

Synthesis and characterization of group 4 metal amides with new C_2 -symmetric binaphthyldiamine-based ligands and their use as catalysts for asymmetric hydroamination/cyclization

Guofu Zi, Furen Zhang, Li Xiang, Yue Chen, Weihai Fang, and Haibin Song

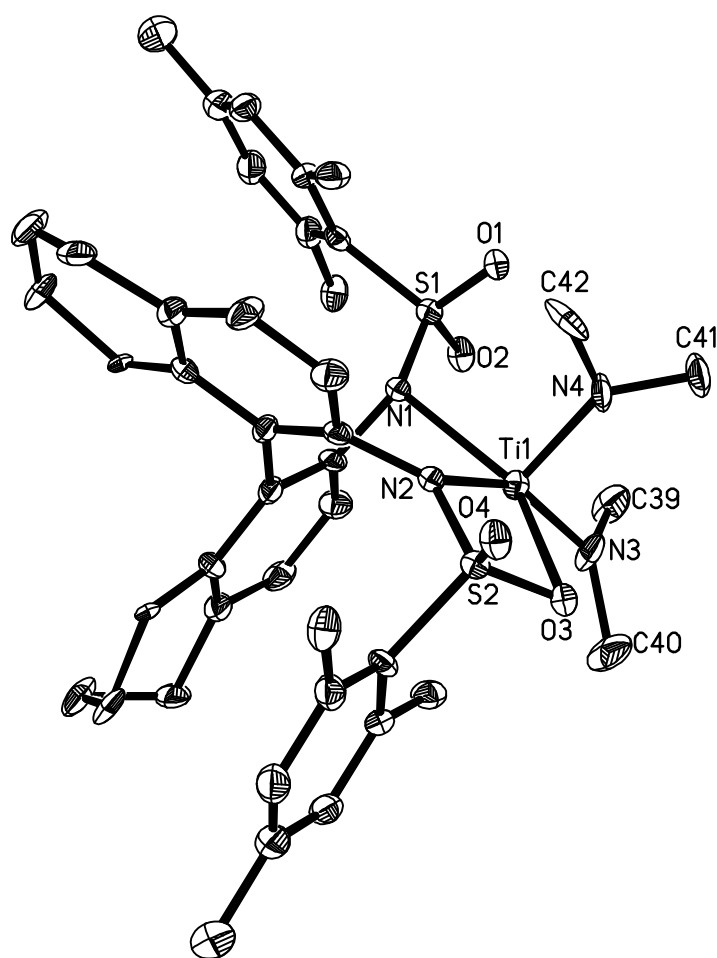


Fig. 1 Molecular structure of **15** (thermal ellipsoids drawn at the 35% probability level).

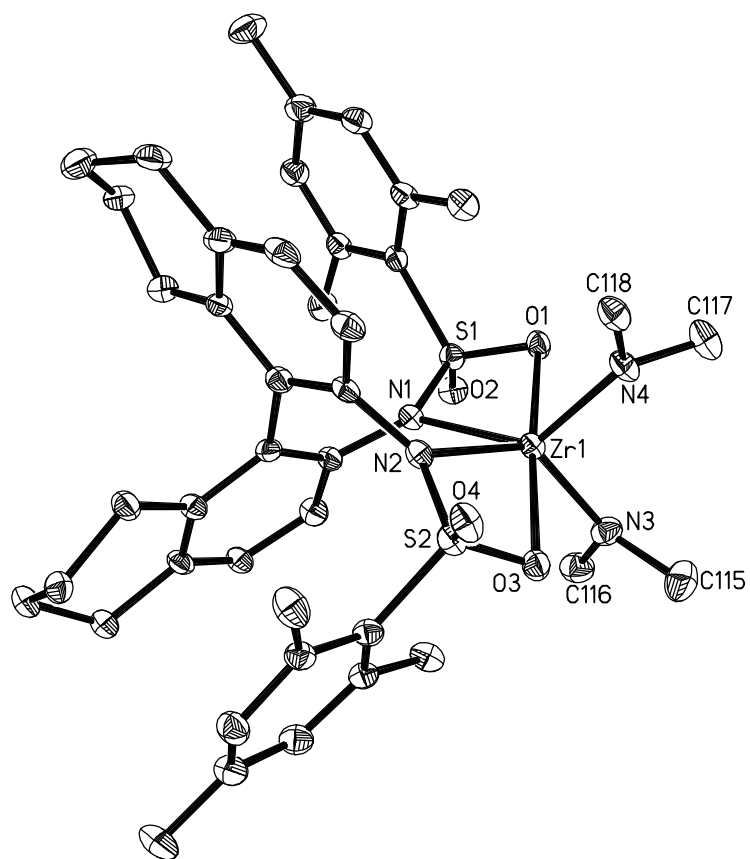


Fig. 2 Molecular structure of **16** (thermal ellipsoids drawn at the 35% probability level).

Table 1 Selected bond distances (Å) and bond angles (deg) for compounds **7-9**, **11-13** and **15-18**

compound	7 (Ti)	8 (Zr)	9 (Zr)	11 (Ti)	12 (Zr)	13 (Ti)	15 (Ti)	16 (Zr)	17 (Zr)	18 (Zr)
M-N (av.)	1.957(3)	2.130(3)	2.159(4)	2.108(3)	2.222(2)	2.061(2)	2.018(11)	2.138(4)	2.203(2)	2.271(2)
M-N (NMe ₂)	1.850(3)	2.018(3)	2.037(4)	1.902(3)	2.043(2)	1.892(2)	1.928(11)	2.015(4)		
	1.874(3)	2.021(2)	2.054(3)	1.902(3)	2.043(2)	1.893(2)	1.864(6)	2.037(4)		
M-O (av.)	2.187(2)	2.335(2)	2.269(3)			2.071(2)	2.444(7)	2.355(3)	2.312(2)	2.225(2)
M-X (av.)	Ti-S	Zr-S	Zr-P			Ti-C	Ti-S	Zr-S	Zr-S	Zr-C
	2.801(1)	2.971(1)	2.925(1)			2.562(2)	2.701(3)	2.984(2)	2.946(1)	2.662(2)
sum angles of N (NMe ₂)	360.0(3)	357.5(3)	358.7(4)	359.9(3)	360.0(2)	358.7(2)	358.6(8)	357.4(4)		
	159.5(3)	359.6(3)	359.6(4)	359.9(3)	360.0(2)	356.5(2)	359.9(7)	359.1(4)		
torsion (aryl-aryl)	62.0(3)	67.5(3)	68.7(5)	65.6(3)	72.0(2)	65.1(6)	67.3(3)	70.0(6)	69.8(6)	69.6(2)
									64.5(6)	66.4(2)

Cartesian coordinates of all stationary points optimized at B3LYP/BSI level and imaginary frequencies of transition states.

Reaction (1): (*R*)-**14** + 2,2-dimethylpent-4-enylamine

R_{fav} (1)

	Coordinates (Angstroms)		
	X	Y	Z

Zr	-0.013211	1.902814	-0.507831
O	-2.242703	2.220431	-0.575105
C	-2.575291	0.968766	-0.486161
N	-1.547007	0.139917	-0.336901
O	1.927352	1.723215	-1.721577
C	2.317381	0.670148	-1.073642
N	1.369860	0.097729	-0.348923
C	-4.035693	0.639437	-0.525268
C	-4.633374	-0.085319	0.528088
C	-4.828764	1.131660	-1.592974
C	-6.016744	-0.315462	0.488668
C	-6.197586	0.852958	-1.598199
C	-6.815430	0.133887	-0.564950
H	-6.479462	-0.864490	1.313559
H	-6.804157	1.216894	-2.432800
C	3.740339	0.220105	-1.203227
C	4.777246	1.061765	-0.742620
C	4.037567	-1.007911	-1.828898
C	6.100857	0.629507	-0.872479
C	5.380536	-1.390473	-1.952435
C	6.425523	-0.594921	-1.472087
H	6.903189	1.272543	-0.498235
H	5.613366	-2.339765	-2.443038
C	2.949971	-1.884539	-2.405168
H	2.239328	-2.222046	-1.637295
H	2.359720	-1.339836	-3.160680
H	3.380132	-2.772759	-2.890319
C	4.484313	2.410930	-0.127520
H	4.225352	3.144111	-0.908504
H	3.627701	2.377574	0.563888
H	5.358365	2.789727	0.422488
C	7.865269	-1.033922	-1.590913
H	8.311218	-1.209640	-0.596902
H	7.957987	-1.965464	-2.168562
H	8.479766	-0.264207	-2.086678
C	-3.839525	-0.614956	1.697603
H	-3.309166	-1.540519	1.421368
H	-3.076245	0.097079	2.043553
H	-4.504587	-0.848886	2.541959
C	-4.238093	1.932415	-2.731412

H	-3.924161	2.929664	-2.389690
H	-3.342631	1.449437	-3.155759
H	-4.971906	2.052671	-3.541721
C	-8.299658	-0.137940	-0.600374
H	-8.637309	-0.661736	0.305932
H	-8.875572	0.798672	-0.685810
H	-8.569544	-0.760893	-1.470153
C	-1.500549	-1.231239	-0.671716
C	-0.512268	-2.080669	-0.111024
C	-2.340486	-1.744628	-1.681592
C	0.404142	-1.663665	1.013509
C	-0.342083	-3.397855	-0.632421
C	-2.208051	-3.049218	-2.127902
H	-3.092402	-1.099267	-2.133222
C	0.294199	-2.281780	2.287464
C	1.456932	-0.746191	0.777042
C	-1.203217	-3.890211	-1.632841
H	-2.878711	-3.417447	-2.909851
C	1.290732	-2.076118	3.263591
C	2.448170	-0.560552	1.755044
C	2.374054	-1.239389	2.962880
H	3.254706	0.149434	1.575032
H	3.154618	-1.084472	3.713460
N	0.360422	2.806833	1.065508
C	0.191125	3.758717	2.117139
H	-0.854633	3.739166	2.486852
H	0.835961	3.520586	2.987444
C	0.518923	5.214196	1.652357
C	2.044035	5.425090	1.637949
H	2.438918	5.424588	2.666992
H	2.561564	4.624867	1.088436
H	2.314045	6.391763	1.178478
C	-0.117617	6.210700	2.635533
H	0.168898	7.249068	2.398392
H	-1.218234	6.149256	2.614377
H	0.210111	6.003382	3.667753
C	-0.087715	5.439352	0.242897
H	-1.179767	5.287934	0.271792
H	0.075714	6.502431	-0.023520
C	0.509840	4.627451	-0.871059
C	-0.151304	4.107297	-1.944968
H	-1.237435	4.202870	-2.040335
H	0.409731	3.733923	-2.806583
H	1.603192	4.574005	-0.890760
C	-0.936959	-3.108189	2.640670
H	-1.747154	-2.400879	2.898403
H	-1.304204	-3.659230	1.764530
C	0.779189	-4.290398	-0.108462
H	0.493625	-4.693939	0.879649
H	1.679515	-3.687052	0.079766
C	1.258134	-2.766047	4.618909
H	1.979617	-3.605903	4.598646

H	1.631738	-2.072542	5.390856
C	-0.118460	-3.309488	5.007380
H	-0.030053	-3.963684	5.890302
H	-0.784443	-2.475052	5.294604
C	-0.734272	-4.058051	3.825040
H	-1.700016	-4.510142	4.105024
H	-0.068126	-4.891117	3.531732
C	-1.055578	-5.277133	-2.238826
H	-2.056351	-5.721278	-2.375061
H	-0.636221	-5.170623	-3.257895
C	-0.155190	-6.212516	-1.430775
H	-0.682614	-6.552219	-0.520310
H	0.077490	-7.115380	-2.018843
C	1.117609	-5.468871	-1.027372
H	1.630155	-5.103680	-1.936561
H	1.824596	-6.140975	-0.514146

R_{dis} (1)

	Coordinates (Angstroms)		
	X	Y	Z
Zr	0.027106	1.867102	-0.547556
O	-2.193138	2.225225	-0.678186
C	-2.549983	0.982962	-0.557231
N	-1.537938	0.140800	-0.375774
O	1.907287	1.661226	-1.829552
C	2.321897	0.622723	-1.167940
N	1.384087	0.034231	-0.443046
C	-4.016443	0.681233	-0.597506
C	-4.636684	0.005819	0.476295
C	-4.788867	1.146113	-1.690534
C	-6.022624	-0.200884	0.431236
C	-6.163669	0.893291	-1.698973
C	-6.804180	0.227183	-0.645313
H	-6.502310	-0.715340	1.268784
H	-6.754636	1.232944	-2.554581
C	3.758635	0.219421	-1.284278
C	4.767390	1.134939	-0.908688
C	4.098292	-1.042167	-1.818658
C	6.106291	0.746980	-1.032123
C	5.452926	-1.375661	-1.943602
C	6.472247	-0.503897	-1.544537
H	6.887161	1.449110	-0.725584
H	5.716823	-2.347769	-2.369882
C	3.042512	-2.016772	-2.285334
H	2.472655	-2.431867	-1.440503
H	2.310161	-1.535870	-2.952631
H	3.500914	-2.855181	-2.829851
C	4.434818	2.512183	-0.381946
H	4.069097	3.161860	-1.192381

H	3.636308	2.483663	0.376491
H	5.321178	2.982487	0.068466
C	7.923720	-0.906681	-1.645034
H	8.265829	-1.388684	-0.711917
H	8.088288	-1.625653	-2.462184
H	8.574273	-0.035528	-1.818262
C	-3.859889	-0.496577	1.669299
H	-3.325695	-1.428725	1.423989
H	-3.101589	0.224609	2.007841
H	-4.536830	-0.708695	2.509927
C	-4.168527	1.884366	-2.855312
H	-3.825994	2.884313	-2.551019
H	-3.285852	1.356962	-3.253232
H	-4.893257	1.994255	-3.675156
C	-8.297631	0.008742	-0.663741
H	-8.595829	-0.807330	0.011497
H	-8.834291	0.917946	-0.339652
H	-8.657125	-0.234733	-1.676016
C	-1.515115	-1.240593	-0.668109
C	-0.535609	-2.089402	-0.090661
C	-2.374675	-1.771684	-1.652227
C	0.412385	-1.652294	1.000099
C	-0.402611	-3.429504	-0.563026
C	-2.275067	-3.093705	-2.052571
H	-3.116988	-1.127517	-2.120566
C	0.310315	-2.216192	2.299043
C	1.485597	-0.774887	0.707766
C	-1.285663	-3.939199	-1.535101
H	-2.960866	-3.474314	-2.815216
C	1.333079	-2.004618	3.246259
C	2.505114	-0.586121	1.655927
C	2.436399	-1.217215	2.889980
H	3.330564	0.089444	1.432722
H	3.237772	-1.059396	3.617701
N	0.457612	2.674708	1.059142
C	0.976582	3.564549	2.046486
H	0.649188	3.269713	3.064164
H	2.086747	3.535273	2.057946
C	0.531637	5.040776	1.802184
C	1.420536	5.978202	2.636103
H	1.395857	5.694253	3.701254
H	2.471282	5.939980	2.303216
H	1.080518	7.024821	2.563299
C	-0.936671	5.215308	2.231018
H	-1.329433	6.203087	1.933352
H	-1.581849	4.438120	1.795287
H	-1.024104	5.140376	3.327244
C	0.717386	5.378646	0.298243
H	0.516958	6.461663	0.176457
H	1.768101	5.222078	0.000492
C	-0.201493	4.676188	-0.659288
C	0.120673	4.176745	-1.883511

H	-1.262995	4.681006	-0.389428
H	-0.667917	3.888633	-2.586217
H	1.149233	4.180180	-2.255642
C	-0.940882	-2.984626	2.707537
H	-1.724468	-2.239239	2.939437
H	-1.336995	-3.564668	1.863283
C	0.700099	-4.330853	-0.015279
H	0.410777	-4.693722	0.987547
H	1.615871	-3.744312	0.148760
C	1.303439	-2.636373	4.629634
H	1.987968	-3.506963	4.630366
H	1.722802	-1.928103	5.363731
C	-0.086168	-3.103688	5.067699
H	-0.007523	-3.717622	5.979971
H	-0.712444	-2.229595	5.324459
C	-0.752385	-3.883117	3.933566
H	-1.728989	-4.284004	4.251216
H	-0.123337	-4.754269	3.670379
C	-1.176842	-5.350684	-2.090793
H	-2.189035	-5.776126	-2.199471
H	-0.767389	-5.290960	-3.117658
C	-0.288480	-6.276907	-1.259479
H	-0.081501	-7.204511	-1.817863
H	-0.813183	-6.573251	-0.332464
C	1.004138	-5.547741	-0.894915
H	1.515126	-5.225853	-1.821238
H	1.701524	-6.216804	-0.364784

TS_{fav} (1) 295.6539 *i*

	Coordinates (Angstroms)		
	X	Y	Z
Zr	-0.034655	1.878333	-0.592033
O	-2.264439	2.170075	-0.357101
C	-2.571608	0.912360	-0.380048
N	-1.520217	0.098236	-0.338470
O	1.913120	1.640840	-1.816569
C	2.322181	0.650336	-1.099459
N	1.368005	0.090650	-0.367219
C	-4.024351	0.553465	-0.438411
C	-4.612631	-0.232724	0.573309
C	-4.818836	1.081904	-1.486939
C	-5.990225	-0.490766	0.512416
C	-6.181282	0.774756	-1.516698
C	-6.790560	-0.007653	-0.524952
H	-6.446637	-1.088620	1.306335
H	-6.789875	1.167665	-2.336529
C	3.765454	0.251050	-1.149808
C	4.747291	1.155024	-0.689844
C	4.136190	-0.990761	-1.706558
C	6.091725	0.768620	-0.742474

C	5.495108	-1.326052	-1.753875
C	6.487664	-0.469002	-1.264585
H	6.852688	1.460886	-0.370032
H	5.784971	-2.285500	-2.191795
C	3.106322	-1.927137	-2.294089
H	2.361419	-2.241670	-1.549529
H	2.547620	-1.439196	-3.110101
H	3.584731	-2.828164	-2.704691
C	4.380482	2.525541	-0.167486
H	4.161034	3.209100	-1.003997
H	3.478010	2.510033	0.463094
H	5.206500	2.955729	0.418140
C	7.942573	-0.872211	-1.282595
H	8.242817	-1.315087	-0.316299
H	8.144830	-1.621812	-2.062711
H	8.599833	-0.006679	-1.460336
C	-3.811226	-0.800024	1.719356
H	-3.276650	-1.711514	1.407110
H	-3.051830	-0.095507	2.089070
H	-4.469956	-1.069426	2.558149
C	-4.232685	1.952263	-2.575101
H	-3.925203	2.929561	-2.174844
H	-3.331978	1.501952	-3.024175
H	-4.964727	2.114126	-3.379559
C	-8.268334	-0.308815	-0.585825
H	-8.863547	0.618402	-0.632318
H	-8.518038	-0.895741	-1.486135
H	-8.601546	-0.881756	0.291955
C	-1.461656	-1.265348	-0.704678
C	-0.471514	-2.110774	-0.142656
C	-2.289309	-1.768094	-1.727051
C	0.423334	-1.682011	0.995685
C	-0.285336	-3.419854	-0.675615
C	-2.138346	-3.065698	-2.190112
H	-3.044085	-1.121500	-2.173118
C	0.315728	-2.306848	2.266828
C	1.449144	-0.728492	0.777014
C	-1.131094	-3.903462	-1.694271
H	-2.796430	-3.430802	-2.983979
C	1.288283	-2.066729	3.259885
C	2.409592	-0.499683	1.776832
C	2.339626	-1.182485	2.982968
H	3.192329	0.239791	1.609441
H	3.099138	-0.998126	3.748340
N	0.492368	3.129643	0.759628
C	0.271608	3.938786	1.938148
H	-0.703008	3.680417	2.394763
H	1.049897	3.736145	2.697092
C	0.275279	5.448228	1.554823
C	1.707079	6.011565	1.626880
H	2.065934	6.022129	2.669350
H	2.418837	5.408405	1.042380

H	1.746719	7.047178	1.249143
C	-0.636878	6.255989	2.487054
H	-0.627280	7.326750	2.222673
H	-1.679678	5.903133	2.432572
H	-0.306003	6.171943	3.536048
C	-0.250878	5.452669	0.105572
H	-1.334621	5.247989	0.091325
H	-0.095108	6.437898	-0.369027
C	0.463347	4.399969	-0.710120
C	-0.115517	3.807124	-1.900221
H	-1.160447	4.066393	-2.113203
H	0.537459	3.726339	-2.774226
H	1.546455	4.543527	-0.769944
C	-0.888026	-3.179100	2.603274
H	-1.719875	-2.503462	2.875530
H	-1.238407	-3.724731	1.717249
C	0.832552	-4.312962	-0.146242
H	0.530978	-4.735884	0.829026
H	1.724842	-3.706915	0.069162
C	1.267959	-2.770609	4.608512
H	2.031239	-3.572583	4.590097
H	1.595958	-2.067728	5.392633
C	-0.084619	-3.386554	4.972627
H	0.027001	-4.051376	5.844833
H	-0.793076	-2.590850	5.268084
C	-0.653803	-4.141855	3.771265
H	-1.600688	-4.641833	4.033494
H	0.052309	-4.937912	3.469280
C	-0.962515	-5.279826	-2.318893
H	-1.957060	-5.730379	-2.477278
H	-0.529042	-5.152782	-3.329576
C	-0.065757	-6.220398	-1.512655
H	0.182819	-7.111707	-2.111643
H	-0.603448	-6.579021	-0.615533
C	1.195096	-5.473613	-1.078503
H	1.718468	-5.089675	-1.973585
H	1.899279	-6.148529	-0.565162

TS_{dis} (1) 302.7385 *i*

	Coordinates (Angstroms)		
	X	Y	Z
Zr	-0.217419	-1.905929	-0.590097
O	1.931701	-2.563039	-0.540866
C	2.457010	-1.380672	-0.476128
N	1.567980	-0.400460	-0.349095
O	-2.017327	-1.310219	-1.919747
C	-2.265839	-0.249383	-1.227629
N	-1.269696	0.111695	-0.429741
C	3.950369	-1.284774	-0.532348
C	4.671825	-0.700001	0.528680

C	4.634576	-1.859250	-1.632632
C	6.072977	-0.685954	0.464094
C	6.030136	-1.798186	-1.661334
C	6.771612	-1.220008	-0.620957
H	6.631131	-0.241961	1.293245
H	6.556852	-2.223312	-2.520823
C	-3.581918	0.448452	-1.388716
C	-4.777767	-0.232086	-1.068824
C	-3.622682	1.752698	-1.925661
C	-5.996574	0.434619	-1.235682
C	-4.868128	2.372556	-2.091377
C	-6.065198	1.739771	-1.739389
H	-6.921476	-0.087641	-0.973864
H	-4.900298	3.379796	-2.516418
C	-2.366569	2.464141	-2.371207
H	-1.686851	2.668829	-1.531989
H	-1.797822	1.856465	-3.093686
H	-2.611516	3.421323	-2.854083
C	-4.766048	-1.657453	-0.567604
H	-4.425179	-2.344233	-1.357537
H	-4.074398	-1.792174	0.279864
H	-5.769361	-1.966790	-0.240559
C	-7.392248	2.444505	-1.885071
H	-7.695737	2.916729	-0.933854
H	-7.347008	3.239091	-2.645185
H	-8.192806	1.743507	-2.168717
C	3.987761	-0.094441	1.730702
H	3.614382	0.917050	1.501812
H	3.122734	-0.687699	2.061823
H	4.689948	-0.008446	2.573109
C	3.898630	-2.518517	-2.776987
H	3.435504	-3.463182	-2.455499
H	3.082311	-1.885670	-3.162377
H	4.584716	-2.727996	-3.610475
C	8.279999	-1.197726	-0.673584
H	8.705244	-0.601469	0.147142
H	8.695374	-2.217410	-0.597691
H	8.641297	-0.774127	-1.625157
C	1.754559	0.970670	-0.630719
C	0.920424	1.944263	-0.025201
C	2.676482	1.382269	-1.613699
C	-0.080260	1.618043	1.056384
C	0.989516	3.299529	-0.465050
C	2.775215	2.713246	-1.985719
H	3.307964	0.640884	-2.101050
C	0.090134	2.129230	2.370057
C	-1.258446	0.896428	0.741214
C	1.932311	3.688524	-1.436912
H	3.503712	3.002609	-2.748782
C	-0.956470	2.029856	3.310506
C	-2.298047	0.818594	1.683982
C	-2.153042	1.404468	2.933988

H	-3.206031	0.267889	1.436603
H	-2.971994	1.338423	3.656140
N	-0.908457	-2.911594	0.880982
C	-1.707015	-3.420778	1.969775
H	-1.139394	-3.388346	2.918500
H	-2.592529	-2.771638	2.108695
C	-2.167190	-4.885230	1.672503
C	-3.603609	-5.124259	2.157087
H	-3.687434	-4.963823	3.245246
H	-4.313969	-4.443157	1.660305
H	-3.926370	-6.158444	1.949972
C	-1.225206	-5.885887	2.369549
H	-1.480114	-6.924817	2.100407
H	-0.170207	-5.714913	2.104829
H	-1.305608	-5.794250	3.465328
C	-2.060795	-5.008746	0.138740
H	-2.097941	-6.067302	-0.174138
H	-2.901909	-4.492015	-0.352850
C	-0.761254	-4.402614	-0.337228
C	-0.558933	-3.939372	-1.694531
H	0.127176	-4.858659	0.112660
H	0.367492	-4.260668	-2.182465
H	-1.441141	-3.900045	-2.343747
C	1.430194	2.713203	2.800862
H	2.103977	1.863298	3.017099
H	1.906727	3.253822	1.972125
C	0.037914	4.343715	0.111997
H	0.379432	4.630650	1.122816
H	-0.956664	3.898684	0.263754
C	-0.850178	2.618485	4.709267
H	-1.414146	3.571284	4.728972
H	-1.363157	1.954765	5.425265
C	0.586543	2.888297	5.161094
H	0.584479	3.485579	6.087623
H	1.091876	1.934022	5.398109
C	1.355075	3.600096	4.047213
H	2.374169	3.861662	4.376240
H	0.846881	4.551807	3.803299
C	2.037400	5.112997	-1.958888
H	3.101983	5.379850	-2.071477
H	1.613415	5.142178	-2.981094
C	1.310706	6.143613	-1.093838
H	1.248073	7.107196	-1.625375
H	1.881915	6.328009	-0.165213
C	-0.077592	5.615949	-0.734058
H	-0.638094	5.401716	-1.662721
H	-0.658793	6.371547	-0.180713

P_{fav} (1)

Coordinates (Angstroms)
X Y Z

```

-----
Zr  -0.113879  1.860128  -0.693914
O   -2.355067  1.997502  -0.529734
C   -2.578628  0.721405  -0.521880
N   -1.474256  -0.014309  -0.427566
O    1.809174  1.683537  -1.967860
C    2.304752  0.774870  -1.201518
N    1.396281  0.180391  -0.434937
C   -4.001071  0.265153  -0.612544
C   -4.569626  -0.529556   0.403992
C   -4.792916  0.710275  -1.701385
C   -5.923933  -0.881451   0.307244
C   -6.130489  0.311832  -1.763939
C   -6.719330  -0.481846  -0.768938
H   -6.366335  -1.485771   1.104136
H   -6.736213  0.640533  -2.613534
C    3.775991  0.498137  -1.235532
C    4.680681  1.524453  -0.879055
C    4.248519  -0.753395  -1.679636
C    6.051760  1.252919  -0.923925
C    5.632412  -0.971159  -1.726001
C    6.550143  0.011007  -1.341052
H    6.753014  2.040699  -0.632909
H    6.000397  -1.938589  -2.079271
C    3.301581  -1.835658  -2.141888
H    2.670462  -2.204614  -1.320389
H    2.617700  -1.465605  -2.922746
H    3.857357  -2.689881  -2.555123
C    4.200682  2.897886  -0.469422
H    3.816443  3.449521  -1.341835
H    3.372134  2.853352   0.255285
H    5.019066  3.480828  -0.022207
C    8.036892  -0.249560  -1.368999
H    8.452409  -0.289375  -0.347186
H    8.271417  -1.204760  -1.861632
H    8.574758  0.550632  -1.903417
C   -3.771598  -1.004948   1.593560
H   -3.152660  -1.876726   1.327050
H   -3.088065  -0.231283   1.973485
H   -4.439356  -1.306684   2.413893
C   -4.230097  1.588143  -2.795673
H   -3.999367  2.593769  -2.414742
H   -3.288235  1.186943  -3.205025
H   -4.945135  1.679682  -3.626013
C   -8.171756  -0.880846  -0.865604
H   -8.489940  -1.466931   0.009047
H   -8.825193  0.004756  -0.936750
H   -8.358222  -1.490050  -1.766300
C   -1.311303  -1.387250  -0.718707
C   -0.280601  -2.126265  -0.084665
C   -2.076541  -2.003827  -1.726588
C    0.563936  -1.561732   1.033027

```

C	0.000645	-3.452915	-0.524132
C	-1.828372	-3.314487	-2.103084
H	-2.860034	-1.436248	-2.227562
C	0.478729	-2.102078	2.343562
C	1.526179	-0.556600	0.759951
C	-0.785423	-4.052850	-1.528667
H	-2.437941	-3.770931	-2.888272
C	1.418584	-1.727646	3.326954
C	2.456079	-0.194877	1.749692
C	2.414694	-0.797506	2.999464
H	3.190258	0.582155	1.536395
H	3.149381	-0.511982	3.757826
N	0.395041	3.264110	0.602738
C	0.489331	3.961510	1.866354
H	0.263362	3.283944	2.704114
H	1.524209	4.334440	2.010962
C	-0.497999	5.173581	1.788244
C	0.122669	6.421340	2.433386
H	0.378227	6.238290	3.491502
H	1.046940	6.723879	1.913431
H	-0.575951	7.274062	2.403191
C	-1.823749	4.825554	2.485151
H	-2.566659	5.628740	2.342973
H	-2.253160	3.897866	2.073136
H	-1.681875	4.689030	3.571128
C	-0.718135	5.350299	0.252056
H	-1.752055	5.083981	-0.017111
H	-0.547091	6.387338	-0.078423
C	0.243018	4.386489	-0.465955
C	-0.214649	3.810869	-1.820347
H	-1.229916	4.140062	-2.087780
H	0.494594	3.999895	-2.634889
H	1.248949	4.835616	-0.563281
C	-0.673024	-3.023311	2.727644
H	-1.551655	-2.384271	2.933633
H	-0.969680	-3.654966	1.880028
C	1.155807	-4.239037	0.089229
H	0.851907	-4.620383	1.080911
H	2.001424	-3.564960	0.290423
C	1.421037	-2.334315	4.722058
H	2.227664	-3.091558	4.767188
H	1.699290	-1.560571	5.457020
C	0.099918	-2.998510	5.115607
H	0.233925	-3.585466	6.038920
H	-0.658682	-2.225400	5.336789
C	-0.401924	-3.877691	3.969473
H	-1.321410	-4.413203	4.257524
H	0.356335	-4.649558	3.740122
C	-0.514399	-5.452508	-2.058568
H	-1.474235	-5.974914	-2.209993
H	-0.063234	-5.361406	-3.065336
C	0.417960	-6.280827	-1.173644

H	0.738418	-7.189442	-1.708857
H	-0.119896	-6.617148	-0.267999
C	1.616649	-5.428369	-0.759163
H	2.138464	-5.066870	-1.664358
H	2.348028	-6.023468	-0.188331

P_{dis} (1)

Coordinates (Angstroms)			
	X	Y	Z

Zr	-0.235304	-1.898379	-0.657873
O	1.891404	-2.597059	-0.647224
C	2.445175	-1.429956	-0.546120
N	1.575056	-0.435703	-0.389756
O	-1.969216	-1.208713	-2.031771
C	-2.220927	-0.171553	-1.309220
N	-1.245617	0.125036	-0.457722
C	3.938963	-1.365118	-0.600372
C	4.673026	-0.820493	0.473678
C	4.609734	-1.928976	-1.714803
C	6.074022	-0.835608	0.408285
C	6.006201	-1.896924	-1.742617
C	6.760342	-1.359251	-0.689609
H	6.642057	-0.424134	1.247384
H	6.523423	-2.313851	-2.611752
C	-3.509677	0.569234	-1.492012
C	-4.734523	-0.092760	-1.246805
C	-3.496012	1.894612	-1.972878
C	-5.927887	0.610691	-1.435844
C	-4.719073	2.552617	-2.164055
C	-5.943796	1.936231	-1.890792
H	-6.875223	0.103200	-1.231215
H	-4.709425	3.577976	-2.544263
C	-2.205632	2.595237	-2.327236
H	-1.572343	2.762274	-1.444387
H	-1.606342	2.000342	-3.035204
H	-2.407602	3.571071	-2.792249
C	-4.774890	-1.534537	-0.798334
H	-4.420954	-2.202436	-1.598559
H	-4.117145	-1.715197	0.067163
H	-5.795855	-1.831260	-0.517806
C	-7.250441	2.668489	-2.079122
H	-7.746066	2.853087	-1.110385
H	-7.101596	3.642075	-2.568966
H	-7.953810	2.082190	-2.693016
C	4.003898	-0.229061	1.691151
H	3.661301	0.799242	1.490737
H	3.120965	-0.805473	2.004151
H	4.706024	-0.188024	2.536929
C	3.859851	-2.546074	-2.873388
H	3.369426	-3.483357	-2.571915

H	3.062235	-1.884266	-3.249351
H	4.543029	-2.757632	-3.708657
C	8.268736	-1.367824	-0.743625
H	8.707659	-0.817288	0.101434
H	8.661344	-2.398711	-0.713514
H	8.638276	-0.910975	-1.676539
C	1.789133	0.942055	-0.613198
C	0.973286	1.904649	0.033552
C	2.723762	1.375591	-1.573965
C	-0.041778	1.551205	1.093910
C	1.075542	3.277006	-0.343137
C	2.852420	2.719245	-1.886016
H	3.341369	0.642384	-2.090739
C	0.126461	2.002622	2.429611
C	-1.231820	0.866301	0.740760
C	2.029701	3.687278	-1.295111
H	3.589285	3.026583	-2.633779
C	-0.931914	1.888628	3.355426
C	-2.281836	0.769957	1.670366
C	-2.137551	1.303591	2.944010
H	-3.197335	0.246686	1.391703
H	-2.964934	1.226969	3.655313
N	-0.964142	-3.053459	0.775225
C	-1.567581	-3.444691	2.037378
H	-0.785412	-3.681033	2.784326
H	-2.156084	-2.606753	2.445708
C	-2.452961	-4.716115	1.765514
C	-3.917245	-4.478329	2.161370
H	-4.017290	-4.315032	3.248163
H	-4.333139	-3.596558	1.647394
H	-4.545038	-5.346501	1.897891
C	-1.903487	-5.924816	2.543950
H	-2.515141	-6.824000	2.360302
H	-0.866248	-6.156911	2.252197
H	-1.907273	-5.733159	3.630504
C	-2.295406	-4.930812	0.235559
H	-2.346434	-5.994854	-0.046821
H	-3.089080	-4.397833	-0.313401
C	-0.944613	-4.311458	-0.136795
C	-0.699024	-3.904614	-1.598047
H	-0.117252	-4.951036	0.223096
H	0.107266	-4.478735	-2.073634
H	-1.617601	-3.933658	-2.202348
C	1.474831	2.537352	2.896941
H	2.124839	1.663630	3.090291
H	1.974416	3.094955	2.093530
C	0.147571	4.317064	0.278431
H	0.496999	4.555966	1.299120
H	-0.856446	3.888396	0.413921
C	-0.828364	2.422529	4.776188
H	-1.372959	3.385438	4.824531
H	-1.362806	1.744158	5.462046

C	0.608470	2.645827	5.252574
H	0.607755	3.209642	6.199751
H	1.091162	1.673355	5.461068
C	1.404853	3.380339	4.173611
H	2.425464	3.607250	4.522833
H	0.920261	4.351050	3.958360
C	2.167982	5.130635	-1.753860
H	3.238638	5.378922	-1.849860
H	1.750943	5.212433	-2.776032
C	1.458800	6.139326	-0.849221
H	1.416802	7.124563	-1.341544
H	2.030849	6.275164	0.087234
C	0.059316	5.625487	-0.514006
H	-0.503970	5.462103	-1.451185
H	-0.507243	6.368827	0.070207
