	3.72853	-3.03254

O	-9.22761	4.23005	-4.89070
O	-6.35729	2.24808	-5.67751
Zn	-10.84567	6.90209	-7.04816
H	-12.83428	2.45309	-8.65924
C	-13.10597	3.07566	-7.77595
H	-14.07027	3.57846	-8.01654
C	-12.00138	4.09027	-7.43821
H	-13.29787	2.37672	-6.93063
H	-11.83050	4.72774	-8.33486
H	-11.05438	3.53580	-7.24822
C	-12.35994	4.94154	-6.21780
H	-13.30324	5.49341	-6.42690
N	-11.27186	5.90961	-5.83178
H	-12.58179	4.25529	-5.37386
H	-11.99692	7.61534	-1.98242
H	-10.58573	5.23523	-5.37072
C	-11.83292	6.60029	-4.61997
H	-12.57532	7.36133	-4.94389
C	-10.75375	7.27697	-3.77333
H	-12.38940	5.89185	-3.97484
H	-10.06889	7.87417	-4.40827
H	-10.12164	6.50133	-3.28681
C	-11.34309	8.18383	-2.68177
H	-11.95441	9.00976	-3.11070
H	-10.54297	8.65891	-2.06857

Structure of the 1-dipropylamine outer complex in Cartesian coordinates

O	-12.27279	8.48745	-9.06719
C	-5.97016	5.56983	-8.79504
C	-6.85545	5.15092	-9.77839
C	-8.09651	5.75161	-9.87443
C	-8.44257	6.75160	-8.99799
C	-7.57495	7.17907	-8.02876
C	-6.32701	6.58197	-7.91620
O	-9.58091	7.32165	-9.10143
C	-7.83752	8.23663	-7.05765
N	-8.98192	8.95030	-7.10681
C	-9.17974	9.92871	-6.13853
C	-8.18593	10.46186	-5.32168
C	-8.50646	11.45967	-4.40149
C	-9.81596	11.92821	-4.30414
C	-10.81030	11.40045	-5.12671
C	-10.49462	10.39822	-6.03935
N	-11.39044	9.81744	-6.93200
C	-12.69740	9.82689	-6.59202
C	-13.71386	9.24337	-7.46701
C	-15.02092	9.38353	-7.01462
C	-16.07011	8.87733	-7.77144
C	-15.81637	8.23072	-8.97504
C	-14.50920	8.09495	-9.41118
C	-13.47523	8.59983	-8.65466

H	-6.57609	4.34733	-10.48047
H	-5.61009	6.90522	-7.13989
H	-7.08837	8.43298	-6.27462
H	-7.14658	10.10272	-5.39484
H	-7.72355	11.88459	-3.74892
H	-10.06131	12.72129	-3.57597
H	-11.84131	11.78153	-5.04997
H	-13.01817	10.28195	-5.64088
H	-15.23896	9.89930	-6.06221
H	-16.64581	7.82916	-9.58209
O	-4.49688	4.37606	-7.37659
C	-17.48263	9.04975	-7.28254
C	-4.61325	4.93248	-8.67639
H	-14.29530	7.58646	-10.36188
H	-8.80617	5.43006	-10.64917
H	-18.23001	8.58915	-7.96148
H	-17.72058	10.13487	-7.24908
H	-4.43784	4.15386	-9.44783
H	-3.82258	5.70120	-8.81208
C	-17.79359	7.10912	-5.90513
H	-18.30457	6.87519	-4.94524
H	-18.47172	6.75952	-6.71243
C	-5.36285	3.26072	-7.19112
C	-5.09737	2.70425	-5.79392
H	-5.15475	2.48230	-7.95714
H	-6.42344	3.57276	-7.29496
H	-4.02863	2.40404	-5.72958
H	-5.24448	3.49717	-5.03085
C	-16.45889	6.36876	-5.94093
H	-15.99390	6.45613	-6.94511
H	-15.76849	6.82789	-5.20272
C	-15.53389	4.19643	-5.45455
C	-14.90625	4.43504	-4.07877
H	-15.84153	3.13036	-5.53107
H	-14.80045	4.37270	-6.26996
H	-15.70713	4.47054	-3.30787
H	-14.36206	5.40317	-4.05479
C	-7.23809	1.84349	-5.11141
C	-7.96152	0.51796	-4.86983
H	-7.23073	2.45497	-4.18554
H	-7.76548	2.42282	-5.89871
H	-8.06258	-0.02194	-5.83673
H	-7.36912	-0.14412	-4.20227
C	-13.43326	3.47051	-2.48950
H	-12.72522	4.32606	-2.44637
H	-14.23395	3.65457	-1.73981
C	-9.28388	1.00184	-2.93261
C	-10.72219	0.93821	-2.41162
H	-8.84917	2.00188	-2.72385
H	-8.67135	0.24601	-2.39379
H	-10.70588	0.76526	-1.31286

H	-11.25811	0.08393	-2.88025
C	-12.71528	2.16373	-2.13838
H	-13.29866	1.29717	-2.51945
H	-12.64988	2.06525	-1.03230
O	-17.60322	8.52240	-5.96676
O	-16.70298	4.99707	-5.62678
O	-14.01099	3.36539	-3.78871
O	-11.39971	2.16174	-2.68529
O	-9.26709	0.72074	-4.33108
O	-5.89839	1.55570	-5.50878
Zn	-10.38316	9.18581	-8.95142
H	-7.08650	8.06958	-12.93776
C	-7.08043	8.81722	-12.11143
H	-6.48973	8.36934	-11.27947
C	-8.50626	9.18219	-11.66849
H	-6.51831	9.70538	-12.47805
H	-9.02983	8.25132	-11.35926
H	-9.06589	9.57561	-12.54942
C	-8.51686	10.22376	-10.54478
H	-7.82758	9.90756	-9.73117
N	-9.89581	10.43158	-9.98571
H	-8.10330	11.17138	-10.95188
H	-10.77427	14.44218	-8.92568
H	-10.42689	10.64928	-10.86525
C	-9.86543	11.79191	-9.35584
H	-9.24879	11.76201	-8.43155
C	-11.27332	12.29382	-9.02410
H	-9.38558	12.53097	-10.03342
H	-11.81388	11.56296	-8.38506
H	-11.86914	12.39063	-9.96211
C	-11.25717	13.65283	-8.30656
H	-10.70646	13.60718	-7.33956
H	-12.28860	14.00606	-8.07541