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Supporting Information

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Supporting Information

Configurationally Labile Lithiated *O*-Benzyl Carbamates - Their Application in Asymmetric Synthesis and Quantum Chemical Investigations on the Equilibrium of Diastereomers

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X-ray crystal structure analysis

Computational Details and Results:

DFT-calculations of the epimeric lithium complexes of the phenylmethyl carbamate 13 and the 1-naphthylmethyl carbamate 19:

If not stated otherwise for all calculations the TURBOMOLE 5.9 suite of programs¹ was used. The structures of the complexes were optimized at DFT level employing the B97-D functional² including an empirical dispersion correction (DFT-D) using a Gaussian AO basis set of triple-zeta quality with polarisation functions on all atoms (TZVP)³ and numerical quadrature multiple grid ("grid m4" option in TURBOMOLE)⁴. The resolution of the identity (RI) approximation was applied for all DFT calculations.⁵ Single point energy calculations were performed with SCS-MP2⁶ using the TZVPP basis set and also employing the RI-approximation.⁷ For comparison single point calculations at the DFT level employing the functionals B3-LYP⁸ and PBE⁹ were performed. Solvent effects (SCS-MP2-level) were simulated using COSMO ($\epsilon(\text{toluene}) = 2.355$).¹⁰ Additional computations using the PCM-model¹¹ for solvent effects were carried out using PBE/6-311G* and Gaussian03¹². The ZPVE contributions were determined at the B97-D level using a split valence basis set (SV(P))¹³ in the harmonic approximation (unscaled) as numerical derivatives of analytically calculated nuclear gradients employing the SNF program.¹⁴

¹ TURBOMOLE V5.9: R. Ahlrichs et al., University of Karlsruhe, Germany, **2006**; see: <http://www.turbomole.com>.

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¹⁰ A. Klamt, G. Schüürmann, *J. Chem. Soc. Perkin Trans. 2* **1993**, 5, 799.

¹¹ B. Barone, M. Cossi, J. Tomasi, *J. Comput. Chem.* **1998**, 19, 404.

¹² Gaussian 03, Revision C.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, **2004**.

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Favoured complexes:

pro-*R* – pro-*S*, in case of (–)-sparteine (**11**) difference between the two epimers of the favoured pair of diastereomers:

ligand	substrate	complex	experiment	B97-D/ TZVP	SCS-MP2/ TZVPP	SCS-MP2/ TZVPP (vib. corr.)
(–)-sparteine (11)	benzyl carbamate 13	14•11	–0.26	0.18	–0.96	–1.01
	(1-naphthyl-) methyl carbamate 19	20•11	0.05	0.49	0.53	0.56
bis(oxazoline) 12 b	benzyl carbamate 13	14•12b	1.51	–0.05	1.20	1.56
	(1-naphthyl-) methyl carbamate 19	20•12b	1.78	2.30	3.53	3.65

Solvent effects:

a) Cosmo at SCS-MP2/TZVPP-level

complex	SCS-MP2	SCS-MP2 (Cosmo)
14•12b	1.20	1.41
20•12b	3.53	3.60

b) PCM at PBE/6-31G*-level

complex	PBE	PBE (PCM)
20•12b	4.43	4.39

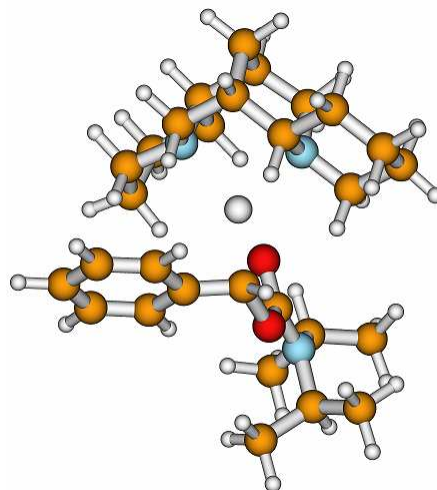
Effect of different functionals

ligand	substrate	experiment	SCS-MP2	B97-D	B3-LYP	PBE
(–)-sparteine (11)	benzyl carbamate 13	–0.23	–0.96	0.18	–1.89	–1.26
	(1-naphthyl-) methyl carbamate 19	0.05	0.53	0.49	–1.78	–1.21
bis(oxazoline) 12 b	benzyl carbamate 13	1.51	1.20	–0.05	3.23	2.84
	(1-naphthyl-) methyl carbamate 19	1.78	3.53	2.30	4.4	4.16

Cartesian coordinates (in Å) obtained for the fully optimized complexes discussed (B97-D/TZVP):

(*S_CR_{Li}*)-14•11:

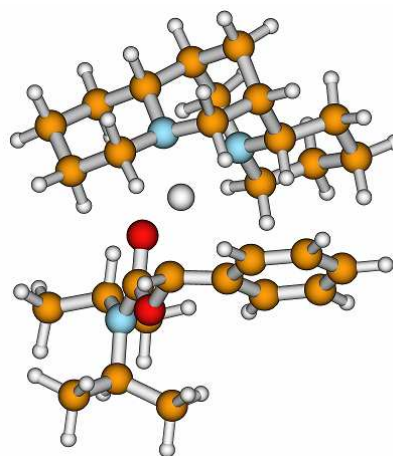
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O	-2.03309682	0.10965699	-1.29543190
C	-0.71266871	-0.34851263	-1.77561526
H	-0.57456742	0.10024746	-2.75906755
C	-0.51569350	-1.76819171	-1.69435730
C	-1.22862465	-2.62702493	-0.80675330
H	-2.04361241	-2.22093966	-0.21332709
C	-0.92013216	-3.98297009	-0.69911735
H	-1.49632174	-4.60115515	-0.01043982
C	0.11226471	-4.55898395	-1.45035406
H	0.34991433	-5.61618042	-1.35823739
C	0.82069157	-3.73501402	-2.34368947
H	1.61488939	-4.15966680	-2.95802440
C	0.51925638	-2.38400007	-2.46583249
H	1.07293846	-1.77164465	-3.17895269
C	-2.15985173	0.41277452	0.00147182
N	-3.42999112	0.78719540	0.34584531
C	-4.57152029	0.82178722	-0.60644236
H	-5.41938140	1.14920681	0.00393641
C	-4.93172136	-0.56668461	-1.15710718
C	-4.39436616	1.87221802	-1.71354068
Li	0.52421689	-0.06034711	0.02541135
N	1.69990272	1.67104218	-0.08854963
N	2.15428397	-1.07652479	0.81980166
C	0.70775129	2.64631783	-0.58060043
H	0.04291432	2.89321803	0.25626961
H	0.10786338	2.11944535	-1.33602877
C	1.33471823	3.90453123	-1.20180139
H	1.89370523	4.46522506	-0.43786076
H	0.53888324	4.56422251	-1.57406539
C	2.28293668	3.49524378	-2.34068969
H	2.77633659	4.37481043	-2.77578695
H	1.69377328	3.02071940	-3.14093940
C	3.32955851	2.49321000	-1.82681569
H	3.98544944	2.99564910	-1.10226222
H	3.96572374	2.13866831	-2.64963476
C	2.65586481	1.27508764	-1.15772230
H	2.03537383	0.77076113	-1.91574390
C	2.32342855	2.06495596	1.18012764
H	1.51261847	2.22665280	1.90120029
H	2.88181658	3.01683873	1.09635387
C	3.30454709	0.99422715	1.68676010
H	3.74163967	1.36881531	2.62236516
C	4.39809901	0.80657931	0.62677156
H	5.15194137	0.08662251	0.97416573
H	4.90672116	1.75818024	0.42770128
C	3.70146419	0.26421710	-0.63139884
H	4.43401299	0.11426062	-1.43583645
C	3.11910658	-1.11697327	-0.29323154
H	2.59680642	-1.54775725	-1.15656156



H	3.96383690	-1.79080359	-0.04053633
C	2.67024766	-0.37647548	2.02182818
H	3.48609922	-0.99257928	2.45830633
C	1.54810603	-0.27053818	3.06280748
H	0.72441829	0.31991764	2.64094404
H	1.93219276	0.26566276	3.94215388
C	1.02132845	-1.66021261	3.44962327
H	0.18648735	-1.56877268	4.15734725
H	1.82230557	-2.22196494	3.95536745
C	0.58116613	-2.41521982	2.18764916
H	-0.29141889	-1.91966531	1.74461500
H	0.28830979	-3.44636642	2.42332802
C	1.70418142	-2.44488685	1.15048476
H	2.56335163	-3.03140642	1.53829277
H	1.35548501	-2.91828269	0.22791116
H	-5.33050009	1.96113418	-2.28102930
H	-4.15733908	2.85047871	-1.27691855
H	-3.59310959	1.58506119	-2.39973376
H	-5.86296325	-0.49557491	-1.73520551
H	-4.14065947	-0.95022283	-1.80665950
H	-5.08710077	-1.27425018	-0.33355762
C	-3.70735101	1.14084321	1.75656167
H	-2.75161538	1.04572813	2.27587235
C	-4.69609307	0.15479306	2.39676049
C	-4.17682867	2.59770975	1.88464261
H	-4.83218729	0.40346369	3.45724152
H	-5.68037992	0.19708169	1.91222544
H	-4.31453027	-0.87058706	2.32281506
H	-4.30743426	2.85212212	2.94446853
H	-3.43545425	3.27848723	1.44883712
H	-5.13809712	2.75980275	1.37963847

(*R_CR_{Li}*)-14•11:

O	-1.41007271	0.83103130	-0.50524632
O	-2.25316156	-0.28957839	1.30174603
C	-0.92558289	-0.31203518	1.92817169
C	-0.22811846	-1.54817066	1.80195199
H	-1.00804465	0.13249178	2.91845895
C	-2.35756728	0.28883842	0.09450553
N	-3.61981672	0.21928785	-0.42556897
C	-4.76248225	-0.45243364	0.25050915
H	-5.59624289	-0.32634214	-0.44773217
C	-5.17216799	0.23938406	1.55913924
C	-4.55311600	-1.96516193	0.41929092
Li	0.38026101	0.48702139	0.32676942
N	1.64676573	-0.10807575	-1.25841213
N	1.94554289	1.66922207	1.05539911
C	0.77277363	-0.99755522	-2.05303811
H	0.01970698	-0.36689125	-2.54060661
H	0.25234652	-1.65018422	-1.34259386
C	1.52863765	-1.87526383	-3.06233397
H	2.01520203	-1.24859923	-3.82464958

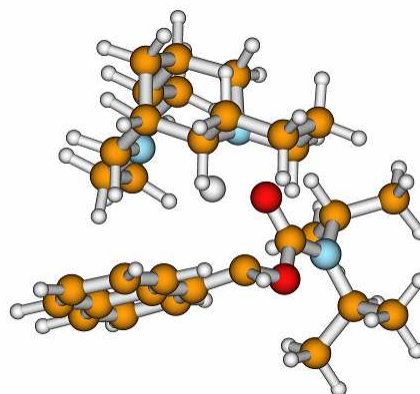


H	0.81210256	-2.52501279	-3.58401465
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H	2.07250201	-3.38926176	-1.62122618
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H	4.11127188	-1.18250741	-2.22070772
H	4.22525832	-2.38193265	-0.92382887
C	2.72896633	-0.86969261	-0.56526797
H	2.21792358	-1.51318436	0.16398207
C	2.11784912	1.04631073	-2.03772564
H	1.22734841	1.57220094	-2.40357926
H	2.70169277	0.73806654	-2.92511639
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H	3.32621117	2.80158040	-1.86464773
C	4.22474383	1.18255567	-0.72231615
H	4.91596479	1.82938928	-0.16377321
H	4.77066544	0.76404469	-1.57661944
C	3.68332373	0.07888208	0.20106725
H	4.50699804	-0.54090798	0.57908597
C	3.04542740	0.75936228	1.41948431
H	2.63532742	0.00589605	2.10053874
H	3.83920342	1.31860976	1.95795937
C	2.31100423	2.64993485	0.00515839
H	3.04940650	3.36341810	0.43200760
C	1.06075876	3.44366692	-0.39818222
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H	1.33703917	4.16118105	-1.18320901
C	0.44166794	4.15907166	0.81072541
H	-0.47986381	4.67836369	0.51579903
H	1.14562783	4.92088834	1.18106676
C	0.15573754	3.14088221	1.92312319
H	-0.61817813	2.43284003	1.59605022
H	-0.20611384	3.64171932	2.83119100
C	1.41410202	2.33810792	2.25588380
H	2.18982946	3.00251204	2.69212517
H	1.17849686	1.55655196	2.98754927
H	-6.11097876	-0.20030746	1.92179970
H	-4.40410760	0.11022600	2.32652468
H	-5.33179646	1.31159355	1.39023769
C	-3.86829768	0.80528440	-1.76313811
H	-2.91800034	1.24657327	-2.07046346
C	-4.91389610	1.92846218	-1.69967372
C	-4.24289912	-0.28016555	-2.78333884
H	-5.01597739	2.39139286	-2.68971484
H	-5.90120855	1.55069413	-1.40309032
H	-4.60524900	2.69824205	-0.98217111
H	-4.36194384	0.16985534	-3.77760496
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C	0.90387883	-1.82299774	2.63799531
C	1.70930557	-2.93635818	2.44098109
C	1.43235795	-3.86686731	1.42090561
C	0.29412121	-3.65483115	0.63244824
C	-0.51961435	-2.53621574	0.81081310
H	1.13181674	-1.13201256	3.45013565
H	2.56267957	-3.09604082	3.10073505

H	2.06251300	-4.74080690	1.27428933
H	0.02996027	-4.37918287	-0.13889577
H	-1.40380817	-2.41269293	0.18982812
H	-5.48667812	-2.42100102	0.77583007
H	-4.28869502	-2.42316328	-0.54190060
H	-3.75986464	-2.17538985	1.14139302

(*S_CR_{Li}*)-20•11:

O	-1.76158961	0.76733354	0.34444344
O	-2.10158264	-0.70877034	-1.36722812
C	-0.66686591	-0.94884991	-1.47461134
H	-0.39284483	-0.86511132	-2.52121740
C	-0.16307783	-2.01132442	-0.68034415
C	-0.89216415	-2.58074419	0.39634865
H	-1.91886369	-2.26744902	0.56154713
C	-0.35152729	-3.57628510	1.22198126
H	-0.97538028	-3.98968134	2.01456107
C	0.94860559	-4.03276009	1.06590539
H	1.36876447	-4.79034408	1.72389119
C	1.74852665	-3.49222192	0.02191072
C	1.20251568	-2.50719613	-0.87923204
C	2.03461055	-2.02577750	-1.92042990
C	-2.52369062	0.13268783	-0.40733412
N	-3.88456528	0.21741312	-0.33001581
C	-4.81831445	-0.56423180	-1.18546776
H	-5.81197766	-0.26134681	-0.84009714
C	-4.71437175	-2.07985909	-0.95738171
C	-4.72997048	-0.17966651	-2.66980433
Li	0.18968614	0.37526435	0.14806677
N	1.17952995	2.07891755	-0.60483034
N	1.61399396	0.32691479	1.70054282
C	0.30869172	2.41882662	-1.74730483
H	-0.61363688	2.85191300	-1.34103436
H	0.03816194	1.46743579	-2.22590531
C	0.96943263	3.34783799	-2.77787578
H	1.18892120	4.32472673	-2.32235323
H	0.27269811	3.52356279	-3.60881768
C	2.27353758	2.70817621	-3.28108261
H	2.78421260	3.36742783	-3.99578726
H	2.03078898	1.77469871	-3.81285614
C	3.19583241	2.38581162	-2.09476848
H	3.52080676	3.32413552	-1.62467645
H	4.09964334	1.86156999	-2.43438893
C	2.47729633	1.50184209	-1.05216171
H	2.21844521	0.55403365	-1.54425973
C	1.29950195	3.17393596	0.36732430
H	0.28327182	3.42599719	0.69457977
H	1.73449434	4.08589235	-0.08371859
C	2.17929207	2.78225681	1.56528046
H	2.23669715	3.65738012	2.22676468
C	3.57456206	2.41809354	1.04071837
H	4.24911233	2.18085959	1.87497981

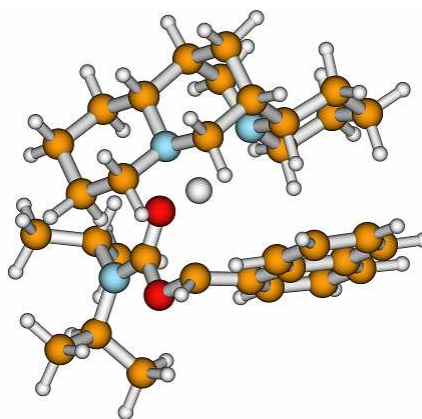


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C	3.39611501	1.17958995	0.14801721
H	4.36113442	0.86171382	-0.26737633
C	2.89376185	0.02474486	1.02677982
H	2.74951321	-0.88177069	0.42979336
H	3.67549586	-0.18897361	1.78389208
C	1.63436151	1.62077768	2.42848718
H	2.33660206	1.52200156	3.28457876
C	0.23773245	1.90809669	2.99578843
H	-0.47656148	1.99399868	2.16801090
H	0.26398053	2.87259890	3.52238005
C	-0.21985820	0.78288903	3.93637660
H	-1.24443660	0.97069462	4.28493723
H	0.43218936	0.76684711	4.82361756
C	-0.13297705	-0.56808127	3.21263090
H	-0.86997295	-0.60497801	2.40098102
H	-0.35619004	-1.39836028	3.89544684
C	1.26026700	-0.77596717	2.61840497
H	2.01468020	-0.83307446	3.43083441
H	1.29832884	-1.71184810	2.05520748
H	-5.54369649	-0.67122577	-3.21947583
H	-4.83410359	0.90578220	-2.79025683
H	-3.77550593	-0.49580840	-3.09936594
H	-5.52785677	-2.58119865	-1.49871311
H	-3.75855772	-2.46979162	-1.31626715
H	-4.81246414	-2.31289845	0.10982621
C	-4.48085257	1.09714012	0.70243706
H	-3.63683404	1.57084839	1.20763924
C	-5.26088348	0.28048623	1.74389434
C	-5.33845419	2.20279244	0.06993637
H	-5.64002812	0.94750177	2.52882876
H	-6.12082353	-0.23196262	1.29330804
H	-4.60911286	-0.47036896	2.20625288
H	-5.70547516	2.87678181	0.85469812
H	-4.74483139	2.78641512	-0.64392890
H	-6.21110376	1.79231963	-0.45453495
C	3.34925942	-2.44133011	-2.06654830
H	1.63925998	-1.29756151	-2.62331873
H	3.95984395	-2.04283189	-2.87501281
C	3.89106929	-3.38416273	-1.16485441
C	3.10155032	-3.89811426	-0.15347943
H	4.92422405	-3.71097365	-1.27246034
H	3.50839276	-4.63527519	0.53835654

$(R_C R_{Li})$ -**20•11**:

O	-1.76378532	0.33376508	-0.68210137
O	-2.26043324	-1.02817646	1.08424127
C	-0.85125696	-1.04389563	1.46348641
C	-0.04806457	-2.01084598	0.80013654
H	-0.78655813	-0.90840995	2.53927332
C	-2.58221712	-0.32966292	-0.02086959
N	-3.90280519	-0.43126975	-0.35293751

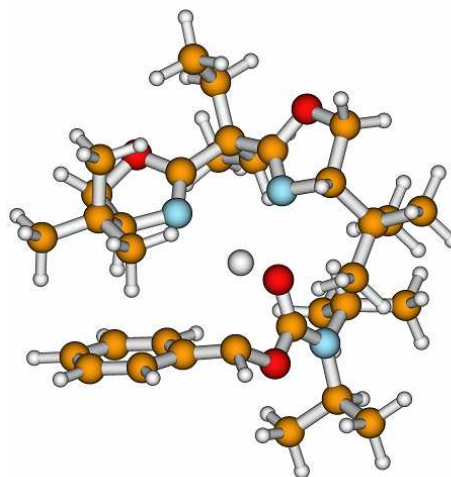
C	-4.90077232	-1.20834683	0.42984286
H	-5.84106342	-1.05178448	-0.10797904
C	-5.10835112	-0.65573763	1.84811965
C	-4.62516256	-2.71905731	0.41467772
Li	0.09337975	0.49698349	0.15658398
N	1.60330981	0.79016528	-1.25527000
N	0.87307827	2.23357829	1.17675276
C	1.32437590	-0.35029100	-2.15586986
H	0.35478459	-0.16585414	-2.63417401
H	1.21353527	-1.23968699	-1.52738631
C	2.43174236	-0.61791585	-3.18597585
H	2.52725240	0.23248421	-3.87847389
H	2.15847034	-1.49840726	-3.78252073
C	3.75970346	-0.84880791	-2.44866485
H	4.57774813	-1.01148327	-3.16371157
H	3.66750365	-1.75121549	-1.82881409
C	4.07464577	0.34662559	-1.53564055
H	4.26787750	1.23506611	-2.15431896
H	4.98119467	0.15531235	-0.94590851
C	2.91231505	0.62817076	-0.55882076
H	2.80203120	-0.25898826	0.08033626
C	1.41843250	2.09184620	-1.91554752
H	0.38650173	2.11986105	-2.28911800
H	2.08457538	2.21122065	-2.79044590
C	1.69269423	3.26853312	-0.96356047
H	1.56547777	4.19138941	-1.54616228
C	3.13776847	3.15308736	-0.45983337
H	3.38866809	4.00630552	0.18575580
H	3.83945697	3.14855304	-1.30290818
C	3.21572678	1.84496313	0.34324084
H	4.22774191	1.70093057	0.74305268
C	2.27602958	1.97317534	1.55103949
H	2.29572218	1.05315834	2.14043284
H	2.65217823	2.79936706	2.19036754
C	0.73773807	3.38415044	0.24654642
H	1.03930676	4.30638881	0.79056516
C	-0.72902396	3.54055497	-0.17137297
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H	-0.80698683	4.39836309	-0.85380728
C	-1.64030106	3.72719558	1.05012816
H	-2.69218174	3.76978025	0.73742106
H	-1.40320639	4.68550123	1.53752535
C	-1.42264865	2.58273527	2.05035659
H	-1.76799329	1.63591848	1.61874367
H	-1.99018849	2.75751971	2.97407544
C	0.06164369	2.43925975	2.39090751
H	0.41781595	3.34164538	2.93168231
H	0.21725288	1.57019704	3.04201459
H	-5.46841825	-3.24434600	0.88221561
H	-4.52115605	-3.07685194	-0.61681536
H	-3.71160587	-2.95801673	0.96495422
H	-5.96661997	-1.16168935	2.30990052
H	-4.22433265	-0.82627709	2.46806828
H	-5.31614276	0.42075979	1.81123520
C	-4.38757953	0.29174360	-1.55198915
H	-3.50626887	0.77492343	-1.97863037



C	-5.39544551	1.38611673	-1.17076076
C	-4.95030109	-0.67851336	-2.60098232
H	-5.69233972	1.94505790	-2.06746873
H	-6.30287825	0.96021265	-0.72346156
H	-4.94764597	2.08438189	-0.45349000
H	-5.23253382	-0.12161283	-3.50368103
H	-4.19653073	-1.42670402	-2.87241545
H	-5.84432993	-1.19888804	-2.23385882
C	1.35951985	-2.18684123	1.17223008
C	2.21744835	-3.02358275	0.36898317
C	1.68857907	-3.73356323	-0.74234955
C	0.34131777	-3.60376523	-1.04705722
C	-0.50551276	-2.76057034	-0.31416843
C	1.93226975	-1.52361794	2.28474156
H	2.34434359	-4.37364810	-1.32819679
H	-0.07719345	-4.16078110	-1.88559968
H	-1.54958870	-2.68730062	-0.60552119
C	3.27915974	-1.62878452	2.59455098
H	1.29907297	-0.89854994	2.90896706
H	3.68537129	-1.09281987	3.45060207
C	4.12455897	-2.42320135	1.78862041
C	3.59716528	-3.10659657	0.70948342
H	5.18466642	-2.50486520	2.02373297
H	4.24106819	-3.73018985	0.08998950

(S_C)-14•12b:

Li	0.13418384	-0.07704988	-0.91499326
O	-1.45827850	-0.05522731	0.36953927
C	-2.41550510	-0.76662192	0.00779995
O	-2.34217908	-1.65251871	-0.98289019
C	-1.01669005	-1.86259256	-1.63133495
H	-1.25213291	-2.07707435	-2.67447969
N	-3.64777874	-0.70333128	0.60165819
C	-3.84702702	0.24895297	1.71672797
C	-4.00822331	-0.48625558	3.05561411
C	-5.01427556	1.20734620	1.43865840
C	-4.76593942	-1.62866118	0.28026621
C	-4.42777426	-3.10120700	0.56246915
C	-5.32477896	-1.40798161	-1.13315729
C	-0.22674571	-2.87743206	-0.97451201
H	-4.59255382	-1.70301255	-1.88987534
H	-5.58338568	-0.35185317	-1.28019196
H	-6.23259186	-2.01201365	-1.26496377
H	-5.33750547	-3.70653989	0.45086806
H	-3.66803325	-3.47275646	-0.12973309
H	-4.05611794	-3.21709581	1.58783301
H	-3.13423980	-1.11939581	3.24980357
H	-4.90556713	-1.11895047	3.05765882
H	-4.10560889	0.24070012	3.87264526
H	-2.93106083	0.84109873	1.76477316
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H	-4.86151877	1.72879541	0.48718268

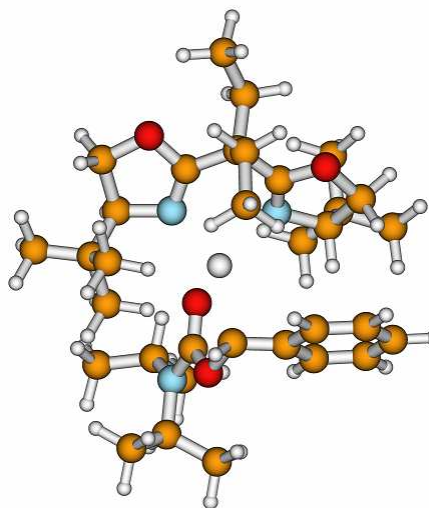


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C	2.87648229	-1.34725065	0.12008604
C	-0.01790015	3.13006301	-1.80551488
C	2.23338296	0.58822262	1.02742415
C	1.05835792	2.62314038	0.08643868
H	-5.55755575	-1.34822161	0.98274837
O	1.01780237	3.98938010	0.15528199
C	1.64485934	1.96026763	1.33166479
O	3.12877114	0.13390431	1.95501580
C	2.73263551	2.87029336	1.97459122
C	0.42591293	1.81198240	2.32014678
H	2.24621353	3.81099455	2.25221897
H	3.06406916	2.38651035	2.89693356
C	3.94343516	3.14493232	1.07544463
H	4.64699482	3.81687772	1.58329508
H	4.47311469	2.21624382	0.83817067
H	3.63899782	3.62289640	0.13618162
H	0.08455079	2.83433502	2.53207420
H	-0.37459864	1.29103105	1.78915386
C	0.71842770	1.07927311	3.63432344
H	-0.18642982	1.08854680	4.25605055
H	0.99421376	0.03482876	3.45284083
H	1.52708788	1.55189907	4.20370878
C	3.42355558	-1.24811701	1.55971564
H	4.50321800	-1.39170451	1.64944447
H	2.89160960	-1.91365699	2.24975236
C	3.95862426	-1.31084313	-1.00066751
H	2.28384722	-2.25537334	-0.01050967
C	0.40778060	4.44090224	-1.08887048
H	-0.43023209	5.09484718	-0.83025555
H	1.16244436	5.00946167	-1.64367835
H	0.46587756	3.05500416	-2.78937699
C	-1.54672797	2.97522183	-2.04052787
C	-2.00490367	4.11439872	-2.97107507
C	-1.81191808	1.62827688	-2.73614198
C	-2.32250420	3.03681277	-0.71421743
H	-3.39577115	2.92517867	-0.91492692
H	-2.01020642	2.22688335	-0.04882043
H	-2.17855803	3.99866020	-0.20381206
H	-3.07364754	4.00356764	-3.19476523
H	-1.85962877	5.10083718	-2.50984404
H	-1.45185752	4.09002973	-3.92063787
H	-1.51377470	0.77648665	-2.11449119
H	-2.88305748	1.52400140	-2.95377636
H	-1.26162206	1.56795006	-3.68529297
C	4.77437161	-2.61318285	-0.91061323
C	3.26266735	-1.24172946	-2.37241219
C	4.88954008	-0.09597279	-0.85212660
H	5.51993633	-2.64296687	-1.71629573
H	5.31041588	-2.68762409	0.04572907
H	4.11439443	-3.48376831	-1.00625409
H	5.63695139	-0.10386566	-1.65619841
H	4.31981322	0.83780052	-0.92464375
H	5.42566097	-0.10475440	0.10609224

H	4.01470968	-1.28875845	-3.17185134
H	2.56505651	-2.07770636	-2.49130283
H	2.70394159	-0.30348635	-2.47342479
C	0.68924539	-3.66569848	-1.73219326
C	1.54500304	-4.58301490	-1.13259254
C	1.53069816	-4.78402017	0.25880789
C	0.61917497	-4.04306489	1.02320003
C	-0.23645244	-3.11262519	0.43178184
H	0.70481496	-3.54585579	-2.81560790
H	2.22163244	-5.16608770	-1.75739670
H	2.19364456	-5.50953904	0.72506133
H	0.57145408	-4.19268817	2.10231484
H	-0.92084257	-2.55417137	1.06395796

(*R*_C)-14•12b:

Li	0.02244154	-0.22454245	-0.02871142
O	1.78760627	-0.31031414	-0.94657658
C	2.76575488	-0.27026151	-0.17923695
O	2.68667453	-0.01984317	1.13586568
C	1.34880365	0.25399789	1.70023225
C	1.07079717	1.65448739	1.84526671
C	-0.00982637	2.07957624	2.67898804
C	-0.37573537	3.41610583	2.77783449
C	0.30516346	4.41247501	2.05351808
C	1.38189760	4.02156832	1.24612001
C	1.76000978	2.68282455	1.13720403
N	4.04949867	-0.47956407	-0.60592876
C	4.28075176	-0.76290857	-2.04008460
C	4.86396250	-2.16946582	-2.24425417
C	5.14756982	0.32414074	-2.69299407
C	5.23778962	-0.44623658	0.28637932
C	5.21849903	-1.55628982	1.34892960
C	5.49703300	0.94434392	0.88588814
H	1.26825604	-0.34265175	2.61001700
H	-0.55383474	1.32760683	3.25135471
H	-1.20076338	3.69379743	3.43483600
H	4.71092982	1.21972364	1.59364557
H	1.94061747	4.77495094	0.69019392
H	0.01713489	5.45814806	2.13481214
H	2.60455461	2.41591515	0.50710428
H	5.53889945	1.69933725	0.09119989
H	6.46196542	0.93808354	1.41085674
H	6.18877967	-1.58136260	1.86313913
H	4.43278617	-1.37656268	2.08750921
H	5.04770527	-2.53195448	0.87746306
H	4.20499892	-2.92468826	-1.79886483
H	5.85913211	-2.26455500	-1.79026806
H	4.96278329	-2.37764826	-3.31761232
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H	5.24577556	0.12246485	-3.76760460

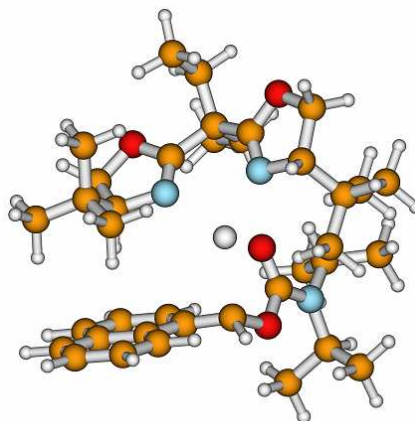


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N	-1.59384669	1.01798428	-0.51053260
N	-1.33864281	-1.86586781	-0.19141252
C	-0.94775305	-3.27400999	-0.43556192
C	-1.42534238	2.48946413	-0.50692186
C	-2.60836307	-1.77802528	-0.30631354
C	-2.79049555	0.75767726	-0.15651580
H	6.07901312	-0.66472117	-0.37955134
O	-3.59255703	1.80635481	0.18938885
C	-3.52513207	-0.57552262	-0.13582777
O	-3.29442539	-2.92989134	-0.58001062
C	-4.26829355	-0.72926722	1.23105216
C	-4.55244482	-0.50091418	-1.33935988
H	-5.04073268	0.04634906	1.26947319
H	-4.77430117	-1.70014595	1.22512757
C	-3.34409754	-0.61383508	2.44825954
H	-3.91958102	-0.74133034	3.37360634
H	-2.56004005	-1.37870559	2.42332153
H	-2.85517656	0.36737736	2.48189899
H	-4.89471535	0.53728126	-1.39871038
H	-3.99510785	-0.70540723	-2.26263570
C	-5.79565707	-1.39855270	-1.26319139
H	-6.41679134	-1.21224506	-2.14931697
H	-5.54087688	-2.46082401	-1.23596995
H	-6.39970259	-1.16125275	-0.37962496
C	-2.30430749	-3.99324955	-0.66201654
H	-2.54001840	-4.72610728	0.11663401
H	-2.39237997	-4.46137618	-1.64749163
C	-0.07012939	-3.88701657	0.69003837
H	-0.34425774	-3.29347991	-1.35424910
C	-2.74599891	2.99988065	0.11389332
H	-3.27471958	3.73677455	-0.49745962
H	-2.60154459	3.37579262	1.13089431
H	-0.58599920	2.74129538	0.14217214
C	-1.10047325	3.03113941	-1.92667259
C	-0.92891024	4.55840705	-1.82495522
C	0.22732685	2.41181247	-2.39863403
C	-2.21888164	2.68931085	-2.92496931
H	-1.96825429	3.08730939	-3.91703169
H	-2.34108864	1.60251630	-3.00989619
H	-3.18034839	3.12532887	-2.62056063
H	-0.62946152	4.96410388	-2.80046976
H	-1.86329579	5.05387495	-1.52787605
H	-0.15707672	4.80687513	-1.08598893
H	0.14619919	1.32400564	-2.49283655
H	0.50724699	2.83066278	-3.37522140
H	1.02560439	2.62760622	-1.67855647
C	0.18557631	-5.36713817	0.34495891
C	1.27284551	-3.14387453	0.74012021
C	-0.76010450	-3.77127015	2.05888074
H	0.86641282	-5.80558280	1.08549068
H	-0.74004533	-5.95860989	0.34950213
H	0.65288701	-5.45996025	-0.64561434
H	-0.14699306	-4.26337578	2.82461642
H	-0.87338262	-2.71708928	2.33494467

H	-1.75104365	-4.24544623	2.06522079
H	1.92630517	-3.59992625	1.49559464
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H	1.12055363	-2.09291703	1.00679670

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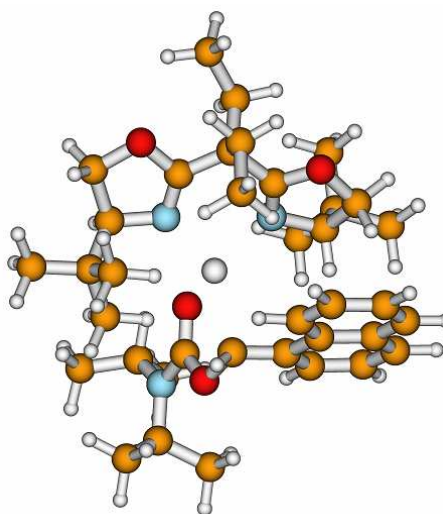
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O	-1.15543712	-2.67069188	-0.50058246
C	0.10313234	-2.18745613	-1.09761325
H	0.12929364	-2.61992129	-2.09342918
N	-2.97286602	-2.36796994	0.81505337
C	-3.81572478	-1.51699167	1.68603505
C	-3.74993488	-1.98000121	3.14883957
C	-5.25873436	-1.43579958	1.16725816
C	-3.35072170	-3.79961562	0.67840054
C	-2.31134679	-4.75440917	1.28624233
C	-3.73208230	-4.17432060	-0.76147572
C	1.25394596	-2.34981603	-0.26212986
H	-2.85805360	-4.13750039	-1.41750717
H	-4.49542232	-3.48598490	-1.14526112
H	-4.14168840	-5.19319427	-0.77554662
H	-2.71701523	-5.77503516	1.28539466
H	-1.38063373	-4.74351461	0.71330243
H	-2.09089176	-4.46857330	2.32187437
H	-2.71217145	-1.97814860	3.50304483
H	-4.15818988	-2.99231414	3.26656653
H	-4.33889768	-1.30266487	3.78094723
H	-3.38204216	-0.51699774	1.62897232
H	-5.83107208	-0.73356960	1.78707150
H	-5.27232848	-1.07975544	0.13118390
H	-5.76389811	-2.40936798	1.21149508
N	-0.95220895	1.92170245	-1.27650121
N	1.31215445	1.31663138	0.36277172
C	2.63864625	0.94908883	0.90637643
C	-1.78923442	2.25546867	-2.44653868
C	0.77462370	2.15419168	1.16362765
C	-1.07068330	2.86059551	-0.41900371
H	-4.25819741	-3.89626817	1.28312604
O	-1.86590463	3.92278834	-0.75240716
C	-0.54074830	2.90914560	1.01201842
O	1.44687190	2.43311119	2.31970322
C	-0.35237996	4.38287450	1.48238913
C	-1.67582199	2.23472017	1.87461665
H	-1.33272257	4.86648793	1.42446088
H	-0.06084902	4.35626169	2.53554345
C	0.68222747	5.18387409	0.68529572
H	0.70022971	6.22543206	1.03075802
H	1.68573023	4.76663376	0.81579271
H	0.44251241	5.18775578	-0.38512757
H	-2.56035492	2.87427885	1.75085524



H	-1.89692397	1.26127216	1.43211157
C	-1.37775218	2.04902345	3.36660800
H	-2.27181742	1.64190393	3.85728490
H	-0.55443346	1.34411078	3.52203413
H	-1.11796021	2.99145219	3.86221640
C	2.57008621	1.49130140	2.34968915
H	3.45438163	2.04695217	2.67042125
H	2.32874059	0.70623341	3.07649795
C	3.80011099	1.52924605	0.04462687
H	2.73030731	-0.13943916	0.90648816
C	-2.32576153	3.67448455	-2.11263450
H	-3.41747574	3.74362425	-2.11096581
H	-1.90638214	4.45619264	-2.75570193
H	-1.14596598	2.28557054	-3.33680681
C	-2.88751882	1.18687527	-2.71412480
C	-3.70862866	1.63361429	-3.93847248
C	-2.21006955	-0.15625169	-3.03532943
C	-3.80794056	1.02308400	-1.49287013
H	-4.58137308	0.27687319	-1.71586990
H	-3.23531580	0.68145147	-0.62544309
H	-4.31565643	1.96341164	-1.23833056
H	-4.45220072	0.86520211	-4.18576217
H	-4.24720572	2.57218742	-3.75066444
H	-3.05894484	1.77479146	-4.81373060
H	-1.59740645	-0.51737257	-2.20179587
H	-2.97124701	-0.91828530	-3.24955078
H	-1.56273586	-0.06147826	-3.91843784
C	5.12721781	1.02617168	0.64210740
C	3.67287965	1.01207333	-1.39779552
C	3.77985977	3.06599234	0.02783777
H	5.96605034	1.37790468	0.02720680
H	5.28055515	1.39990399	1.66406224
H	5.14508156	-0.06941317	0.66110123
H	4.63105898	3.43837331	-0.55725153
H	2.85891489	3.43206514	-0.44013238
H	3.85304635	3.49127527	1.03754419
H	4.50344630	1.39957530	-2.00322347
H	3.70710695	-0.07963399	-1.42765181
H	2.72939423	1.34713083	-1.84567140
C	2.59530580	-2.40776122	-0.84466965
C	3.75033886	-2.49492906	0.01469173
C	3.59319523	-2.53418261	1.42766093
C	2.31627452	-2.49722928	1.96389499
C	1.17606197	-2.40019940	1.15039795
C	2.81431166	-2.38844191	-2.24623641
C	5.04327547	-2.54504693	-0.57740553
H	4.47482796	-2.60950476	2.06109523
H	2.18319391	-2.54651856	3.04506474
H	0.20325340	-2.38093510	1.63092478
C	4.08608583	-2.44447857	-2.79242160
H	1.96560549	-2.30824666	-2.91956166
H	4.21382487	-2.42267934	-3.87315279
C	5.21555851	-2.51999825	-1.94743783
H	5.90776712	-2.60604050	0.08346053
H	6.21610079	-2.55900346	-2.37518756

(R_C)-20•12b:

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O	-2.06757490	0.48665030	-0.99849194
C	-2.97279376	0.11734472	-0.23036608
O	-2.76299712	-0.42676085	0.97951262
C	-1.37382619	-0.64077894	1.40683774
C	-0.90915669	-1.97491895	1.20444680
C	0.32684176	-2.42925777	1.84116766
C	0.80943646	-3.76765584	1.60431307
C	0.10256498	-4.63823121	0.73072851
C	-1.05255276	-4.18344478	0.11433556
C	-1.54890153	-2.88913890	0.33533661
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C	-4.67581616	0.80887733	-1.84839788
C	-5.47054112	2.11184301	-1.67374678
C	-5.42232880	-0.21279436	-2.71924471
C	-5.40345054	-0.20541428	0.35956023
C	-5.46290803	0.60122261	1.66599193
C	-5.42017100	-1.72303443	0.59783942
H	-1.28768752	-0.22531207	2.40899502
C	1.10699811	-1.57693891	2.66151942
C	2.01325753	-4.18227774	2.24103045
H	-4.55481634	-2.03920366	1.18608722
H	-1.60135229	-4.84542794	-0.55587515
H	0.47652647	-5.64640499	0.56366791
H	-2.46863377	-2.58917661	-0.15823497
H	-5.41293557	-2.25852885	-0.35947913
H	-6.33610875	-1.99349700	1.14043664
H	-6.38667487	0.34907451	2.20388241
H	-4.60820816	0.37075037	2.30751739
H	-5.46711255	1.67683003	1.45040036
H	-4.89812809	2.83221237	-1.07679471
H	-6.43352562	1.93510537	-1.17682067
H	-5.67623819	2.55441837	-2.65702044
H	-3.73269691	1.04936983	-2.34333807
H	-5.62795842	0.22302886	-3.70548761
H	-4.81430916	-1.11513429	-2.85435230
H	-6.38285763	-0.50143839	-2.27241014
N	1.50272506	-0.38687461	-0.96735167
N	0.82147351	2.31138028	-0.09390384
C	0.19323221	3.64202941	0.08514673
C	1.59814629	-1.84567676	-1.21165820
C	2.06533027	2.48648976	-0.33035628
C	2.67045324	0.03498718	-0.66847029
H	-6.31325217	0.03599593	-0.19935035
O	3.66501762	-0.88628638	-0.55250122
C	3.16991323	1.47130360	-0.57891064
O	2.52543830	3.77477145	-0.34776492
C	4.22622772	1.60834491	0.55959194
C	3.82702050	1.72766249	-1.99715442
H	5.06685783	0.95344720	0.30742930
H	4.59312310	2.63872674	0.55036364



C	3.67401076	1.25379301	1.94412407
H	4.46088284	1.35205495	2.70274654
H	2.84904076	1.92145677	2.22216546
H	3.30136204	0.22394722	1.96991117
H	4.37424190	0.81289646	-2.25113358
H	3.00987155	1.81992784	-2.72439436
C	4.79449015	2.91090953	-2.13117382
H	5.19686979	2.91910685	-3.15290377
H	4.30677202	3.87045212	-1.94202063
H	5.64081934	2.81048901	-1.44173489
C	1.37793624	4.62982801	-0.08723167
H	1.59595155	5.20832300	0.81625358
H	1.26055649	5.30750605	-0.93921220
C	-0.58031604	3.78777595	1.42446267
H	-0.53971886	3.77436894	-0.72309870
C	3.01163479	-2.19287980	-0.69910388
H	3.61289117	-2.77877814	-1.39921677
H	2.99263589	-2.66802523	0.28629877
H	0.84029166	-2.35661759	-0.61859342
C	1.31545374	-2.19098316	-2.70095097
C	1.39753628	-3.72121835	-2.85515805
C	-0.11245573	-1.73085235	-3.04777605
C	2.32553798	-1.51172481	-3.63946829
H	2.10725750	-1.78157811	-4.68112260
H	2.26680203	-0.42056904	-3.54703959
H	3.35485180	-1.82520436	-3.41806347
H	1.12732929	-4.00576109	-3.88082372
H	2.41216320	-4.09416613	-2.65996221
H	0.70986932	-4.21276818	-2.15585764
H	-0.20770830	-0.64261938	-2.96598215
H	-0.36105034	-2.03005205	-4.07535939
H	-0.83606200	-2.18636291	-2.36079383
C	-1.10529689	5.23288413	1.52638799
C	-1.77514098	2.82371455	1.41789832
C	0.32740315	3.46531420	2.62295965
H	-1.71903993	5.33854013	2.42994476
H	-0.29060976	5.96676884	1.58760372
H	-1.73171721	5.48025547	0.65766896
H	-0.22827468	3.60776415	3.55843996
H	0.66299876	2.42304053	2.57460106
H	1.21231529	4.11572486	2.65496135
H	-2.35796804	2.93909814	2.34129075
H	-2.43410444	3.02351121	0.56277193
H	-1.43327703	1.78615280	1.35587238
C	2.28074307	-2.00695561	3.26106182
H	0.78362693	-0.55020828	2.81341842
H	2.85502402	-1.32428414	3.88427684
C	2.73495470	-3.32897422	3.05459654
H	2.36381147	-5.19888322	2.06339838
H	3.65474180	-3.66997005	3.52734965