

# Supplementary Materials

## Theoretical Study of The Halogen Concentration Effect on The 1,3-Butadiene Polymerization Catalyzed by the Neodymium-Based Ziegler–Natta System

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**TABLE S1:** Atomic Cartesian coordinates (in Å) for optimized structures of *i*-C<sub>4</sub>H<sub>9</sub>-AS+η-*trans*-C<sub>4</sub>H<sub>6</sub>

### AS(I)

Atom	x	y	z
C	-0.70916628561647	-1.71313625977091	-0.32542353377025
Al	1.03517405488812	-1.56074772828490	-1.32674438676138
C	0.47039473957466	-1.24275553353853	-3.38778178995632
Nd	1.47577987915394	1.18121971575609	-3.22864643128328
C	1.71967708476618	1.04333089710162	-5.64345153561784
C	2.58266409165779	-2.81860522262289	-1.65372069779705
C	1.92413646620542	0.22487188949592	-0.62153480767080
Cl	1.76021036561576	3.83379548817408	-2.71731114386795
Al	4.31581385564987	3.82594368364638	-2.84946152929271
C	4.73287531692404	4.29220997467836	-0.96147533975129
C	4.32463825244279	1.81452948856626	-3.22683881352166
C	4.63166416438280	4.95341413779304	-4.46094167156721
C	-1.67329586543294	1.84180044857694	-4.61539272986636
H	-1.98104545933759	0.80749299256395	-4.71499941392842
H	-1.58710608337292	2.41628229726752	-5.52695552538709
C	-1.42582329305078	2.38665192891795	-3.41637580472745
C	-1.49362688661344	1.65004268074858	-2.16030818242546
C	-1.10608999541091	2.15029398773781	-0.97957346544148
H	-1.15562926115823	1.55161173403952	-0.08021890114035
H	-0.72873912327621	3.16257295424744	-0.89004415181715
H	-1.85383039180196	0.62668143809803	-2.20661477611517
H	-1.12479335759565	3.42851239884054	-3.35558609910217
H	-0.70862986751007	-0.96369306065489	0.48090227766050
H	-1.48326057873372	-1.36390212705686	-1.02574237793221

H	2.64320649492105	-2.99349496175858	-2.73931236583346
H	3.47672675079676	-2.21697088612346	-1.42568612856237
H	4.67918121163438	4.30123406133043	-5.34482216444238
H	3.76127964837722	5.60409969553961	-4.62465317610535
H	3.96240840156103	3.82665519587072	-0.33067632904903
H	5.67226819813984	3.79615994383105	-0.67520222227626
H	2.42137054715140	0.20056589430135	-5.79404898810827
H	0.75656370588994	0.69997284763877	-6.06067809933155
H	2.93544589238818	0.41831081538510	-1.01775568247012
H	1.35069900546696	1.16476654702930	-0.72659847191320
H	3.88422639531981	1.29596790649297	-2.35741628229021
H	3.72909323132944	1.63193738830723	-4.13831881133740
H	-0.23703928667778	-0.48156653260568	-3.77450892903522
H	1.34296002990040	-1.19496696605412	-4.06792169017295
C	2.21571505260232	2.21608779707351	-6.48903195021257
C	1.23886195379956	3.39456656554385	-6.49126753807297
C	-1.21635606025727	-3.03195689249522	0.28059218823921
C	-2.68142260163651	-2.89227717189489	0.71624322328322
C	-0.36124585020597	-3.45599989936347	1.47598409848543
C	2.77753619724202	-4.18040080360409	-0.96584268960651
C	4.19544265128339	-4.70872605272345	-1.22614324959934
C	1.75134940089175	-5.20828042057251	-1.44471999097258
C	4.84690224045476	5.77435838577200	-0.57452630042408
C	5.19836811373775	5.90397320545738	0.91378342987747
C	5.89260035591449	5.83194188527339	-4.44009491679076
C	6.03038730419051	6.61023981678795	-5.75447512831744
C	7.14773594162947	4.99150567126470	-4.19347934842965
C	3.55665563575099	6.53967095768746	-0.87487237200080
C	2.45620943092536	1.73489120377297	-7.93303373527829
H	5.66390802180335	6.24104110844292	-1.14999987357117
H	5.30094793785681	6.95441439407921	1.19160923834493
H	4.41751114364688	5.45234285519321	1.52863306304598
H	6.14095092500142	5.39463399330308	1.12125211804061
H	3.66475212125441	7.59192846431683	-0.60660264462591
H	3.32271484891963	6.47639034751884	-1.94362738687301
H	2.72022106671941	6.12070131150606	-0.31054302985362
H	5.81106866302662	6.56875935429528	-3.62387482821212
H	8.03642327926190	5.62335728165196	-4.15146259289531
H	7.05729859407790	4.45871404081174	-3.23851139690601
H	7.28233148401674	4.25525512622866	-4.98994491135596
H	6.91303260450034	7.25173535728938	-5.72884719200885
H	6.12181780556557	5.92078717414262	-6.59604377873646
H	5.14927936341480	7.23436099447112	-5.91166310840735
H	-1.17219407593462	-3.83183462003770	-0.47727498468510
H	2.66490429980243	-4.06827686612307	0.12517239716037
H	-0.69268240458860	-4.41982012812399	1.86603428808718

H	0.68670530201178	-3.54703917605140	1.17454792470991
H	-0.42654152933036	-2.71513438962123	2.27639113761475
H	-3.04050484886567	-3.82466262770876	1.15574627891758
H	-2.78265201015078	-2.09432920701827	1.45456078348103
H	-3.30732200034078	-2.64988221875653	-0.14411536346809
H	1.86805980030017	-6.14874936715514	-0.90332553142061
H	0.73666663010079	-4.83627043692633	-1.27510630330376
H	1.87366665744432	-5.40482299646659	-2.51219787513607
H	4.33629507149272	-5.67981282101246	-0.74802502360192
H	4.36836020795589	-4.81742371278745	-2.29872085604864
H	4.93421497337257	-4.01283469130032	-0.82498124423709
H	3.18620921746461	2.57265798207020	-6.10315635339311
H	1.65368437098778	4.22736143304335	-7.06116133067381
H	0.28854551267230	3.10424439198561	-6.94173702913737
H	1.05233372597546	3.73693534289106	-5.47006349299257
H	2.82460126501646	2.56087548756263	-8.54262426173134
H	3.19465010821655	0.93332997115275	-7.94229973366763
H	1.52793156573618	1.36026442845988	-8.36507576468124
C	2.12641155439947	0.14772893549234	0.90896588602425
H	1.15273479872089	-0.01720324907044	1.39978166531181
C	3.06116671299508	-0.98898595025024	1.31959087953524
C	2.68052841291948	1.48025062327566	1.43205082918780
H	3.22652492615620	-0.97650683314075	2.39824994824641
H	2.62110781280180	-1.95516145827542	1.05387353932893
H	4.02841542258279	-0.89634039036689	0.81959985371966
H	2.80124687912808	1.44678689409246	2.51621828978851
H	3.65365520935965	1.68633050289987	0.97889300015320
H	2.00079343672707	2.29721691307690	1.18337456629651
C	5.65010685839614	1.08362043661684	-3.49574777346595
C	5.38063470710490	-0.36825148051194	-3.91329463815809
H	6.17636728043821	1.57861703951846	-4.32909764750297
C	6.56148677486018	1.11074058991285	-2.26825607682217
H	6.31572341697815	-0.90655061752598	-4.07578412818228
H	4.81240613031250	-0.88402851346158	-3.13375832401451
H	4.80134778824866	-0.39273952697135	-4.83817583027271
H	7.49168438289350	0.57644456146177	-2.46743386044920
H	6.80823596740709	2.14377958682343	-2.00504790065509
H	6.06855897992001	0.64259431937103	-1.41235799556605
C	-0.21775711063221	-2.58700702779351	-3.73889518274323
C	0.39230726081592	-3.21707556915751	-4.99519301930836
H	-0.08001324633855	-3.31459253638499	-2.91178247126567
C	-1.72416668990489	-2.41440681117674	-3.93957950383897
H	-0.10086350380878	-4.16296098748932	-5.22845261577769
H	0.28047659709350	-2.54346464456309	-5.84715384741485
H	1.45651040381795	-3.41003398783934	-4.84518258372583
H	-2.19850959960602	-3.38284410062101	-4.11208300888710

H	-2.18197172574562	-1.96043800929983	-3.05860499187085
H	-1.92196635131825	-1.77277669145431	-4.80064094362040

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## AS(II)

Atom	x	y	z
C	-0.71878623471922	-1.90351939601519	-0.58859858885257
Al	1.21447035208794	-1.87945966486930	-1.10041891809474
Cl	0.93737065197123	-1.31696788427129	-3.56066558859937
Nd	1.55040687029394	1.31003354132522	-3.73449192961881
C	1.72726305682777	1.13506421058662	-6.10820206008901
C	2.41167294778376	-3.46419107275700	-1.21100717314708
C	2.13546752963587	-0.11047847373576	-0.73954382733368
Cl	1.62886283785727	3.98392451213571	-3.22190317877125
Al	4.15792735928243	4.00612197822508	-3.25897369398007
C	4.51345323740784	4.64535439782388	-1.41023792713820
C	4.28920437206245	1.96762051745465	-3.56699650425740
C	4.52963796895220	4.98376292551988	-4.95382132270037
C	-1.50272049923164	1.27404597404744	-4.83113272306168
H	-1.54720797183872	0.19085327513080	-4.80565068175799
H	-1.55575316098341	1.74802600656284	-5.80117407091906
C	-1.39108611108642	1.99644612140662	-3.70605726370144
C	-1.28102892798012	1.41238488575363	-2.37334553778885
C	-0.96383622269848	2.12157245690586	-1.28242105549905
H	-0.86692759641422	1.64420075546085	-0.31651883883289
H	-0.78942501550661	3.19022701419826	-1.32997633035945
H	-1.43126792844641	0.33999260606018	-2.28876237295467
H	-1.34171808964918	3.08029882508084	-3.76998206592850
H	-1.01554283626215	-0.89011854927200	-0.27670144879958
H	-1.32510800914769	-2.12894280735087	-1.47806093957040
H	3.14856320252683	-3.27279386695681	-2.00599635832786
H	3.00461354246380	-3.51012291721854	-0.28486613242924
H	4.66359199016019	4.24735180962621	-5.75985696862909
H	3.63931321969800	5.56291458243459	-5.23641880941024
H	3.72407432556996	4.25551671384097	-0.75359582297082
H	5.44308537484649	4.18780435826312	-1.04214830893816
H	2.50863624560288	0.35806573134702	-6.21897554004742
H	0.79865621535041	0.68368548819241	-6.49782328397696
H	3.05754464719196	-0.03322832147588	-1.33838888738682
H	1.44502446640665	0.68583555946063	-1.07637170009881
H	3.86608402835929	1.34320780492615	-2.75642276234927
H	3.80527707373370	1.72935060554215	-4.53341703662230
C	2.10037060212759	2.32544703777475	-6.98256967979788
C	1.01189446786139	3.40250542216179	-6.99350295648672
C	-1.13593526068872	-2.87675339128568	0.52209902556146
C	-2.63253334254656	-2.72718337822309	0.82612216356618

C	-0.31424960539762	-2.65215722505632	1.79332248740270
C	1.79393132678202	-4.85223543710786	-1.43852443066182
C	2.89423186695306	-5.92275369497554	-1.45042271103014
C	0.99257788808707	-4.91479046428046	-2.74018369340123
C	4.62016768841375	6.16239078204869	-1.19377272881714
C	4.93311700065964	6.46327797678203	0.27814842561669
C	5.73917760868645	5.93121025089688	-4.96662494518826
C	5.90762775604809	6.56829584698781	-6.35188935790237
C	7.02266675332713	5.19993290316137	-4.56690343724555
C	3.34015650248089	6.88729134539751	-1.61371389504544
C	2.37170670031633	1.83800435012089	-8.41936331474161
H	5.45321024641706	6.55999321834526	-1.79720514168209
H	5.03615902502693	7.53860130068253	0.43332396574148
H	4.13266897732243	6.09032925418748	0.91984284604469
H	5.86605506673911	5.97759885165768	0.56913938834264
H	3.44299868364599	7.96324009675209	-1.46375774246061
H	3.13487124999962	6.70323218302512	-2.67449237332018
H	2.48806475056383	6.53399147191546	-1.02832718867418
H	5.57282577021901	6.74681651569037	-4.24373861741754
H	7.87123015941299	5.88580657429262	-4.55407012538354
H	6.90987692117740	4.77101509645624	-3.56364768493950
H	7.24042263122895	4.39056874120448	-5.26821694302812
H	6.74862860092991	7.26387587808364	-6.35330896347302
H	6.08759948065076	5.79826226328854	-7.10464786518056
H	5.00262933459139	7.11400354658406	-6.62351940718109
H	-0.96660117015677	-3.91256871529173	0.18474608831577
H	1.11186073807232	-5.08842279655696	-0.60488908018757
H	-0.60413936411288	-3.35832351399732	2.57286626666408
H	0.75133090600515	-2.79505711161089	1.57585150015408
H	-0.45829829047855	-1.63725187258072	2.17205061631710
H	-2.93773517025656	-3.43671451817115	1.59693551846712
H	-2.85007176170839	-1.71546685229752	1.17336080182248
H	-3.21611086680157	-2.91780129028820	-0.07580085984515
H	0.56682289341099	-5.90995694924938	-2.87899805158371
H	0.17313326074149	-4.18859712651986	-2.71217616919704
H	1.63076327591174	-4.68680231005581	-3.59715953008635
H	2.45905522099575	-6.91459571531376	-1.58376023381163
H	3.59714968646042	-5.73502358794051	-2.26422566919386
H	3.44277026866478	-5.90630529567180	-0.50720604567771
H	3.03613360144566	2.77966511789406	-6.61232116105302
H	1.33047682880380	4.25506125349312	-7.59466968418289
H	0.08516368082678	3.00741678657315	-7.41271025191505
H	0.81447154661897	3.75388090365338	-5.97696119634550
H	2.65948143202612	2.68151718422464	-9.04770882628760
H	3.17909644607374	1.10609531520556	-8.41990803932130
H	1.47693823810047	1.37366198489526	-8.83428850005991

C	2.50446395748023	0.27813743925375	0.70282753310474
H	1.59588697531567	0.25030066906334	1.32724185111009
C	3.52322552568711	-0.69405003950321	1.29992810801995
C	3.05700984034379	1.70739511411860	0.75250254230186
H	3.79528742303989	-0.39281027657499	2.31271971084562
H	3.09989847274326	-1.70259430056309	1.34367302609852
H	4.42999762667279	-0.72439182821105	0.69062456746225
H	3.27669502070476	2.00353010219754	1.77938242434328
H	3.97694757997835	1.77411487041360	0.16597138395830
H	2.32733270160560	2.40583774012564	0.33690602977795
C	5.71147839129670	1.40407194649288	-3.76138799060180
C	5.64467519551385	-0.05480436615599	-4.23158893217143
H	6.22690052634239	1.98510845091958	-4.54501966258701
C	6.53778218434529	1.49558807626652	-2.47849598078199
H	6.64681125537659	-0.46562791606207	-4.36474540857064
H	5.11221608595177	-0.66424262218554	-3.49591583640766
H	5.11478881065399	-0.11982057523636	-5.18371340912155
H	7.53638553853423	1.08493625747868	-2.63620171434291
H	6.64166912972741	2.53972086975270	-2.16876278360366
H	6.05897859489831	0.93867447805855	-1.66966739810017

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### AS(III)

Atom	x	y	z
C	-0.71411807585702	-1.90827782598643	-0.60541508847748
Al	1.21056430557512	-1.90530841567359	-1.15035899151160
Cl	0.88965961980037	-1.35341762821869	-3.61556932541869
Nd	1.54410862183391	1.25883167501390	-3.75061633180134
C	1.70583665230150	1.06743646214535	-6.11445695122417
C	2.38187642074225	-3.50877988366714	-1.27366041362497
C	2.12894856398959	-0.12737313492657	-0.82090611220525
Cl	1.54826357423754	4.03776199112153	-3.21500810548831
Al	3.90227583126823	4.24234428805510	-3.25610244381295
C	4.48630644631692	4.65402946708691	-1.42138115061353
Cl	4.24255238243883	1.93147207388665	-3.55666099989318
C	4.30883823243325	5.16021568044919	-4.95419511628276
C	-1.51713298247015	1.27969050087526	-4.87490985594598
H	-1.55455818385602	0.19608027267018	-4.85909225376824
H	-1.56901713308815	1.76132271175828	-5.84121818990231
C	-1.41437000859434	1.99276619337127	-3.74428402361753
C	-1.30615343856093	1.39885329885378	-2.41504506840814
C	-0.99519237369216	2.09945389356972	-1.31739292863662
H	-0.89878097805264	1.61448510787848	-0.35526130675262
H	-0.82688267647967	3.16950297878690	-1.35468197533620
H	-1.45309306417578	0.32518924107417	-2.33834085578183
H	-1.37146621698676	3.07735489591095	-3.79891848427950

H	-0.99329390238825	-0.89192873921412	-0.28653821046113
H	-1.33912116283588	-2.12521710139199	-1.48389411595218
H	3.10692985554548	-3.33433700086925	-2.08306011145219
H	2.99005124939492	-3.56033363456817	-0.35788588781095
H	4.18421930171395	4.45683908715823	-5.78640528669328
H	3.55666267252965	5.94566458435672	-5.11296041404409
H	3.74472228634993	4.25332178478042	-0.71980880717150
H	5.41696253642414	4.10752951116732	-1.21509119137556
H	2.50471344889486	0.29972714107453	-6.16026661041371
H	0.80811038314675	0.60810581829883	-6.55996839255376
H	3.03003198172524	-0.00473497219604	-1.44609314123908
H	1.39739123688099	0.64911764597931	-1.11547299780534
C	2.13667640061824	2.25457430654014	-6.95996842070784
C	1.05777992091407	3.33881974275931	-7.04118113677876
C	-1.12230130128292	-2.87798017982622	0.51134516044772
C	-2.61283255442418	-2.71442481153723	0.83775639315800
C	-0.27901403372165	-2.66063446411212	1.76952722526589
C	1.73424245665231	-4.88549830485677	-1.48260759342471
C	2.81587681256772	-5.97487069681650	-1.50421546687573
C	0.91191109209133	-4.94187169034940	-2.77133968947568
C	4.70911639888634	6.14130369829088	-1.11104199068924
C	5.14847643817701	6.31555780440358	0.34775435763115
C	5.70559658905692	5.79184277752085	-5.04862865044301
C	5.88969705560691	6.47038601915365	-6.41148838041775
C	6.80425459878593	4.75034162234049	-4.82570149284479
C	3.44867312458392	6.96508831239325	-1.38367326340147
C	2.49453709560511	1.76258559782284	-8.37707576059982
H	5.51784966827760	6.53092621377824	-1.75164944988754
H	5.33038446467689	7.36882946444252	0.56750432725206
H	4.37677790833001	5.94369036291285	1.02439114705123
H	6.06812325890560	5.75710400596252	0.52978149978574
H	3.62336361441840	8.01887328518140	-1.16134729340621
H	3.16355988774828	6.87730850926438	-2.43946725374770
H	2.61654662904191	6.61310924081500	-0.76900887689799
H	5.80818765361349	6.56897855083299	-4.27285985596657
H	7.79059879683490	5.21125784693355	-4.89682897656513
H	6.70221842810088	4.30382911098533	-3.82852741363955
H	6.73821637798572	3.95364283037215	-5.57087028173342
H	6.86982028459080	6.94644026148944	-6.47083991081035
H	5.80668759424986	5.73623117057569	-7.21525218729529
H	5.12196368300670	7.23205243849464	-6.55670587766948
H	-0.96811622737574	-3.91508366983671	0.17099452265468
H	1.06147826389089	-5.10425093547108	-0.63690030894244
H	-0.56025459390319	-3.36679642909911	2.55209981208452
H	0.78233893376840	-2.80881178826751	1.53467159134687
H	-0.41131448628042	-1.64563736281652	2.15206595216972

H	-2.91194724656881	-3.42053813250560	1.61396576806834
H	-2.81594449766577	-1.70043224644986	1.18686804387324
H	-3.21154794595132	-2.90139108276883	-0.05493879092615
H	0.46691755296590	-5.93028904934778	-2.89647957089131
H	0.10576628456289	-4.20129309763683	-2.73536352438287
H	1.54051119045238	-4.73045646852829	-3.63946554803879
H	2.36067354131364	-6.95923324506312	-1.62444686405737
H	3.50912427610951	-5.80442852869536	-2.32992061721467
H	3.37877321659540	-5.96214058990565	-0.56949231665646
H	3.05232755884487	2.69942718628731	-6.53227470535437
H	1.41474107109396	4.18276580013499	-7.63253686801305
H	0.15284749207855	2.94479859662346	-7.50617482199383
H	0.80717363359998	3.70142174771374	-6.04034891915336
H	2.83246061070314	2.60350071569866	-8.98311531442729
H	3.29136880571157	1.02127637226840	-8.32528575336634
H	1.62256764336857	1.30977117184887	-8.84886609718435
C	2.53116501875434	0.24781473397534	0.61675803062903
H	1.64103299025605	0.18983375241461	1.26529960263223
C	3.58761622651849	-0.71006808984150	1.16982744253333
C	3.05247846010037	1.68833529732347	0.67231664871679
H	3.88550877608258	-0.41426050773268	2.17683837395903
H	3.18517468735626	-1.72726445073279	1.21575122170831
H	4.47474030493406	-0.71594339269047	0.53168217027047
H	3.29358735562126	1.97389937657272	1.69731906433662
H	3.95415193106504	1.78454845498723	0.06216787291435
H	2.29455141959312	2.37536486816216	0.28935215214800

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#### AS(IV)

Atom	x	y	z	
C	0.37501435631223	-0.28203889217552	-0.90234257341685	
C	0.03783865244820	0.04290683060365	0.55842403456994	
C	1.28139582299441	0.45944157221650	1.34594251140219	
Al	1.74143684174820	-1.67059873717667	-1.19716391099401	
C	2.22105209213571	-3.31203424039476	-0.21822029476899	
C	1.05379882832879	-4.06220973805066	0.43971693202384	
C	-0.04565418145422	-4.39194846110442	-0.57244341194366	
Cl	3.77630970782009	-0.55597512307923	-1.58640872611962	
Nd	3.46056735355982	-0.44570930385763	-4.33908100624277	
C	4.94728792995750	-2.10488253729797	-5.26835286101801	
Cl	1.80097090455237	1.94494721331560	-4.29715852004890	
Al	3.59830673883677	3.33406571302224	-3.74628623202508	
C	3.63047901016448	4.66549985807464	-5.20135817373600	
C	4.49548983098987	5.91084381636747	-4.96463125045700	
C	5.95281068225181	5.53673988781605	-4.68774332667385	
Cl	5.24551836939067	1.69481750071867	-4.20540189075461	

Cl	1.48479842063575	-2.23830253060677	-3.46977421196650
C	3.69219969631522	3.52139051693122	-1.78911815417657
C	2.98350734929354	4.73814193724048	-1.18257975247117
C	1.48990797906795	4.73784346302416	-1.51208400331982
C	-1.02201601933360	1.14928947233762	0.62054043890491
C	1.56127668384644	-5.34679631498169	1.10589869379015
C	4.40794535536428	6.84808214465326	-6.17566408341819
C	3.19218429031979	4.76260738401152	0.33658536596050
C	2.92412385562638	0.47286953073922	-7.31616378738636
C	2.12281653166392	-0.73298618672166	-7.13345050057190
C	0.90128922601677	-0.74115719885708	-6.58099548156150
H	0.70187954912163	0.63609981759744	-1.40912670101026
H	-0.54880436080300	-0.58807162422204	-1.41364876887785
H	2.74136668071923	-3.98993385091614	-0.90838415202735
H	2.95659911507370	-3.05796389004988	0.55777627226039
H	3.95875432982447	4.17432033215415	-6.12826924774671
H	2.59659050910588	4.98891638443941	-5.38970125473511
H	3.29358845004655	2.60625822508002	-1.33132584736946
H	4.75285427961050	3.55438222445750	-1.50183598282506
H	5.75941678093128	-1.63101702518977	-5.84694537749648
H	4.32909583557138	-2.68052947978887	-5.98356857741210
H	3.42590388735986	5.66077586176414	-1.59509863571857
H	2.69794652238960	5.63114361279415	0.77428801928800
H	2.78210457608348	3.85837420381915	0.79028756362950
H	4.25755643575393	4.81329602164708	0.56643428443780
H	1.00328914796173	5.61830794053815	-1.09029248575625
H	1.34499395749028	4.74767449914248	-2.59929575097347
H	1.00916435981926	3.84564266344393	-1.10383384634963
H	4.11086417343028	6.45993149287587	-4.08929622947777
H	6.55550189370676	6.43242016195650	-4.53098853005912
H	6.01406846450117	4.91596226566498	-3.78527598345441
H	6.37380410201719	4.97563968738676	-5.52547585325965
H	4.99979685912746	7.74804707208453	-6.00209130057821
H	4.78118327391169	6.34815798349477	-7.07113308510662
H	3.37061076006038	7.13992612187614	-6.34696241812841
H	-0.38699037591677	-0.85418486486185	1.03999283891631
H	0.61430996004708	-3.42789553513740	1.22706471091311
H	1.02665064489511	0.65816736943468	2.38789610308650
H	2.03035689388645	-0.34193896347938	1.31881129545628
H	1.72351335345083	1.36288799904446	0.91901717912200
H	-1.29015398506887	1.36022054240636	1.65691909572415
H	-0.64142050788320	2.06437332931458	0.16291008187949
H	-1.91905790926814	0.83871224418543	0.08297053324430
H	-0.86287641560590	-4.92929767921152	-0.08919428826914
H	-0.44808046298806	-3.46643995495317	-1.00346464524220
H	0.34721267718921	-5.01113183952290	-1.38271786776360

H	0.74171344585790	-5.86358775431364	1.60758571047544
H	1.99479000927182	-6.01562713678897	0.36015055372322
H	2.32741325460069	-5.10636375790816	1.84466356867021
H	2.43224766684578	1.42010805552944	-7.11923451352872
C	4.22126095471557	0.45784100596358	-7.64755986032376
H	2.57837632966095	-1.67248521028278	-7.43342105569644
H	0.35804259118169	-1.66340791419925	-6.42827653973353
H	0.41947235647457	0.17618042425627	-6.26381933539199
H	4.79126553989059	1.37340691322620	-7.72972394126046
H	4.74556834728636	-0.47112980540730	-7.83727899093056
C	5.55949204676986	-3.08013432526781	-4.27512047873203
H	4.77308654315919	-3.48786897600514	-3.61382335337255
C	6.15638411396678	-4.27260683312528	-5.05090826557464
C	6.63746758283819	-2.41650446855094	-3.41378652626409
H	7.03830289196663	-3.12826402197010	-2.69190111571586
H	7.45447956862831	-2.05490761586041	-4.04011111802633
H	6.21863356845946	-1.56887708136451	-2.86436059952913
H	6.59542031913482	-4.98211861023345	-4.34969898229101
H	5.37721712824445	-4.77557857693759	-5.62254258373381
H	6.92724297364069	-3.92395496879812	-5.73773425266426

**TABLE S2:** Atomic Cartesian coordinates (in Å) for optimized structures of *i*-C<sub>4</sub>H<sub>9</sub>-AS+ $\eta$ -*trans*-C<sub>4</sub>H<sub>6</sub>

**AS(I)**

Atom	x	y	z
C	-0.50765694836898	0.46360603610219	-0.26014353125039
Al	-0.01631739354995	-0.37995435502306	1.49163362483184
C	2.12962274358129	-0.64759021159983	1.37689947627031
Nd	2.27319649371817	1.15724807993501	3.17203374485218
C	-0.53745352976590	-2.07964124543926	2.43799677425520
C	-0.42675047843387	1.25730303380837	2.79554233224103
Cl	2.70113222344060	3.03522334821037	1.26004521873544
Al	1.40424944688988	5.11374603249483	1.86357625687711
C	-0.21347628663003	4.82864955637449	0.72693120109997
C	1.19578908610492	4.54373565301182	3.79986006765078
C	2.80583598194083	6.50121731070438	1.55268071248155
H	-1.00676180788277	1.41826684824482	-0.04249576499329
H	0.45634608814671	0.76279003359903	-0.69779526875431
H	0.34373099497729	-2.73567563152291	2.49546667104630
H	-0.72255019338914	-1.78466870351023	3.48140347577651
H	3.19296062079119	6.83044157615906	2.52715633818753
H	3.65642100003735	6.01566773828103	1.05229578207765
H	-0.39835612016272	3.74615954188149	0.68690907720049
H	-1.08279339634333	5.25122166222033	1.25309534485952
C	5.64881101511095	2.62661238592667	5.63021079772851

H	5.68095011864762	1.61432430155699	6.05032023908892
H	6.64627153389783	2.84216931189500	5.23590701517937
C	3.97602030673553	-0.31585579940326	4.50589523097713
C	4.80509777292851	0.28807863368282	3.53725283335538
C	4.95376741773818	1.64676895572380	3.37268881508615
C	4.63925997499727	2.64760162917725	4.45619575430417
H	3.89655022825941	-1.39654509607253	4.51806580862730
H	3.89028364658675	0.14396851343836	5.48519979885203
H	5.15814813779515	-0.33837421732895	2.72090151225393
H	5.50698001910977	2.01524127298973	2.51944463544304
H	4.58612104462862	3.64974880019838	4.02950998112262
H	3.64738863559793	2.47765047378092	4.92371981529469
C	0.92923289767083	-0.34773001582211	5.77806637285344
C	1.04386704225870	0.78703651510583	6.48335059596966
C	2.08030149671468	1.02288645677126	7.47575958106559
C	2.16506507563910	2.12690155845115	8.22260845641790
H	2.94381180085098	2.24924075505854	8.96409841588127
H	1.44740714825661	2.93293009197179	8.12615847229033
H	2.80820242872701	0.22806350059434	7.61274831954934
H	0.31693675410690	1.58332954814755	6.33952305973353
H	0.11430586174772	-0.51116755587772	5.08733099870911
H	1.62487760596433	-1.16614421702734	5.91244306907414
H	2.18232396889470	4.19992111427418	4.15190653857639
H	0.49448678238005	3.69953048504744	3.89311700125809
H	2.79221441804444	0.16844757673298	1.02605654785177
H	2.62376464154513	-1.10929136914012	2.25376264171234
H	-0.13039436020145	1.43127710607734	3.84557193942057
H	-0.19427065209828	2.18661774400481	2.25432574851059
C	7.63518947627861	6.09555824080518	6.11557226369794
H	7.21107128221121	6.92574819557514	6.68713970200648
H	8.70266627536325	6.29476187063241	5.97765160322990
C	5.26787897643100	3.60233924147144	6.70955249494412
C	6.05512899597925	4.51365830824858	7.26913010130221
H	4.23778097445183	3.51058544736457	7.04905161517048
H	5.64085253660141	5.15313530633069	8.04502455091771
C	7.49317000312459	4.79300927320324	6.93609591455851
H	8.05635940556841	4.91397860562745	7.86702210834532
H	7.94364254019740	3.96777734256810	6.37767537778878
C	6.98163183553776	5.96414180455898	4.76794046121569
C	5.79025250953564	6.43597478603790	4.41795203701044
H	7.55491793381574	5.39139112305057	4.04252949847238
H	5.43572521117989	6.26862511828275	3.40216653167273
C	4.85688225390948	7.24457870388576	5.27440405404515
C	4.77810165086142	8.69031574436396	4.75611143762373
H	3.86178671933026	6.78785829325201	5.23379812398884
H	5.17905511159052	7.24659961529976	6.31964529778284

H	5.79678183952820	9.07940948076795	4.65144271153275
H	4.32204805411702	8.68999875431688	3.75985407547844
C	-1.32005915145257	-0.24268727231045	-1.35687660003862
C	-1.22807177509683	0.53095370582561	-2.67889135473633
C	-2.78766275089499	-0.38512421292002	-0.94897190078114
C	-1.73295268570879	-2.94258245318700	1.99886893784989
C	-2.10481658254233	-3.94690815566555	3.09795285090888
C	-1.42908252634718	-3.69254786244916	0.70084148317968
C	-0.22890269218445	5.35789000540013	-0.71342268868913
C	-1.59936960373721	5.10378845599631	-1.35681144177020
C	2.42811619641334	7.74813428899385	0.74039540250170
C	3.64736950727344	8.65994346803285	0.55055506234056
C	1.29275673017338	8.52506925357729	1.40967519906728
C	0.87167745757814	4.71917098054177	-1.56214053357081
H	-0.06715144783982	6.44895461383802	-0.70666653129065
H	-1.62150023637606	5.49223338537384	-2.37654668715764
H	-1.81185228951435	4.03318961643068	-1.38496364795227
H	-2.38233489742663	5.59683956168098	-0.77825525440166
H	0.85939840248207	5.12528406732712	-2.57500740942448
H	1.85288876590523	4.92109763979704	-1.11951873571718
H	0.73337281713094	3.63671198827763	-1.62033118060221
H	2.08714153315107	7.44324213080929	-0.26258994526115
H	1.01027231234008	9.39237508333272	0.81060589768538
H	0.41412595795170	7.87959216572526	1.51995007540720
H	1.59423112176625	8.87120538383113	2.40105628155194
H	3.38501789865953	9.52844463964467	-0.05622619001904
H	4.01566178946126	9.00748465606570	1.51766726433424
H	4.44896640943643	8.11334726547789	0.05132892881789
H	-0.91044553806678	-1.25137842509981	-1.53621162268765
H	-2.61304598132926	-2.29934166344428	1.82844813770735
H	-3.34475220836002	-0.94993946605619	-1.69852903165671
H	-2.86453511628104	-0.90986646574371	0.00840641661535
H	-3.25060555332327	0.59861620700990	-0.83959687139751
H	-1.80938681297736	0.03287457136272	-3.45721125502679
H	-1.61217334917850	1.54506023813257	-2.55082248700693
H	-0.18904965749326	0.59341297746822	-3.00669761006995
H	-2.30806592759268	-4.24068362483757	0.35713279072848
H	-1.13288524355874	-2.98794223169742	-0.08222666291435
H	-0.61267327879647	-4.40287751087726	0.85054071782951
H	-2.94315734802954	-4.57009523835597	2.78090492521105
H	-1.25383703100808	-4.59262544649043	3.32417880586652
H	-2.39013683929567	-3.41806455922210	4.00890384187016
C	3.98854972832174	9.62754413074946	5.68351276259382
C	4.08867113282174	11.06608661718850	5.16205412112425
C	2.51908925719518	9.21280632904436	5.80653751273165
H	4.44356265568998	9.59061048645650	6.68418307158409

H	1.97269971375184	9.93857996400271	6.41044394906975
H	2.05013352385322	9.16065639855986	4.82165617832996
H	2.43190237110958	8.23813756294692	6.28658516271452
H	3.55969212134234	11.74849084309737	5.82865623955649
H	5.13233594701850	11.37837763746001	5.10525815554711
H	3.64882583297252	11.14335188659119	4.16597649610706
C	0.73656148160977	5.62640038013139	4.78993663135522
C	0.71830290819425	5.08840180579500	6.22542887832304
H	1.45338227892138	6.46395624149886	4.75843570234831
C	-0.64290692280656	6.17455530602732	4.42113976660268
H	-1.39273280903094	5.38028283368384	4.44344695148760
H	-0.94636090329075	6.95749413237635	5.11822450442488
H	-0.61944168269609	6.60145821190231	3.41250896400111
H	0.41020460359311	5.86587516856380	6.92673989004556
H	0.02431664520905	4.24962884742147	6.30527290684319
H	1.71533490226391	4.74417776931805	6.50354015257919
C	2.20296653678836	-1.71377580775396	0.25340020692752
C	2.92538138082752	-2.97793535783354	0.72705023468075
H	1.18231194911987	-2.02545308770132	-0.05855284863572
C	2.90026634761173	-1.16187988775957	-0.99174333684464
H	2.94973908612387	-3.72494248620283	-0.06924588777968
H	3.95172725778759	-2.74336824269816	1.01690889742584
H	2.41340963050589	-3.41034424903181	1.58929437939447
H	2.90037483561683	-1.90678603798861	-1.79040461831814
H	2.38761004491515	-0.26858885676704	-1.35477647302628
H	3.93447426564472	-0.89633897016507	-0.76259032514828
C	-1.97536973590026	1.17525224723880	2.86470525046720
C	-2.63027271001469	2.52277221525811	2.54685422066165
H	-2.35542253647146	0.45007922280985	2.11248496112516
C	-2.45896074766726	0.69629701110149	4.23420735551306
H	-3.71640181542289	2.45182425719208	2.63558692620167
H	-2.27296824908606	3.28933981628358	3.23825988084388
H	-2.38877678711003	2.83140661584045	1.52845184705509
H	-3.54828364441856	0.61987369690953	4.24487000537329
H	-2.04733020556070	-0.28613178152170	4.47098232490489
H	-2.15371331789483	1.39733993786717	5.01365800008890

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## AS(II)

Atom	x	y	z
C	-1.09494915418962	0.09160318875800	-0.41263771013743
Al	-0.16912328578645	-0.67403565708411	1.17435799423698
C	1.87908700705533	-0.65829365995733	1.14961502782363
Nd	2.49716866810149	1.47138501357404	3.09636085023494
C	-0.86523800347385	-2.18113330702905	2.29065440842893
Cl	-0.25332896844507	1.19384259077401	2.77307829469924

Cl	3.13657628930673	2.90898647915069	0.88844436953860
Al	1.66347967034781	4.80656013253115	1.55640274238123
C	0.01493754708338	4.38028469745489	0.52546561165580
C	1.59199746780695	4.23245824042851	3.53246978721201
C	2.90343705348113	6.34931854935860	1.30409698096538
H	-0.81398040086673	1.15094601512620	-0.49511116124674
H	-0.69702394392238	-0.38291581413873	-1.32133659099763
H	-0.01870033916255	-2.65257236409132	2.81363037420136
H	-1.51331622548654	-1.77624096009269	3.08134118375730
H	3.21485853239685	6.71686492626799	2.29200036532322
H	3.82132870249835	5.96016084066628	0.84018134402923
H	-0.09035245405953	3.28675053386351	0.50451118821641
H	-0.85835508154578	4.73447423561208	1.09327543611533
C	5.67902621799199	2.45556241896178	6.21008879184517
H	5.67234043965904	1.38816138031747	6.45699857166979
H	6.68573486598270	2.69859559358689	5.85739097729331
C	4.26223552985745	-0.16354056655182	4.15456966907577
C	5.06624356579346	0.77199839075184	3.47782664571803
C	5.09101088193480	2.12549230801168	3.73838320822614
C	4.67307491032963	2.72413678392773	5.05782255657822
H	4.28694224611957	-1.19923297297758	3.84085579689468
H	4.05597753575234	-0.02235059957376	5.21096350215988
H	5.50821954340715	0.45725418321894	2.53383012639736
H	5.64966506642214	2.76959996056621	3.07187653212154
H	4.55408073849242	3.80247603592308	4.94679416477996
H	3.69421086790072	2.35211654636186	5.41356432278866
C	1.18809677946236	-0.76357051962792	5.26826364290995
C	1.03326918152518	0.33035065220037	6.02735714549617
C	1.88308258605538	0.66130024482848	7.16088203990340
C	1.68098758888140	1.70611342203195	7.96786483071071
H	2.32932604657537	1.90507321335798	8.81107051845215
H	0.85027357721636	2.38571665672080	7.81555677570201
H	2.71725046536824	-0.00836363779912	7.35315639115735
H	0.21134680353092	1.00882368526828	5.81021336658239
H	0.50467452002806	-0.99162626253393	4.46213922796490
H	1.97989045611685	-1.47521935078646	5.46595004933085
H	2.60976409672651	3.99929157497457	3.89106714688307
H	0.91472037896682	3.38667199876360	3.74407690795855
H	2.27234950318585	0.32306072170022	0.82732715456242
H	2.23113766593354	-0.89167504378201	2.17580116143639
C	7.25082277042023	6.06869796763273	6.66398900712320
H	6.68850918754274	6.80310782222190	7.24664335942085
H	8.26111647553981	6.46541714435710	6.51335737501160
C	5.32144177817332	3.27230018285564	7.41993195268458
C	6.03604140080345	4.26248484925951	7.94345649918139
H	4.36153208258256	3.01909360144796	7.86426452731767

H	5.63677041107176	4.79043838992834	8.80629692888086
C	7.37508277740451	4.76080568551004	7.47681472309319
H	7.99659919781272	4.96605754134429	8.35436737966865
H	7.89267013005543	4.01194112653900	6.87035803799471
C	6.62656325984471	5.82859372558698	5.31838473244185
C	5.49943711822757	6.35190224296544	4.84810863864946
H	7.18631368428908	5.14075543042475	4.68785299000152
H	5.18361083113328	6.09042182560205	3.83851145304302
C	4.59490832040382	7.33318283965131	5.53785412871534
C	4.55516744086558	8.65760784249258	4.75825414452869
H	3.58688444291793	6.90761826512183	5.58034765207432
H	4.91810655300202	7.52304318688699	6.56546159233369
H	5.57928180557758	9.03381555922462	4.65972287984777
H	4.17557025781127	8.47059430141421	3.74706057277900
C	-2.62627447168039	-0.01702557357119	-0.46172130338065
C	-3.15682357837848	0.52639609428662	-1.79483433736737
C	-3.28639890809534	0.72134464456895	0.70382848864458
C	-1.64558749791666	-3.28491037792258	1.56075869566616
C	-2.06460623022868	-4.38647417888195	2.54311081714737
C	-0.82355999430114	-3.88614896283547	0.41854056640938
C	-0.10385366781584	4.91205371972299	-0.90903503625303
C	-1.46545595635234	4.53645879840742	-1.50711195242708
C	2.42503873817778	7.54997069697071	0.47428682354964
C	3.55132580129560	8.58094498101224	0.32333118858657
C	1.19602996263146	8.21003932228000	1.10193728618857
C	1.02015720653601	4.38484709771209	-1.80271975558870
H	-0.04258481255734	6.01353432881415	-0.89643110387739
H	-1.57318248245928	4.95615110324794	-2.50878276801729
H	-1.56044051416778	3.45065195716333	-1.57083446447222
H	-2.27147924458762	4.91911279035456	-0.87886776763233
H	0.92234564980249	4.77986559990682	-2.81527088085165
H	1.99322867460738	4.69175080108501	-1.40317921681716
H	0.99315331088846	3.29304902863934	-1.85130556778228
H	2.15029866901098	7.21080911623636	-0.53831109297447
H	0.84892777608960	9.04336925173499	0.48883151156742
H	0.38201438144981	7.48163255655070	1.18735641557197
H	1.42959587936479	8.58782076228041	2.10002549970506
H	3.21766198138338	9.42714222123743	-0.27985875785520
H	3.86165608551066	8.94990765006537	1.30287624712978
H	4.41432585697648	8.12363992203546	-0.16326732020166
H	-2.91862606062787	-1.07940838721589	-0.40172681377280
H	-2.56583419282545	-2.85729218712291	1.12973481799510
H	-4.37264272568476	0.63225548535839	0.64702661230699
H	-2.95325709075876	0.29411174009034	1.65595632029679
H	-3.02368936773961	1.78200655839636	0.68734943679555
H	-4.24229599001213	0.42385331466883	-1.84377227117610

H	-2.89950481247210	1.58151557600966	-1.90285780980940
H	-2.71587512210535	-0.02468588458160	-2.62711825740485
H	-1.39228266198257	-4.65629735878060	-0.10507435932300
H	-0.55816520519915	-3.10306158260060	-0.30214310278122
H	0.09783796564479	-4.33349981313954	0.79980047523009
H	-2.64490434682879	-5.15569211473567	2.03051865310919
H	-1.18398372743222	-4.85101862051231	2.99093973058217
H	-2.67583004460980	-3.96114040678571	3.34066695728145
C	3.69596038338339	9.73414065061446	5.44114416606075
C	3.90329571470442	11.08157212713733	4.73915298364847
C	2.20863914653831	9.36665038186471	5.44005977443926
H	4.02840011558660	9.83468053928114	6.48469738655495
H	1.62385275823140	10.16903226681173	5.89205393667866
H	1.85318861456927	9.21335517252977	4.41902425255903
H	2.03252335387414	8.45527663265185	6.01123516501639
H	3.32186614292126	11.85982084184007	5.23526919031582
H	4.95577711631258	11.36675289638251	4.76583505148995
H	3.58570650144055	11.02322281670154	3.69651320762860
C	1.10113105878099	5.35213395264334	4.47210270015933
C	1.19693729451140	4.91756704787128	5.93864011325022
H	1.74323706253251	6.23906479964580	4.34309440271863
C	-0.33683309679169	5.75813462740967	4.14659261344470
H	-0.67501976384507	6.54950783037402	4.81762097250929
H	-0.39886489362064	6.13081117867896	3.11827429422814
H	-1.01202230325310	4.90474156864126	4.24679220269217
H	0.85633386873956	5.71324142288273	6.60340660137175
H	0.58029106019862	4.03297482618905	6.10809273938879
H	2.22990218889693	4.67350921452297	6.19146380808361
C	2.60813112066199	-1.68198277159269	0.25705861016467
C	4.11445409931782	-1.67944085850460	0.54551822556663
H	2.22906182130273	-2.69439516787988	0.47700693376492
C	2.36842092246592	-1.39316588678800	-1.22578726012505
H	4.64016456852077	-2.35850470083894	-0.12795480231829
H	4.52254700641080	-0.67391846006232	0.41549386192938
H	4.29971829767992	-2.00126923152611	1.57159570540627
H	2.91138702970274	-2.10597866733464	-1.84850490847592
H	1.30329237452863	-1.47737451455881	-1.45959772826289
H	2.70159913731070	-0.38430323522061	-1.48129909971573

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### AS(III)

Atom	x	y	z	
C	-0.19374000038149		0.24827312318746	-0.61509772865974
Al	-0.19987517589688		-0.49445629409480	1.21099750639851
Cl	2.04999037586051		-0.84153093394288	1.79386221866176
Nd	2.33927569659752		1.41659639227381	3.39729465953046

C	-1.20675771673301	-2.02013346906690	1.96628354687142
Cl	-0.48152579925262	1.23633723347426	2.72143798630028
Cl	2.75065829432716	2.88150290768074	1.14531242086635
Al	1.32376658147855	4.79495714171741	1.79271226537744
C	-0.35022096092320	4.45231873125468	0.76015592615942
C	1.27672868946955	4.25642283881469	3.77896517146084
C	2.57670162706210	6.32139423608781	1.49570294692316
H	0.07654330078243	1.30973122561090	-0.55205039888157
H	0.61126670871637	-0.23193148653589	-1.18833085943089
H	-0.64241137070536	-2.43014144015156	2.81503132441989
H	-2.14739020106876	-1.63866238540089	2.38796773920906
H	3.00342879858354	6.61271996108370	2.46559597720947
H	3.42657539085083	5.94630056937841	0.90722643407839
H	-0.45023495321279	3.36853431065753	0.61844351707874
H	-1.21235932416411	4.73811725641154	1.38042475610220
C	5.89464296224295	2.73196581521149	5.67862740762660
H	5.92136006061834	1.72306701642314	6.10529782063081
H	6.86504691727642	2.90806122711477	5.20545213609956
C	4.02977256956162	-0.13809917073737	4.73699520305594
C	4.80351715873306	0.40341663634387	3.70374062470048
C	4.98771514273354	1.75878797991619	3.48966346949692
C	4.79902585767991	2.78026563196975	4.58142845077752
H	3.85717737430068	-1.20576234798991	4.76160872467037
H	3.99090733501511	0.35467849334387	5.70267435529325
H	5.06536346025536	-0.25609081039509	2.87879583564832
H	5.51059200041691	2.08491086473793	2.60087594783810
H	4.75655516022610	3.78308105825977	4.15300774129615
H	3.83895868617168	2.64907122842091	5.12484869470658
C	0.70840142898078	-0.63481832623580	5.41826333027148
C	0.73303192936222	0.45830405985153	6.19370720202189
C	1.67735621162374	0.66035787485024	7.28351885704908
C	1.68873847841518	1.73076439691377	8.08066116466157
H	2.40797709829423	1.83110260712256	8.88311795261977
H	0.97068291677842	2.53373416648570	7.96271193534928
H	2.40290539596901	-0.13187068872748	7.44240781975503
H	-0.00548531460259	1.24035319372234	6.02809919501955
H	-0.03406532589042	-0.75815470433247	4.64283381952087
H	1.41588296411676	-1.44188744798463	5.56151523499055
H	2.31509086240885	4.07961823335827	4.10975021240187
H	0.65993209019904	3.36821756202439	4.00777375520864
C	7.66494233912779	6.36349704983555	5.69357666762563
H	7.21215532653210	7.16783710435637	6.27960187769955
H	8.68211398867082	6.67171147025162	5.43167786913386
C	5.62880629887597	3.73205485676095	6.76896472877203
C	6.42390247296328	4.72762062252552	7.14508003527771
H	4.67837268021652	3.59163848321976	7.27986930272067

H	6.09456681647349	5.37650962356976	7.95326372469134
C	7.76119888981310	5.09201155423584	6.56736624474695
H	8.45635992993340	5.29564653384328	7.38809779618515
H	8.17865368583091	4.27742275391359	5.96914686018894
C	6.89546456780018	6.10379604112310	4.42873472725657
C	5.64111996937772	6.46448304376877	4.18025685671915
H	7.44336149177668	5.54473545955960	3.67370420679472
H	5.20894723967551	6.22713963488012	3.20995844527799
C	4.73866208522238	7.24002368578531	5.09943096598112
C	4.76466306271573	8.73665024863998	4.74340797470610
H	3.71817112413933	6.85829338056762	4.99354706908991
H	5.03765771702861	7.11000891321408	6.14393360742459
H	5.80493590831634	9.07900888340060	4.76009039043771
H	4.39141756676473	8.87255243406805	3.72235342885895
C	-1.50801958040258	0.10813418105126	-1.39451966077814
C	-1.37457799402615	0.74301605816953	-2.78345369230423
C	-2.67903837433149	0.73740093113102	-0.63749109991727
C	-1.53438792111708	-3.16077997116705	0.99089170101977
C	-2.32092455872651	-4.26479116316713	1.70784940638701
C	-0.26627803980196	-3.74119976795522	0.36125598037981
C	-0.48876148669886	5.14533479204819	-0.60107598608809
C	-1.88763953597569	4.91167997103478	-1.18599782417314
C	2.05091461549136	7.58973635294254	0.80839217712517
C	3.18114346527994	8.61214167623105	0.63058175741089
C	0.89825425259849	8.21706837555024	1.59421186312907
C	0.57914083623144	4.66732351114866	-1.58558856989849
H	-0.37143873479132	6.23437471111554	-0.47119597448631
H	-1.99413142584224	5.43288968812839	-2.13887750477177
H	-2.05599488410246	3.84595931007780	-1.34951373571392
H	-2.64904190976025	5.28163846188902	-0.49746215336740
H	0.48721384246392	5.19298399836020	-2.53739079282046
H	1.57829954841136	4.85863677512821	-1.17818230141013
H	0.47932980587545	3.59504440072071	-1.76953615146960
H	1.67951777967753	7.33525140420766	-0.19752711605782
H	0.51457123055737	9.09969918133297	1.08011172654572
H	0.08080462262537	7.49501648115315	1.69871370436347
H	1.22828671994627	8.51325227050795	2.59239587914508
H	2.81085608465871	9.50686353279954	0.12725041562756
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H	0.26845716251318	-2.96150579631297	-0.19527627641041
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H	1.32451437492073	6.28808982866536	4.52978071106651
C	-0.72515378455049	5.65866160688243	4.45443153276058
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#### AS(IV)

Atom	x	y	z
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Al	2.14026228067785	4.67190691847301	1.17146587007951
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C	2.39095753134760	2.27097699482786	7.15627564172571
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C	1.05803008323817	9.51608029746235	6.52863639476097
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H	0.05673152791573	9.41447165026758	6.94955655798749
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H	0.99771802813755	10.14651995878110	5.63960963415210