

Experimental procedure

Synthesis of [Zn{MeZn}₄{HN-NMe₂}₂{O-NEt₂}₄] (1): Me₂Zn (5.00 mL of a 2.0 M solution in toluene; 10.0 mmol) was added dropwise via syringe to a stirred solution of H₂NNMe₂ (0.40 mL, 5.22 mmol) and Et₂NOH (0.50 mL, 4.87 mmol) in *n*-hexane (20 mL) at 0 °C. The reaction mixture was gradually warmed to room temperature and stirred for 6 h. The solvents were removed under reduced pressure, the resulting residue was dissolved in *n*-hexane and filtered. The clear, colourless filtrate was stored at -10 °C to afford colourless, platelike crystals.

Mp 164 °C (decomp); ¹H NMR (400 MHz, C₇D₈, 200 K): δ = -0.40 [s, 6 H, ZnCH₃], -0.27 [s, 6 H, ZnCH₃], 0.98 [t, ³J_{H,H} = 6.9 Hz, 6 H, N(CH₂CH₃)₂], 1.16 [t, ³J_{H,H} = 6.7 Hz, 6 H, N(CH₂CH₃)₂], 1.18 [t, ³J_{H,H} = 6.7 Hz, 6 H, N(CH₂CH₃)₂], 1.34 [t, ³J_{H,H} = 6.7 Hz, 6 H, N(CH₂CH₃)₂], 1.61, 1.64 [s, 2 H, N-H], 1.81 [s, 6 H, N(CH₃)₂], 2.17 [s, 6 H, N(CH₃)₂], 2.29 [q, ³J_{H,H} = 6.7 Hz, 2 H, N(CH₂CH₃)₂], 2.65 [q, ³J_{H,H} = 6.7 Hz, 2 H, N(CH₂CH₃)₂], 2.74 [q, ³J_{H,H} = 6.9 Hz, 2 H, N(CH₂CH₃)₂], 2.83 [q, ³J_{H,H} = 6.9 Hz, 2 H, N(CH₂CH₃)₂], 2.90 [q, ³J_{H,H} = 6.9 Hz, 2 H, N(CH₂CH₃)₂], 3.00 [q, ³J_{H,H} = 6.8 Hz, 2 H, N(CH₂CH₃)₂], 3.16 [q, ³J_{H,H} = 7.2 Hz, 2 H, N(CH₂CH₃)₂], 3.86 [q, ³J_{H,H} = 7.5 Hz, 2 H, N(CH₂CH₃)₂] ppm; ¹H NMR (400 MHz, C₇D₈, 250 K): δ = -0.51 [s, 6 H, ZnCH₃], -0.40 [s, 6 H, ZnCH₃], 0.96 [t, ³J_{H,H} = 6.9 Hz, 6 H, N(CH₂CH₃)₂], 1.11 [m, 12 H, N(CH₂CH₃)₂], 1.29 [t, ³J_{H,H} = 7.3 Hz, 6 H, N(CH₂CH₃)₂], 1.45 [s, 2 H, N-H], 1.94 [s, 6 H, N(CH₃)₂], 2.23 [s, 6 H, N(CH₃)₂], 2.32-2.49 [m, 4 H, N(CH₂CH₃)₂], 2.67 [q, ³J_{H,H} = 7.0 Hz, 2 H, N(CH₂CH₃)₂], 2.74-2.91 [m, 6 H, N(CH₂CH₃)₂], 3.01 [q, ³J_{H,H} = 7.0 Hz, 2 H, N(CH₂CH₃)₂], 3.81 [q, ³J_{H,H} = 7.6 Hz, 2 H, N(CH₂CH₃)₂] ppm; ¹H NMR (400 MHz, C₇D₈, 300 K): δ = -0.60 [s, 6 H, ZnCH₃], -0.50 [s, 6 H, ZnCH₃], 0.95 [t, ³J_{H,H} = 7.0 Hz, 6 H, N(CH₂CH₃)₂], 1.07 [t, ³J_{H,H} = 7.1 Hz, 12 H, N(CH₂CH₃)₂], 1.26 [t, ³J_{H,H} = 7.3 Hz, 6 H, N(CH₂CH₃)₂], 1.54 [s, 2 H, N-H], 2.04 [s, 6 H, N(CH₃)₂], 2.28 [s, 6 H, N(CH₃)₂], 2.36 [q, ³J_{H,H} = 6.8 Hz, 2 H, N(CH₂CH₃)₂], 2.65-2.91 [m, 10 H, N(CH₂CH₃)₂], 3.01 [q, ³J_{H,H} = 7.1 Hz, 2 H, N(CH₂CH₃)₂], 3.77 [q, ³J_{H,H} = 7.6 Hz, 2 H, N(CH₂CH₃)₂] ppm; ¹³C {¹H} NMR (100.6 MHz, C₇D₈, 200 K): δ = -10.59, -9.32 [ZnCH₃], 12.74, 13.75, 14.05, 14.4 [N(CH₂CH₃)₂], 52.14, 53.50

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[N(CH₃)₂], 55.04, 55.22, 56.67, 62.24 [N(CH₂CH₃)₂ ppm; ¹³C {¹H} NMR (100.6 MHz, C₇D₈, 300 K): δ = -10.77, -10.27[ZnCH₃], 12.23, 13.02, 13.72 [N(CH₂CH₃)₂], 52.61, 53.44 [N(CH₃)₂], 55.49, 55.90, 61.57 [N(CH₂CH₃)₂ ppm; elemental analysis for C₂₄H₆₆N₈O₄Zn₅ (857.78): calcd: C 33.60, H 7.76, N 13.06; found: C 33.43, H 7.73, N 12.91; EI-MS [*m/z* (%): 843 (12), [M⁺ - CH₃], 674 (100), [M⁺ - ZnONEt₂ - 2 CH₃]; IR [KBr, cm⁻¹]: 3184 (br, N-H).

Synthesis of [Zn{EtZn}₄{HN-N(CH₂)₅}₂{O-NEt₂}₄] (2): The experimental procedure was the same as for compound **1**, but Et₂Zn (5.0 mL of a 2.0 M solution in *n*-hexane; 10.0 mmol) was used instead of Me₂Zn and 1-aminopiperidine (0.54 mL, 5.00 mmol) was used instead of *N,N*-dimethylhydrazine. An *n*-hexane solution of compound **2** was stored at -10 °C for several days to afford colourless platelike crystals.

Mp 195 °C (decomp); ¹H NMR (200.1 MHz, C₆D₆, 300K): δ = 0.32-0.54 [m, 8 H, ZnCH₂CH₃], 1.02-3.70 [m, 74 H, ZnCH₂CH₃, N(CH₂CH₃)₂, N(CH₂)₅, NH, N(CH₂CH₃)₂] ppm; ¹³C {¹H} NMR (50.3 MHz, C₆D₆, 300K): δ = 2.54, 3.20, 3.73 [ZnCH₂CH₃], 11.88, 12.31, 12.83, 13.12 [ZnCH₂CH₃], 13.79, 13.89, 14.09, 14.43, 14.70, 15.28 [N(CH₂CH₃)₂], 22.83, 22.95, 23.12, 23.38, 23.97, 24.16, 24.34, 24.97, 26.44, 26.75, 61.15 [N(CH₂)₅], 53.42, 55.79, 55.89 [N(CH₃)₂], 63.25, 63.89, 64.64, 65.31, 65.66 [N(CH₂CH₃)₂] ppm; elemental analysis for C₃₄H₈₂N₈O₄Zn₅: calcd: C 41.08, H 8.31, N 11.27; found: C 40.79, H 8.04, N 11.60; IR [KBr, cm⁻¹]: 3177 (br, N-H).

Computational Details

All calculations were carried out using the Turbomole (Version 5.7) [1] program package. The four isomeric species **3**, **4a**, **4b** and **4c** were optimized at the DFT level of theory, employing Turbomoles RIDFT [2-4] program deck, which is making use of the "RI two-electron-integral" routine [5] for the approximate evaluation of two-electron integrals. All-electron SV(P) basis sets [6] for all elements including Zn were employed, since relativistic effects are expected to be small. The calculations were done with a standard grid of m3 size [7].

Both the comparison of the solid state structure of **1** and extensive test calculations up to the RI-CC2(fc)/TZVPP level of theory on the ZnONH₂⁺ cation suggest that, DFT/SV(P) with the Becke-Perdew local density functional [8] is both sufficient and efficient in the reproduction of structural features of the considered compounds.

As a starting point for the calculations on the twofold dimethylhydrazine substituted species **4a**, **4b** and **4c** one molecular subunit from the solid state structure of **1** was chosen, and two Me₂NO groups were replaced by two Me₂NNH groups. For the generation of the different steric orientations of the hydrazine group substituents **4a**, **4b** and **4c**, the N-N bonds were rotated from one starting geometry by 180°. All starting geometries lead to converging optimisations.

References

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Coordinates in Bohr Units

Compound 3

0.00071527859868	0.00329145075180	-1.99708219804109	zn
-3.08428637670607	-5.00721666698577	0.38298575014271	zn
-3.45062199749069	4.62101670971681	-0.34803590493626	zn
3.08699058437470	5.00546861033120	0.37436348915589	zn
3.45451577750036	-4.61756882968785	-0.36421563232857	zn
-6.20141374331880	-7.07713946730516	0.73597119175645	c
-5.78491750665178	-9.14048797601802	0.66822377020163	h
-7.58457058182809	-6.67060655749414	-0.80143843063379	h
-7.19056129125722	-6.71865733266240	2.56012474866606	h
-6.40248549855414	6.93709075063919	-0.69666000987749	c
-7.53156753986595	7.02188435874958	1.08012926923309	h
-7.71260539913870	6.33725450301424	-2.23452741396675	h
-5.83001689446562	8.91605774753862	-1.13684737121826	h
6.19852575021090	7.08413655234158	0.72562236502905	c
7.16810109195771	6.75819334280006	2.56632378731142	h
5.78271899996166	9.14597977688976	0.61708482657179	h
7.59762609559966	6.65054490558785	-0.78971456274229	h
6.40466107696333	-6.93423122187506	-0.72404278020201	c
7.43412353719899	-7.16099100650041	1.10015701170998	h
7.80161890401545	-6.23824238543178	-2.14015723218259	h
5.84161091869226	-8.86839941955250	-1.34083935757732	h
0.94143917789833	-3.46424272163887	-3.26183611309229	n
1.85524662230277	-3.49759437340170	-5.00469558603800	h
-1.22532696276070	-5.13597961099919	-3.43486364149981	n
-0.42761030060744	-7.74939955277289	-3.95494345584944	c
0.55417721142971	-7.89486260186371	-5.82532619782110	h
-2.10884963883323	-9.00676172429217	-3.96369524611206	h
0.89131774161463	-8.37750512123169	-2.45368700172678	h
-3.02727472921892	-4.26015076255634	-5.36107239831751	c
-3.68346213054143	-2.33909432366556	-4.84041380219082	h
-4.68829864049400	-5.54356999644635	-5.40755995713726	h
-2.13825320845035	-4.21485132256616	-7.28298446240723	h
-3.09541479716106	-1.13377611750694	-0.20656646646227	o
-4.68056003229304	0.77893607662609	0.84897295230253	n
-7.27096399218837	0.32821893374706	-0.04793897961938	c
-7.30534190030493	0.48432371132728	-2.13831315477877	h
-8.53713119305635	1.79702097749261	0.75337335705676	h
-7.93660020994013	-1.59226417463360	0.51672580583286	h
-4.52226518849602	0.61498426787084	3.61561555486100	c
-5.67105307123793	2.15499808638210	4.46225023207429	h
-5.20922701420424	-1.26102872336671	4.29925339777729	h
-2.52376862382989	0.89225026874049	4.16688051304601	h
-0.40553323592633	5.07793781730692	1.92334157520989	o
-1.01296975187421	6.41533848285519	4.21464289416143	n
-0.75151543229408	9.11352336168549	3.75502822343002	c
-1.22775149563633	10.15820115401164	5.51676114955823	h
1.21039271584949	9.65508334640490	3.14409869092500	h
-2.11471082806534	9.69342602832410	2.26737993608450	h
0.67835807591352	5.53490431534712	6.18569843146155	c
0.39598089170031	3.47744335673258	6.48820893294154	h
0.22622873410172	6.53773664142582	7.97713829819803	h
2.72808683162275	5.87000655785604	5.71946614878267	h
3.12675030888776	1.13642364427172	-0.25379653653584	o
4.67009098325179	-0.77939540840068	0.85871390780493	n
4.42994985110969	-0.60544024911643	3.61892052871818	c
5.53713851100326	-2.15415329987679	4.50412514557091	h
2.41336167296568	-0.86352715337820	4.10972206289677	h
5.11305071082006	1.26639443475934	4.31761021197137	h
7.28761820804870	-0.34034696761707	0.03805873558857	c
7.38341366183427	-0.50175915025297	-2.04981114165806	h

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8.52359364878628	-1.81116508408963	0.88132547476212	h
7.94206979393490	1.57936536014664	0.61806039260751	h
0.41484031291166	-5.09732668650748	1.91089256684763	o
1.02865045392286	-6.41866183325913	4.20912119252171	n
0.80860023395702	-9.12144082991025	3.75413058828636	c
1.29083868176812	-10.15547325524724	5.52055050820098	h
2.18712789679192	-9.68444190576431	2.27416483546711	h
-1.14241983695562	-9.69228004716147	3.13445047758474	h
-0.68606295809328	-5.55806946353365	6.16882996628543	c
-0.43601270614758	-3.49577781129280	6.46690398231550	h
-0.22858729208782	-6.54884518689360	7.96563607184089	h
-2.72805346205155	-5.92525996192421	5.69286715500837	h
-0.95021674139828	3.46833711673006	-3.25796528039936	n
-1.87024782119157	3.50303152585965	-4.99752911148537	h
1.21468759317869	5.14219403917231	-3.43702198626128	n
3.01258332795775	4.26947923984068	-5.36919314260600	c
3.67584597874354	2.35077927621354	-4.84907077327171	h
4.67006258873848	5.55725013803033	-5.42116280104173	h
2.11704282406828	4.22233185517885	-7.28802461290408	h
0.41149943681942	7.75434045691955	-3.95466521254009	c
2.09033837986920	9.01486511352060	-3.96610484870106	h
-0.90646666478318	8.37976283571445	-2.45131363376842	h
-0.57394142790953	7.89844942254091	-5.82323478672521	h

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Compound 4a

6.17589894596235	7.12117539714370	-0.92741697041344	c
3.34600082672494	4.77624571589879	-0.11277477207732	zn
4.90920216180007	0.92363039829060	0.59622923637290	n
3.01418858741512	-0.98435247042298	0.26072627579638	o
3.13557694645426	-5.01089854778502	0.34689177343796	zn
6.34494508411011	-6.96542069196576	0.24348037880003	c
0.00002112066746	-0.00001589486029	-1.70574542641142	zn
-3.34595377388397	-4.77617092974332	-0.11307894983240	zn
-4.90931538077243	-0.92362661679551	0.59591337600185	n
-5.79511398765820	-0.75703094615567	3.22377503393204	c
1.03453270057370	3.30628611803166	-3.14794219423636	o
-1.17285062615132	4.91094094680953	-3.42451110801964	n
-0.27459917064850	7.45133110291513	-4.09545940854966	c
-3.13559704812471	5.01091660216050	0.34685157192325	zn
-6.34487186216104	6.96560808720785	0.24341624628200	c
-3.01423541521886	0.98436128194109	0.26059060484945	o
-1.03432367327500	-3.30620554780426	-3.14820805166548	o
1.17307526465067	-4.91083308710948	-3.42457524317363	n
0.27467257839703	-7.45119055070891	-4.09552698544210	c
-2.70620725364676	3.86499241357962	-5.48289220627077	c
0.26395156054250	4.78088819413766	2.24821518058279	n
0.67940218145480	6.26948607042881	4.53739445445947	n
-1.36427765530675	5.85685793266391	6.33017597746569	c
0.89351254003693	8.91758996095195	3.85274053942345	c
6.98115649589979	0.44995421767055	-1.19468132282863	c
5.79538184282818	0.75643068151188	3.22391293845074	c
2.70669480050046	-3.86458328197257	-5.48264103943309	c
-0.26410505235142	-4.78111317169786	2.24808497881317	n
-0.67975925287689	-6.26963751479956	4.53729575659495	n
1.36385548846319	-5.85715272389748	6.33018391770745	c
-6.17551828036518	-7.12147778114768	-0.92772095368325	c
-0.89408366285950	-8.91774865230972	3.85270136957104	c
-6.98146029300700	-0.44951981885260	-1.19463615863976	c
7.68606322970026	7.07344955733436	0.54251216655789	h
5.57020899249993	9.13131768788267	-1.09340791464207	h
7.07628268329947	6.60985469993512	-2.76232784200655	h
-7.55748232069783	6.58520091336476	1.92232997674233	h
-7.50403480553078	6.53636727284340	-1.46385176607566	h
-5.97119283933286	9.03867600827618	0.22838241695495	h
-1.61542392627518	3.79948226555959	-7.28818898467619	h
-4.42326156534496	5.04898946070914	-5.72198976633543	h
-3.30837823666422	1.92148027909836	-4.97583032367810	h
0.88894837419713	7.40279488268423	-5.85476355202415	h
0.89953187271000	8.21238302658166	-2.53378514439302	h
-1.93934115854402	8.70151602636431	-4.36281379324422	h
2.53101789730248	9.18062982682579	2.56414411899288	h
1.22394192023162	10.05786430990861	5.58486947581306	h
-0.85467925973874	9.65736133521142	2.88234115668022	h
-1.42400017548254	3.82964010674212	6.89053974026341	h
-3.27193877031245	6.37733656249318	5.53892742570426	h
-1.01706820530255	6.99320965297519	8.06409631698306	h
7.76484564953062	-1.49246247320125	-0.94247114990847	h
8.48584127993353	1.87988146750002	-0.88812167500191	h
6.25822188635876	0.67000272207423	-3.14997405088873	h
6.58727887088681	-1.15650195147322	3.63365784272338	h
4.18793312939844	1.13612057946112	4.51342515367966	h
7.26601263677612	2.22073683002106	3.54018366782794	h
-7.68617272758350	-7.07319906978495	0.54168581177617	h
-5.56972972969296	-9.13166905442700	-1.09275631310750	h
-7.07529266260039	-6.61086927342505	-2.76312987591034	h
7.557470271109386	-6.58504989641780	1.92246139173699	h
7.50415090035002	-6.53602690184682	-1.46371833727777	h

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5.97132426360984	-9.03849765113061	0.22830701904582	h
1.61612865547954	-3.79873286451074	-7.28805099787228	h
4.42384665273634	-5.04841867120180	-5.72167492282937	h
3.30872134245015	-1.92109799656999	-4.97518019056511	h
-0.88866215047337	-7.40262718299781	-5.85496775558838	h
-0.89968568145439	-8.21210702669237	-2.53394585502554	h
1.93933944514906	-8.70151585161694	-4.36265798781493	h
-2.53153288247006	-9.18062003241779	2.56399654006976	h
-1.22472049254892	-10.05791440245524	5.58486156633911	h
0.85408878263940	-9.65771634942571	2.88241655878267	h
1.42372517916760	-3.82993214656783	6.89051913491233	h
3.27151431552602	-6.37781181913204	5.53905501112517	h
1.01645547501300	-6.99345418817882	8.06409898483438	h
-7.76546428264796	1.49273401806375	-0.94212099833922	h
-8.48598900143326	-1.87960814110965	-0.88806551942622	h
-6.25853159409892	-0.66889656110699	-3.14999757430708	h
-6.58679950390600	1.15585737693758	3.63412288929100	h
-4.18754299602191	-1.13720794690108	4.51299076381537	h
-7.26581275022737	-2.22130691102888	3.53987051569646	h
0.21427623874632	2.92952154089838	2.88355617759796	h
-0.21440646236778	-2.92969321781066	2.88329384080694	h

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Compound **4b**

6.06860800339239	7.24968211465072	-1.20922399072520	c
3.25628113568806	4.88505032059133	-0.32050533711186	zn
4.83028320595088	1.06246480288414	0.48027475092363	n
3.08379055701863	-0.90753944300672	-0.13230341294932	o
3.18657277231694	-4.91326132403935	0.12779796419636	zn
6.39784014220770	-6.85346647909844	-0.10220054757486	c
-0.08839048606298	0.10538935963756	-1.73093367749951	zn
-3.29073099807717	-4.73100495047300	-0.07169284854402	zn
-4.88086999985823	-0.90388303421528	0.74250216026400	n
-5.72724227777506	-0.81342578382714	3.38509830977289	c
0.81539006696118	3.44338915513501	-3.21527812728189	o
-1.42768615421965	5.01020584127553	-3.37065414168053	n
-0.61143968911940	7.57655994399588	-4.05434566392215	c
-3.22317137773018	4.93185487456135	0.45691426140827	zn
-6.46288502202851	6.83903284938967	0.70026297762059	c
-2.98847466246198	1.01121149689761	0.42128542486145	o
-1.14640830030338	-3.19821156993647	-3.18302848656838	o
1.07212301502730	-4.76969245157029	-3.56022990700359	n
0.17889976848925	-7.30223267067436	-4.26489566074225	c
-3.02492668129917	3.96242614230141	-5.38153795538317	c
0.26769407897911	5.70561366373263	2.08467649481891	n
0.68910066418682	4.93507378566508	4.67469553756056	n
-1.60249863976332	5.13775668949623	6.18799219613410	c
2.72844321782251	6.40961685564674	5.78629530995214	c
7.09363267698267	0.70588795373944	-1.10094106452090	c
5.43456051062480	0.80778080023736	3.18336496379722	c
2.54095761499639	-3.65831763565281	-5.63237426001092	c
-0.12778539896720	-4.69168742468721	2.17516853174075	n
-0.44915360366262	-6.18507879882998	4.47753001588481	n
1.64966928746798	-5.74594684338946	6.19934669949866	c
-6.13102826742767	-7.09949839175351	-0.77701403486221	c
-0.65359310443194	-8.83555680156116	3.79996890225854	c
-6.98438228767788	-0.41066488019188	-1.00436830339107	c
7.65076047689092	7.17299110116303	0.18258002997866	h
5.42905572761806	9.25673416423261	-1.26493561485322	h
6.89258086168106	6.82077625600777	-3.09975489170049	h
-7.56193503231455	6.33395157241996	2.42453848563632	h
-7.72794892886810	6.50151712688821	-0.95079118386395	h
-6.12271999004512	8.91645334074531	0.79251386679380	h
-2.00177054155077	3.94027142966139	-7.22626565118505	h
-4.77133089473473	5.11681277612232	-5.53611383200644	h
-3.56808672329753	2.00051101124710	-4.88002820901640	h
0.42836315673376	7.57562084144355	-5.88976933782750	h
0.66629910728140	8.33058259107447	-2.57221846354196	h
-2.30701837627836	8.80711629933233	-4.18561220050869	h
4.47281363607170	6.20607854028945	4.63425067008852	h
3.12586121494614	5.74367495668235	7.74000866366191	h
2.26415934980362	8.49033489568371	5.87919796009466	h
-3.09844155121313	3.91924791933506	5.36371056174372	h
-2.34872814943184	7.12924569181025	6.29110716028940	h
-1.21656012629398	4.47513638976198	8.14625126320452	h
7.92267524856526	-1.20819824486290	-0.78740766771116	h
8.49859762389113	2.19144093362268	-0.63300294278012	h
6.55412888356484	0.91328136204937	-3.11528830997374	h
6.19801419846285	-1.11665694215780	3.59317442689051	h
3.68223762711148	1.15820103016900	4.28131398943181	h
6.87062746686047	2.25031871612684	3.69919505872014	h
-7.54984721205472	-7.11334628571455	0.78207181460343	h
-5.50460889220686	-9.09450289161501	-1.02738965309551	h
-7.14840939457195	-6.56234749745303	-2.54197385122948	h
7.65734820057413	-6.48768402294038	1.54540645478706	h
7.50015605530732	-6.38130425230326	-1.83559030564546	h

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6.04454192717244	-8.92979425603021	-0.14075881979796	h
1.39672864461247	-3.54686712283303	-7.40207486632682	h
4.25099615470239	-4.83279788281575	-5.95585343513505	h
3.15902460524006	-1.73274026255777	-5.07933558479709	h
-1.03091819419364	-7.22624921526801	-5.99190129839954	h
-0.94708071331526	-8.10826504177725	-2.69013949974514	h
1.84672268511234	-8.53096547296823	-4.60295810724457	h
-2.33200332727213	-9.12033257097625	2.56951308830512	h
-0.90772621534460	-9.98076893294450	5.54161463233963	h
1.06777901401919	-9.55406595691078	2.76773260047975	h
1.70302464311749	-3.71759367280460	6.75457796695817	h
3.53502795042148	-6.24576358662445	5.34328670047323	h
1.37561636227063	-6.88469110437220	7.94475140069877	h
-7.77806215498591	1.52116046931265	-0.70506708858520	h
-8.47374885541594	-1.85543280810190	-0.69376705282357	h
-6.29738284821001	-0.59740202475031	-2.97605828362859	h
-6.58154517301757	1.06154585756394	3.84335873262773	h
-4.08665326441468	-1.16285945507659	4.63928953271269	h
-7.14346541517048	-2.33219381289596	3.69264470227940	h
0.18518864843703	7.68911303822402	2.10848263367880	h
-0.08595765289026	-2.83861259695340	2.80751248308363	h

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Compound 4c

6.07103073650424	7.15909224016117	-1.19759153855540	c
3.19517786214542	4.86955703304115	-0.31578697661632	zn
4.75565010787458	1.06872573005577	0.74210855990512	n
3.04570480266688	-0.94894969553337	0.17012364513597	o
3.30565767245579	-4.86222880890349	0.22423886541293	zn
6.59150640781288	-6.70186385220727	0.32148353938085	c
-0.00013671280638	0.00029227135934	-1.66074121125789	zn
-3.19527052576635	-4.86911135465053	-0.31622697902435	zn
-4.75564741518065	-1.06860026214123	0.74216933111688	n
-5.23846617812347	-0.99570636498952	3.47820028809604	c
0.90426554260735	3.29803829166660	-3.24095077548549	o
-1.36957976979030	4.80211752726789	-3.53143378885817	n
-0.58529465587259	7.34246329674206	-4.33756202546671	c
-3.30559345176207	4.86268813947861	0.22485418227000	zn
-6.59144931558030	6.70226266428629	0.32317842487569	c
-3.04586882139940	0.94931893413942	0.17041263916895	o
-0.90468294071189	-3.29735361670084	-3.24119104050599	o
1.36920517955022	-4.80135741592865	-3.53208094039259	n
0.58498120917391	-7.34159970527952	-4.33863522005619	c
-2.90537740860708	3.60741393118764	-5.50935390027889	c
0.11667561121902	5.80142809241452	1.92193666551926	n
0.45389416537120	5.22774436885554	4.57287426914120	n
-1.88626180427843	5.53154424947043	5.99057012291264	c
2.45104779364767	6.78723679024538	5.64290129427225	c
7.09216593718255	0.65697598735628	-0.71104908611580	c
5.23901788210595	0.99501237715545	3.47803204586569	c
2.90486661838991	-3.60629659559690	-5.50988484344493	c
-0.11654510876546	-5.80106893266991	1.92120464714543	n
-0.45352318763883	-5.22986833838136	4.57272284722287	n
1.88701154838496	-5.53487235964556	5.98957147304230	c
-6.07097498098308	-7.15903166771555	-1.19754889446077	c
-2.45023805881985	-6.79092633806853	5.64131500180386	c
-7.09245493886399	-0.65683438017999	-0.71046438038881	c
7.59567820869996	7.14253420191003	0.25908396549467	h
5.45120715123957	9.16503575687180	-1.37804076876223	h
6.96517741277186	6.63086714615270	-3.03019414553672	h
-7.72955242954093	6.20496381442292	2.02427276601310	h
-7.79365107466607	6.29433741221353	-1.35811003244239	h
-6.30473563523728	8.78868729240393	0.38106969265702	h
-1.83960060612857	3.48708675423352	-7.32598023618778	h
-4.66050890581549	4.72842635678208	-5.77509505858924	h
-3.43940503822748	1.67616349440347	-4.89233877092293	h
0.49476499757575	7.26137931577700	-6.14787359599186	h
0.64566910626033	8.19843999210093	-2.87095859723874	h
-2.29836266470546	8.53309844626278	-4.57127569824252	h
4.23304390963552	6.51354092215320	4.56546107047191	h
2.78700934222053	6.25994435706781	7.64982564956194	h
1.97804766759937	8.86704127798538	5.57450791489973	h
-3.35615107235599	4.25655887853883	5.20569010887535	h
-2.63522079623721	7.52458560893470	5.92873649729543	h
-1.56648087996730	5.00737833449440	8.00171306068944	h
7.93181392819733	-1.22321191209661	-0.25322285273457	h
8.45378462188717	2.18733678213098	-0.26145817435388	h
6.64992611803611	0.74677962432844	-2.75740919081404	h
6.06177566079510	-0.86612847023861	4.03799520124877	h
3.42685951481937	1.33492787700488	4.47582445372273	h
6.59419498606680	2.52362758946265	3.96371832736983	h
-7.59510050209490	-7.14300156412329	0.25968153302712	h
-5.45084155669186	-9.16483353676470	-1.37850941178549	h
-6.96589421791003	-6.63072267454410	-3.02974141968250	h
7.72994528816232	-6.20510264528954	2.02250122251049	h
7.79327712512090	-6.29320351664084	-1.35993693871996	h

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6.30493950841835	-8.78832654441609	0.37863677112404	h
1.83895564212153	-3.48557043204710	-7.32639599991753	h
4.65996074927418	-4.72728220544141	-5.77601346641289	h
3.43901287583447	-1.67518734541919	-4.89251575890224	h
-0.49521902735653	-7.26022270743749	-6.14884761469734	h
-0.64583930651122	-8.19793640764091	-2.87211683478533	h
2.29808769851902	-8.53211729105249	-4.57269588444906	h
-4.23271168759688	-6.51556320600767	4.56510691333751	h
-2.78527202754115	-6.26680014936861	7.64921395049730	h
-1.97719762682346	-8.87059112684335	5.56941836299891	h
3.35618604907285	-4.25785494109720	5.20662471218286	h
2.63683682200911	-7.52746501235724	5.92422052715151	h
1.56730214344033	-5.01432868968623	8.00166376475804	h
-7.93266607598111	1.22301545414330	-0.25247314844850	h
-8.45332772334329	-2.18805523325206	-0.26140534277033	h
-6.65052118049387	-0.74708498723847	-2.75688690526465	h
-6.06146031802643	0.86492132125197	4.03934324172584	h
-3.42615975547394	-1.33631498739675	4.47557380426601	h
-6.59271769557540	-2.52524941265532	3.96365286074880	h
-0.00027580724761	7.78053684366091	1.79855195279084	h
0.00031964582812	-7.78009139430137	1.79604742966096	h