

Electronic Supplementary Information

DFT-calculation of the Structures of (1-methyl-4-phenyl-1-azabuta-1,3-diene)tetracarbonyliron(0) and (4-phenyl-1-oxabuta-1,3-diene)tetracarbonyliron(0).

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 - 4.4 η^3 C-acyl
 - 4.5 η^2 N=C cisoid
 - 4.6 η^2 N=C transoid
 - 4.7 σ^2 N cisoid
 - 4.8 σ^2 N transoid

1. Colour versions of Figures 1, 2 and 4.

Figure 1 Calculated structures of the (1-methyl-4-phenyl-1-azabuta-1,3-diene)tetracarbonyliron(0) complexes 1-8.

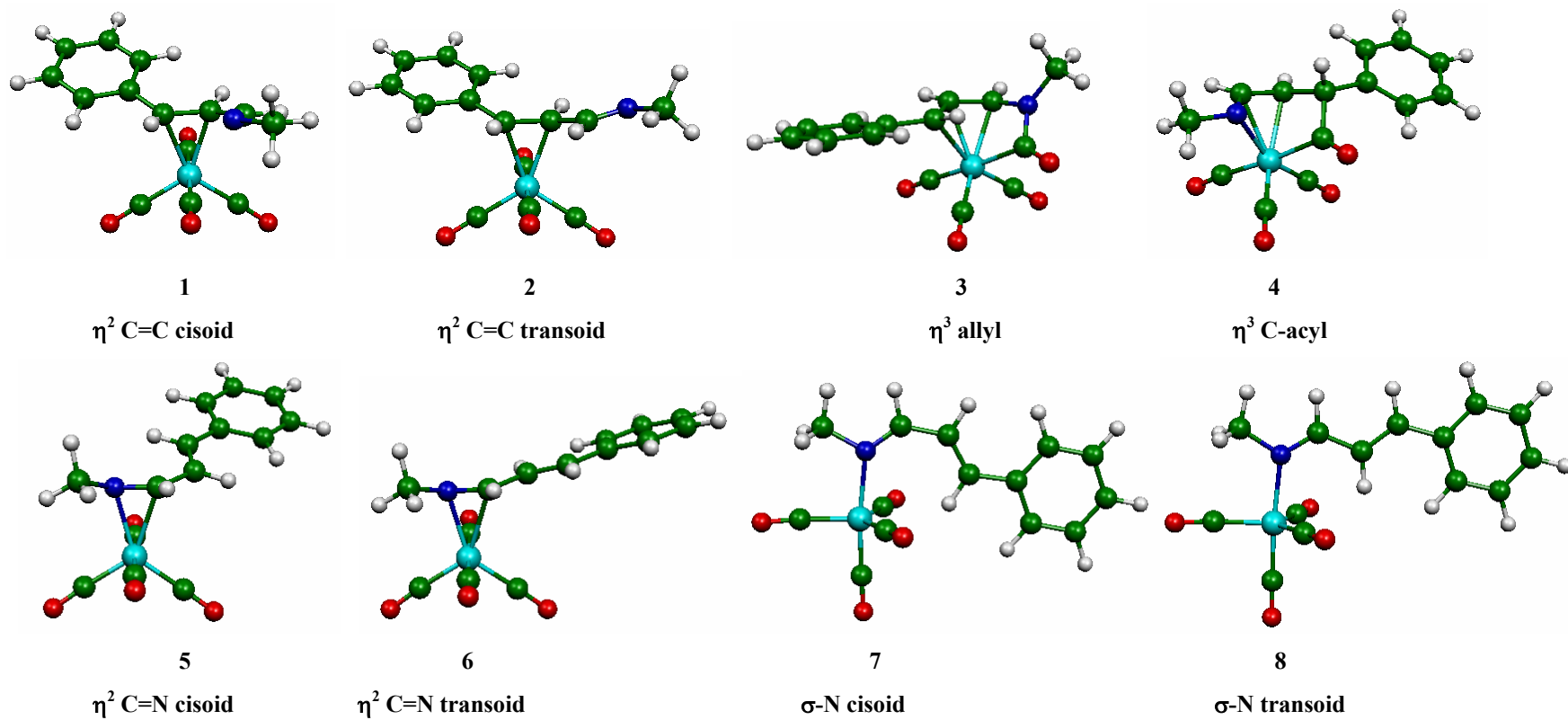


Figure 2 Calculated structures of the (4-phenyl-1-oxabuta-1,3-diene)tetracarbonyliron(0) complexes **9-16**.

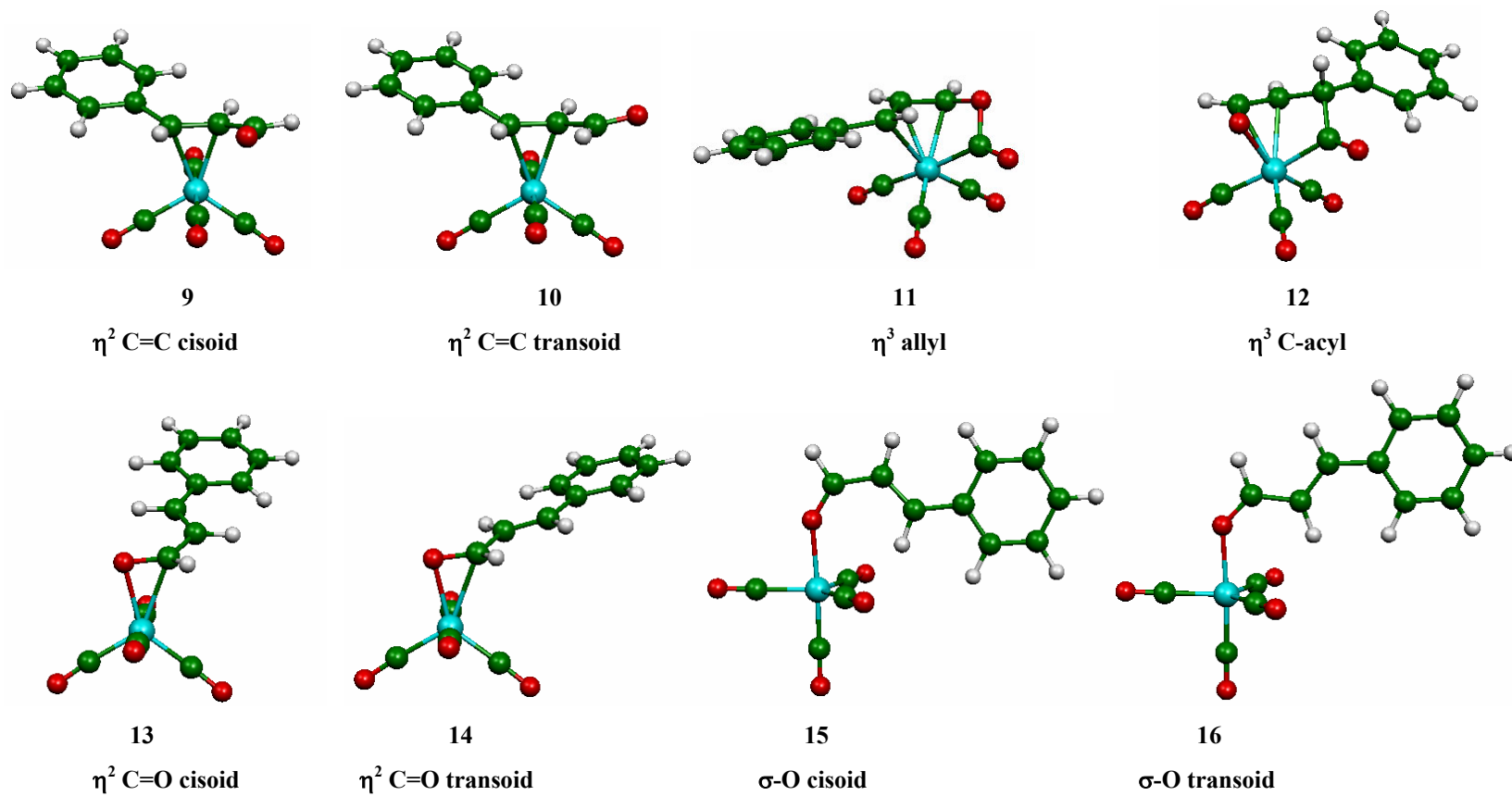
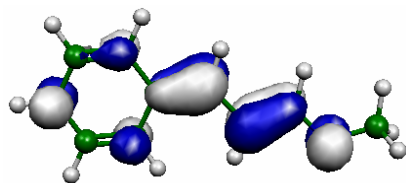
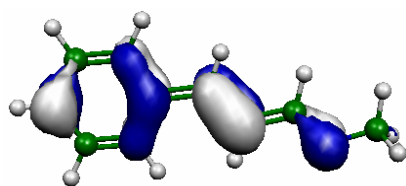


Figure 4 Relevant orbitals and orbital energies of 1-methyl-4-phenyl-1-azabuta-1,3-diene and 4-phenyl-1-oxabuta-1,3-diene in *transoid* conformation (orbital energies of the corresponding *cisoid* conformation are given in parenthesis).

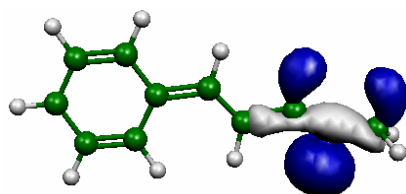
1-methyl-4-phenyl-1-azabuta-1,3-diene



LUMO, $E = -1.54$ eV (-1.59 eV)

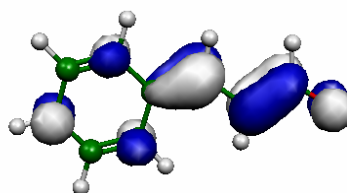


HOMO, $E = -5.94$ eV (-5.85 eV)

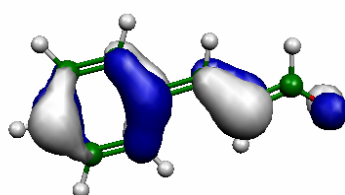


HOMO-1, $E = -6.74$ eV (-6.72 eV)

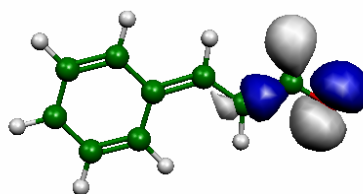
4-phenyl-1-oxabuta-1,3-diene



LUMO, $E = -2.09$ eV (-2.12 eV)



HOMO, $E = -6.58$ eV (-6.47 eV)



HOMO-1, $E = -6.74$ eV (-6.76 eV)

2. Calculated absolute energies and zero point energies of the (1-azabuta-1,3-diene) and (1-oxabuta-1,3-diene)tetracarbonyliron(0) complexes.

	Gas phase values (B3LYP/LANL2DZ/6-31G*)		PCM single point calculations, $\epsilon = 8.93$ (CH ₂ Cl ₂)
	Absolute energy (a.u.)	ZPE-correction (a.u.)	Absolute energy (a.u.)
Ligand 1^a			
η^2 (C=C) cisoid	-1019.2267957	0.219855	-1019.233815
η^2 (C=C) transoid	-1019.2271899	0.219703	-1019.234993
η^3 (C=C-C) allyl	-1019.2271101	0.222446	-1019.238952
η^3 (N=C-C) C-acyl	-1019.2026560	0.221294	-1019.212763
η^2 (C=N) cisoid	-1019.2169111	0.219680	-1019.223679
η^2 (C=N) transoid	-1019.2193954	0.219310	-1019.226528
σ -N cisoid	-1019.2333448	0.221031	-1019.243429
σ -N transoid	-1019.2443459	0.220909	-1019.255005
Ligand 2^a			
η^2 (C=C) cisoid	-999.7940696	0.179479	-999.8032785
η^2 (C=C) transoid	-999.7928552	0.179435	-999.8030563
η^3 (C=C-C) allyl	-999.7782345	0.181750	-999.7903995
η^3 (O=C-C) C-acyl	-999.7638468	0.180872	-999.774797
η^2 (C=O) cisoid	-999.7836852	0.178989	-999.7917758
η^2 (C=O) transoid	-999.7850315	0.178742	-999.794685
σ -O cisoid	-999.7890824	0.179352	-999.7992019
σ -O transoid	-999.7956896	0.179426	-999.8088429

^a 1: 1-methyl-4-phenyl-1-azabuta-1,3-diene; 2: 4-phenyl-1-oxabuta-1,3-diene

3. Z-matrix coordinates of the 1-azabuta-1,3-diene complexes

3.1 η^2 olefin cisoid

```

fe
c 1 cfe2
c 1 cfe3          2 cfec3
c 1 cfe4          3 cfec4          2 dih4
c 1 cfe5          4 cfec5          3 dih5
o 2 oc6          1 ocfe6          5 dih6
    
```

o	3	oc7	1	ocfe7	5	dih7
o	4	oc8	1	ocfe8	5	dih8
o	5	oc9	1	ocfe9	2	dih9
c	7	co10	3	coc10	1	dih10
n	10	nc11	7	ncol11	3	dih11
c	11	cn12	10	cnc12	7	dih12
c	12	cc13	11	ccn13	10	dih13
c	13	cc14	12	ccc14	11	dih14
c	14	cc15	13	ccc15	12	dih15
c	15	cc16	14	ccc16	13	dih16
c	16	cc17	15	ccc17	14	dih17
c	17	cc18	16	ccc18	15	dih18
c	18	cc19	17	ccc19	16	dih19
c	19	cc20	18	ccc20	17	dih20
h	10	hc21	11	hcn21	12	dih21
h	10	hc22	11	hcn22	12	dih22
h	10	hc23	11	hcn23	12	dih23
h	12	hc24	13	hcc24	14	dih24
h	13	hc25	14	hcc25	15	dih25
h	14	hc26	15	hcc26	20	dih26
h	16	hc27	15	hcc27	20	dih27
h	17	hc28	16	hcc28	15	dih28
h	18	hc29	19	hcc29	20	dih29
h	19	hc30	20	hcc30	15	dih30
h	20	hc31	19	hcc31	18	dih31
cfe2			1.817314			
cfe3			1.828171			
cfec3			179.776			
cfe4			1.791578			
cfec4			89.548			
dih4			-37.547			
cfe5			1.792594			
cfec5			113.681			
dih5			90.018			
oc6			1.147456			
ocfe6			178.299			
dih6			12.174			
oc7			1.145975			
ocfe7			176.580			
dih7			-71.897			
oc8			1.152052			
ocfe8			179.005			
dih8			-36.466			
oc9			1.152928			
ocfe9			178.009			
dih9			-97.430			
co10			3.862419			
coc10			89.106			
dih10			159.655			
nc11			1.449280			
ncol11			52.673			
dih11			33.763			

cn12	1.273911
cnc12	118.144
dih12	-105.599
cc13	1.477207
ccn13	123.269
dih13	179.536
cc14	1.410001
ccc14	123.074
dih14	-2.430
cc15	1.481489
ccc15	126.486
dih15	146.584
cc16	1.406987
ccc16	118.675
dih16	178.633
cc17	1.391926
ccc17	121.238
dih17	178.703
cc18	1.397244
ccc18	120.140
dih18	-0.211
cc19	1.395745
ccc19	119.370
dih19	-0.488
cc20	1.394459
ccc20	120.446
dih20	0.361
hc21	1.103342
hcn21	113.809
dih21	1.615
hc22	1.097163
hcn22	109.289
dih22	-120.012
hc23	1.096772
hcn23	109.353
dih23	123.381
hc24	1.103728
hcc24	115.037
dih24	178.250
hc25	1.087285
hcc25	119.313
dih25	-7.756
hc26	1.086732
hcc26	113.557
dih26	150.727
hc27	1.087710
hcc27	118.999
dih27	-179.405
hc28	1.086723
hcc28	119.697
dih28	179.934
hc29	1.086437

hcc29	120.285
dih29	179.793
hc30	1.086814
hcc30	119.488
dih30	179.844
hc31	1.086144
hcc31	119.052
dih31	-178.389

3.2 η^2 olefin transoid

fe			
c	1 cfe2		
c	1 cfe3	2 cfec3	
c	1 cfe4	3 cfec4	2 dih4
c	1 cfe5	4 cfec5	3 dih5
o	2 oc6	1 ocfe6	5 dih6
o	3 oc7	1 ocfe7	5 dih7
o	4 oc8	1 ocfe8	5 dih8
o	5 oc9	1 ocfe9	2 dih9
c	3 cc10	1 ccfe10	5 dih10
n	10 nc11	3 ncc11	1 dih11
c	11 cn12	10 cnc12	3 dih12
c	12 cc13	11 ccn13	10 dih13
c	13 cc14	12 ccc14	11 dih14
c	14 cc15	13 ccc15	12 dih15
c	15 cc16	14 ccc16	13 dih16
c	16 cc17	15 ccc17	14 dih17
c	17 cc18	16 ccc18	15 dih18
c	18 cc19	17 ccc19	16 dih19
c	19 cc20	18 ccc20	17 dih20
h	10 hc21	11 hcn21	12 dih21
h	10 hc22	11 hcn22	12 dih22
h	10 hc23	11 hcn23	12 dih23
h	12 hc24	13 hcc24	14 dih24
h	13 hc25	14 hcc25	15 dih25
h	14 hc26	15 hcc26	20 dih26
h	16 hc27	15 hcc27	20 dih27
h	17 hc28	16 hcc28	15 dih28
h	18 hc29	19 hcc29	20 dih29
h	19 hc30	20 hcc30	15 dih30
h	20 hc31	19 hcc31	18 dih31
cfe2=	1.819515		
cfe3=	1.816436		
cfec3=	179.646		
cfe4=	1.790802		
cfec4=	89.583		
dih4=	-74.577		
cfe5=	1.795071		
cfec5=	114.018		
dih5=	90.397		
oc6=	1.147041		

ocfe6=	178.389
dih6=	21.507
oc7=	1.149130
ocfe7=	177.752
dih7=	-98.714
oc8=	1.152263
ocfe8=	178.658
dih8=	-23.113
oc9=	1.151519
ocfe9=	178.186
dih9=	-106.515
cc10=	4.809208
ccfe10=	89.133
dih10=	72.232
nc11=	1.449197
ncc11=	52.833
dih11=	15.075
cn12=	1.273843
cnc12=	117.947
dih12=	30.589
cc13=	1.468813
ccn13=	121.685
dih13=	179.001
cc14=	1.412153
ccc14=	122.427
dih14=	-162.797
cc15=	1.481932
ccc15=	126.386
dih15=	146.249
cc16=	1.406724
ccc16=	118.776
dih16=	-179.285
cc17=	1.392033
ccc17=	121.198
dih17=	178.552
cc18=	1.397061
ccc18=	120.146
dih18=	-0.207
cc19=	1.395817
ccc19=	119.362
dih19=	-0.435
cc20=	1.394187
ccc20=	120.474
dih20=	0.323
hc21=	1.096908
hcn21=	109.317
dih21=	-123.144
hc22=	1.103540
hcn22=	113.970
dih22=	-1.366
hc23=	1.097305
hcn23=	109.230

dih23= 120.369
hc24= 1.105022
hcc24= 116.493
dih24= 15.727
hc25= 1.086343
hcc25= 119.890
dih25= -7.034
hc26= 1.088856
hcc26= 112.619
dih26= 152.544
hc27= 1.087986
hcc27= 119.120
dih27= -179.429
hc28= 1.086675
hcc28= 119.684
dih28= 179.894
hc29= 1.086396
hcc29= 120.317
dih29= 179.786
hc30= 1.086687
hcc30= 119.417
dih30= 179.841
hc31= 1.085746
hcc31= 119.074
dih31= -178.471

3.3 η^3 allyl

fe
c 1 cfe2
c 1 cfe3 2 cfec3
c 1 cfe4 2 cfec4 3 dih4
c 1 cfe5 2 cfec5 3 dih5
o 2 oc6 1 ocfe6 4 dih6
o 3 oc7 1 ocfe7 4 dih7
o 4 oc8 1 ocfe8 5 dih8
o 5 oc9 1 ocfe9 4 dih9
c 3 cc10 1 ccfe10 4 dih10
n 10 nc11 3 ncc11 1 dih11
c 11 cn12 10 cnc12 3 dih12
c 12 cc13 11 ccn13 10 dih13
c 13 cc14 12 ccc14 11 dih14
c 14 cc15 13 ccc15 12 dih15
c 15 cc16 14 ccc16 13 dih16
c 16 cc17 15 ccc17 14 dih17
c 17 cc18 16 ccc18 15 dih18
c 18 cc19 17 ccc19 16 dih19
c 19 cc20 18 ccc20 17 dih20
h 10 hc21 11 hcn21 12 dih21
h 10 hc22 11 hcn22 12 dih22
h 10 hc23 11 hcn23 12 dih23
h 12 hc24 13 hcc24 14 dih24

h	13	hc25	14	hcc25	15	dih25
h	14	hc26	15	hcc26	20	dih26
h	16	hc27	15	hcc27	20	dih27
h	17	hc28	16	hcc28	15	dih28
h	18	hc29	19	hcc29	20	dih29
h	19	hc30	20	hcc30	15	dih30
h	20	hc31	19	hcc31	18	dih31
cfe2		1.834715				
cfe3		2.030337				
cfec3		174.334				
cfe4		1.787065				
cfec4		96.463				
dih4		-170.464				
cfe5		1.783225				
cfec5		94.448				
dih5		-68.199				
oc6		1.148970				
ocfe6		177.199				
dih6		-85.568				
oc7		1.214607				
ocfe7		137.210				
dih7		15.899				
oc8		1.147675				
ocfe8		176.830				
dih8		96.645				
oc9		1.150530				
ocfe9		179.604				
dih9		-56.913				
cc10		2.527455				
ccfe10		123.845				
dih10		-158.700				
nc11		1.457053				
ncc11		25.942				
dih11		-10.267				
cn12		1.428598				
cnc12		124.658				
dih12		166.060				
cc13		1.410460				
ccn13		120.317				
dih13		-104.318				
cc14		1.412135				
ccc14		122.334				
dih14		-20.442				
cc15		1.477355				
ccc15		124.382				
dih15		-172.189				
cc16		1.406122				
ccc16		118.288				
dih16		-163.883				
cc17		1.393148				
ccc17		121.200				
dih17		179.452				

cc18	1.395578
ccc18	120.129
dih18	-0.162
cc19	1.397114
ccc19	119.414
dih19	0.101
cc20	1.392701
ccc20	120.429
dih20	0.119
hc21	1.097870
hcn21	111.721
dih21	60.228
hc22	1.091932
hcn22	107.047
dih22	179.927
hc23	1.096386
hcn23	110.544
dih23	-61.181
hc24	1.087808
hcc24	119.613
dih24	178.903
hc25	1.086850
hcc25	119.760
dih25	-5.872
hc26	1.085357
hcc26	113.939
dih26	171.170
hc27	1.087523
hcc27	119.150
dih27	179.866
hc28	1.086554
hcc28	119.640
dih28	179.933
hc29	1.086252
hcc29	120.274
dih29	-179.817
hc30	1.086719
hcc30	119.492
dih30	179.834
hc31	1.086189
hcc31	118.759
dih31	179.334

3.4 η^3 C acyl

fe			
c	1 cfe2		
c	1 cfe3	2 cfec3	
c	1 cfe4	2 cfec4	3 dih4
c	1 cfe5	2 cfec5	3 dih5
o	2 oc6	1 ocfe6	4 dih6
o	3 oc7	1 ocfe7	4 dih7

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o	4	oc8	1	ocfe8	5	dih8
o	5	oc9	1	ocfe9	4	dih9
c	1	cfe10	4	cfec10	8	dih10
n	1	nfe11	4	nfec11	8	dih11
c	1	cfe12	4	cfec12	8	dih12
c	12	cc13	1	ccfe13	4	dih13
c	13	cc14	12	ccc14	1	dih14
c	14	cc15	13	ccc15	12	dih15
c	15	cc16	14	ccc16	13	dih16
c	16	cc17	15	ccc17	14	dih17
c	17	cc18	16	ccc18	15	dih18
c	18	cc19	17	ccc19	16	dih19
c	15	cc20	14	ccc20	13	dih20
h	10	hc21	11	hcn21	12	dih21
h	10	hc22	11	hcn22	12	dih22
h	10	hc23	11	hcn23	12	dih23
h	12	hc24	13	hcc24	1	dih24
h	13	hc25	12	hcc25	1	dih25
h	14	hc26	13	hcc26	12	dih26
h	16	hc27	15	hcc27	14	dih27
h	17	hc28	16	hcc28	15	dih28
h	18	hc29	17	hcc29	16	dih29
h	19	hc30	18	hcc30	17	dih30
h	20	hc31	15	hcc31	14	dih31
cfe2=			1.867993			
cfe3=			1.989624			
cfec3=			174.690			
cfe4=			1.791119			
cfec4=			95.738			
dih4=			164.751			
cfe5=			1.782199			
cfec5=			94.487			
dih5=			-95.752			
oc6=			1.147982			
ocfe6=			174.176			
dih6=			-73.375			
oc7=			1.203225			
ocfe7=			133.995			
dih7=			8.376			
oc8=			1.146621			
ocfe8=			176.904			
dih8=			113.573			
oc9=			1.150550			
ocfe9=			178.945			
dih9=			52.750			
cfe10=			3.165679			
cfec10=			83.683			
dih10=			-70.772			
nfe11=			2.118691			
nfec11=			96.064			
dih11=			-51.889			
cfe12=			2.181515			

cfec12=	131.432
dih12=	-59.591
cc13=	1.408511
ccfe13=	71.047
dih13=	144.375
cc14=	1.532715
ccc14=	118.714
dih14=	-80.567
cc15=	1.528350
ccc15=	114.353
dih15=	-171.109
cc16=	1.401077
ccc16=	122.149
dih16=	-138.676
cc17=	1.396748
ccc17=	120.603
dih17=	-178.168
cc18=	1.394076
ccc18=	120.535
dih18=	0.432
cc19=	1.395971
ccc19=	119.350
dih19=	0.337
cc20=	1.403884
ccc20=	119.433
dih20=	44.154
hc21=	1.103028
hcn21=	113.304
dih21=	32.915
hc22=	1.097648
hcn22=	109.360
dih22=	-88.103
hc23=	1.092606
hcn23=	109.530
dih23=	154.414
hc24=	1.099434
hcc24=	120.030
dih24=	-116.385
hc25=	1.084198
hcc25=	118.118
dih25=	119.355
hc26=	1.102152
hcc26=	109.883
dih26=	-48.884
hc27=	1.083960
hcc27=	119.739
dih27=	1.118
hc28=	1.086798
hcc28=	119.387
dih28=	-179.704
hc29=	1.086615
hcc29=	120.380

dih29= 179.947
hc30= 1.086906
hcc30= 120.194
dih30= 179.253
hc31= 1.087118
hcc31= 119.916
dih31= -0.864

3.5 η^2 N=C cisoid

fe
c 1 cfe2
c 1 cfe3 2 cfec3
c 1 cfe4 3 cfec4 2 dih4
c 1 cfe5 3 cfec5 2 dih5
o 2 oc6 1 ocfe6 5 dih6
o 3 oc7 1 ocfe7 5 dih7
o 4 oc8 1 ocfe8 5 dih8
o 5 oc9 1 ocfe9 4 dih9
c 1 cfe10 5 cfec10 9 dih10
n 1 nfe11 5 nfec11 9 dih11
c 11 cn12 1 cnfe12 5 dih12
c 12 cc13 11 ccn13 1 dih13
c 13 cc14 12 ccc14 11 dih14
c 14 cc15 13 ccc15 12 dih15
c 15 cc16 14 ccc16 13 dih16
c 16 cc17 15 ccc17 14 dih17
c 17 cc18 16 ccc18 15 dih18
c 18 cc19 17 ccc19 16 dih19
c 19 cc20 18 ccc20 17 dih20
h 10 hc21 11 hcn21 12 dih21
h 10 hc22 11 hcn22 12 dih22
h 10 hc23 11 hcn23 12 dih23
h 12 hc24 13 hcc24 14 dih24
h 13 hc25 14 hcc25 15 dih25
h 14 hc26 15 hcc26 20 dih26
h 16 hc27 15 hcc27 20 dih27
h 17 hc28 16 hcc28 15 dih28
h 18 hc29 19 hcc29 20 dih29
h 19 hc30 20 hcc30 15 dih30
h 20 hc31 19 hcc31 18 dih31
cfe2= 1.820657
cfe3= 1.829281
cfec3= 177.167
cfe4= 1.788873
cfec4= 91.647
dih4= -115.911
cfe5= 1.790015
cfec5= 90.571
dih5= 131.117
oc6= 1.149369

ocfe6=	178.007
dih6=	72.044
oc7=	1.144804
ocfe7=	178.175
dih7=	44.461
oc8=	1.153601
ocfe8=	177.606
dih8=	16.432
oc9=	1.152831
ocfe9=	176.671
dih9=	12.445
cfe10=	3.033230
cfec10=	89.550
dih10=	-153.518
nfe11=	2.133209
nfec11=	105.808
dih11=	-174.181
cn12=	1.332197
cnfe12=	77.300
dih12=	167.688
cc13=	1.466254
ccn13=	123.682
dih13=	100.407
cc14=	1.350253
ccc14=	124.025
dih14=	18.804
cc15=	1.463898
ccc15=	127.323
dih15=	178.399
cc16=	1.407713
ccc16=	118.589
dih16=	-177.309
cc17=	1.393274
ccc17=	121.264
dih17=	179.776
cc18=	1.395410
ccc18=	120.053
dih18=	-0.100
cc19=	1.398625
ccc19=	119.492
dih19=	0.199
cc20=	1.391004
ccc20=	120.440
dih20=	-0.034
hc21=	1.098807
hcn21=	108.399
dih21=	90.113
hc22=	1.103235
hcn22=	113.674
dih22=	-29.697
hc23=	1.092516
hcn23=	110.097

dih23= -152.143
hc24= 1.101307
hcc24= 114.570
dih24= -142.369
hc25= 1.088044
hcc25= 121.007
dih25= 2.245
hc26= 1.088737
hcc26= 115.583
dih26= -177.807
hc27= 1.087526
hcc27= 118.938
dih27= 179.790
hc28= 1.086744
hcc28= 119.776
dih28= 179.878
hc29= 1.086549
hcc29= 120.211
dih29= -179.911
hc30= 1.086829
hcc30= 119.605
dih30= 179.876
hc31= 1.086245
hcc31= 119.176
dih31= 179.657

3.6 η^2 N=C transoid

fe

c	1	cfe2		
c	1	cfe3	2	cfec3
c	1	cfe4	3	cfec4
c	1	cfe5	3	cfec5
o	2	oc6	1	ocfe6
o	3	oc7	1	ocfe7
o	4	oc8	1	ocfe8
o	5	oc9	1	ocfe9
c	1	cfe10	5	cfec10
n	1	nfe11	5	nfec11
c	11	cn12	1	cnfe12
c	12	cc13	11	ccn13
c	13	cc14	12	ccc14
c	14	cc15	13	ccc15
c	15	cc16	14	ccc16
c	16	cc17	15	ccc17
c	17	cc18	16	ccc18
c	18	cc19	17	ccc19
c	15	cc20	16	ccc20
h	10	hc21	11	hcn21
h	10	hc22	11	hcn22
h	10	hc23	11	hcn23
h	12	hc24	13	hcc24

h	13	hc25	14	hcc25	15	dih25
h	14	hc26	15	hcc26	16	dih26
h	16	hc27	17	hcc27	18	dih27
h	17	hc28	16	hcc28	15	dih28
h	18	hc29	17	hcc29	16	dih29
h	19	hc30	20	hcc30	15	dih30
h	20	hc31	15	hcc31	16	dih31
cfe2		1.820529				
cfe3		1.823660				
cfec3		175.591				
cfe4		1.788184				
cfec4		92.002				
dih4		-112.301				
cfe5		1.784702				
cfec5		91.192				
dih5		134.656				
oc6		1.150274				
ocfe6		178.209				
dih6		57.167				
oc7		1.147228				
ocfe7		177.954				
dih7		65.760				
oc8		1.153484				
ocfe8		177.459				
dih8		14.828				
oc9		1.153714				
ocfe9		175.832				
dih9		11.238				
cfe10		3.034523				
cfec10		87.962				
dih10		-156.309				
nfe11		2.134018				
nfec11		106.063				
dih11		-175.341				
cn12		1.328308				
cnfe12		81.237				
dih12		163.239				
cc13		1.453715				
ccn13		123.849				
dih13		93.956				
cc14		1.351857				
ccc14		122.157				
dih14		169.493				
cc15		1.461695				
ccc15		127.748				
dih15		-178.803				
cc16		1.409581				
ccc16		123.390				
dih16		-0.146				
cc17		1.390807				
ccc17		120.819				
dih17		-179.701				

cc18	1.398777
ccc18	120.452
dih18	0.021
cc19	1.395526
ccc19	119.519
dih19	-0.033
cc20	1.408039
ccc20	117.922
dih20	0.023
hc21	1.098626
hcn21	108.532
dih21	87.540
hc22	1.102746
hcn22	113.518
dih22	-32.524
hc23	1.091900
hcn23	109.907
dih23	-154.662
hc24	1.101490
hcc24	115.112
dih24	5.541
hc25	1.086490
hcc25	121.414
dih25	-1.295
hc26	1.090824
hcc26	114.799
dih26	179.175
hc27	1.086124
hcc27	119.235
dih27	-179.905
hc28	1.086751
hcc28	119.571
dih28	179.893
hc29	1.086443
hcc29	120.202
dih29	179.808
hc30	1.086698
hcc30	119.757
dih30	-179.856
hc31	1.087640
hcc31	119.027
dih31	-179.894

3.7 σ^2 N cisoid

fe				
c	1	cfe2		
c	1	cfe3	2	cfec3
c	1	cfe4	2	cfec4
c	1	cfe5	4	cfec5
o	2	oc6	1	ocfe6
o	3	oc7	1	ocfe7
			3	dih4
			2	dih5
			3	dih6
			2	dih7

o	4	oc8	1	ocfe8	3	dih8
o	5	oc9	1	ocfe9	3	dih9
c	3	cc10	1	ccfe10	2	dih10
n	1	nfe11	3	nfec11	7	dih11
c	11	cn12	1	cnfe12	3	dih12
c	12	cc13	11	ccn13	1	dih13
c	13	cc14	12	ccc14	11	dih14
c	14	cc15	13	ccc15	12	dih15
c	15	cc16	14	ccc16	13	dih16
c	16	cc17	15	ccc17	14	dih17
c	17	cc18	16	ccc18	15	dih18
c	18	cc19	17	ccc19	16	dih19
c	19	cc20	18	ccc20	17	dih20
h	10	hc21	11	hcn21	12	dih21
h	10	hc22	11	hcn22	12	dih22
h	10	hc23	11	hcn23	12	dih23
h	12	hc24	13	hcc24	14	dih24
h	13	hc25	14	hcc25	15	dih25
h	14	hc26	15	hcc26	20	dih26
h	16	hc27	15	hcc27	20	dih27
h	17	hc28	16	hcc28	15	dih28
h	18	hc29	19	hcc29	20	dih29
h	19	hc30	20	hcc30	15	dih30
h	20	hc31	19	hcc31	18	dih31
cfe2=			1.775692			
cfe3=			1.806657			
cfec3=			91.499			
cfe4=			1.802044			
cfec4=			89.980			
dih4=			-114.267			
cfe5=			1.802086			
cfec5=			131.301			
dih5=			89.922			
oc6=			1.153925			
ocfe6=			178.970			
dih6=			179.427			
oc7=			1.155816			
ocfe7=			175.518			
dih7=			0.004			
oc8=			1.156660			
ocfe8=			178.031			
dih8=			41.823			
oc9=			1.156723			
ocfe9=			178.066			
dih9=			-43.700			
cc10=			2.895159			
ccfe10=			75.738			
dih10=			179.635			
nfe11=			2.092054			
nfec11=			95.103			
dih11=			-179.902			
cn12=			1.296579			

cnfe12=	130.726
dih12=	-179.604
cc13=	1.452013
ccn13=	132.743
dih13=	0.014
cc14=	1.355233
ccc14=	130.049
dih14=	-0.457
cc15=	1.460743
ccc15=	126.594
dih15=	-179.880
cc16=	1.408605
ccc16=	117.903
dih16=	-179.760
cc17=	1.392566
ccc17=	121.121
dih17=	179.991
cc18=	1.395467
ccc18=	119.908
dih18=	0.013
cc19=	1.399281
ccc19=	119.780
dih19=	0.004
cc20=	1.389960
ccc20=	120.324
dih20=	-0.015
hc21=	1.096990
hcn21=	111.848
dih21=	-0.134
hc22=	1.093596
hcn22=	109.379
dih22=	-121.018
hc23=	1.093618
hcn23=	109.439
dih23=	120.765
hc24=	1.095109
hcc24=	111.725
dih24=	179.512
hc25=	1.087657
hcc25=	118.543
dih25=	-0.025
hc26=	1.084629
hcc26=	115.360
dih26=	-179.742
hc27=	1.087082
hcc27=	119.009
dih27=	-179.998
hc28=	1.086295
hcc28=	119.870
dih28=	-180.000
hc29=	1.086404
hcc29=	120.050

dih29= 179.995
hc30= 1.086535
hcc30= 119.704
dih30= -179.978
hc31= 1.085746
hcc31= 119.141
dih31= 179.986

3.8 σ^2 N transoid

fe
c 1 cfe2
c 1 cfe3 2 cfec3
c 1 cfe4 2 cfec4 3 dih4
c 1 cfe5 4 cfec5 2 dih5
o 2 oc6 1 ocfe6 3 dih6
o 3 oc7 1 ocfe7 2 dih7
o 4 oc8 1 ocfe8 3 dih8
o 5 oc9 1 ocfe9 3 dih9
c 3 cc10 1 ccfe10 2 dih10
n 1 nfe11 3 nfec11 7 dih11
c 11 cn12 1 cnfe12 3 dih12
c 12 cc13 11 ccn13 1 dih13
c 13 cc14 12 ccc14 11 dih14
c 14 cc15 13 ccc15 12 dih15
c 15 cc16 14 ccc16 13 dih16
c 16 cc17 15 ccc17 14 dih17
c 17 cc18 16 ccc18 15 dih18
c 18 cc19 17 ccc19 16 dih19
c 15 cc20 16 ccc20 17 dih20
h 10 hc21 11 hcn21 12 dih21
h 10 hc22 11 hcn22 12 dih22
h 10 hc23 11 hcn23 12 dih23
h 12 hc24 13 hcc24 14 dih24
h 13 hc25 14 hcc25 15 dih25
h 14 hc26 15 hcc26 16 dih26
h 16 hc27 17 hcc27 18 dih27
h 17 hc28 16 hcc28 15 dih28
h 18 hc29 17 hcc29 16 dih29
h 19 hc30 20 hcc30 15 dih30
h 20 hc31 15 hcc31 16 dih31
cfe2 1.777101
cfe3 1.804647
cfec3 90.864
cfe4 1.801855
cfec4 90.154
dih4 -116.605
cfe5 1.801800
cfec5 127.016
dih5 90.422
oc6 1.153521
ocfe6 179.290

dih6	176.792
oc7	1.156356
ocfe7	176.668
dih7	1.299
oc8	1.156964
ocfe8	178.533
dih8	54.864
oc9	1.156950
ocfe9	178.484
dih9	-53.847
cc10	2.922611
ccfe10	76.541
dih10	179.991
nfe11	2.092281
nfec11	93.592
dih11	-178.728
cn12	1.293644
cnfe12	126.397
dih12	-179.879
cc13	1.441296
ccn13	126.504
dih13	-0.013
cc14	1.354618
ccc14	120.388
dih14	179.746
cc15	1.459138
ccc15	127.604
dih15	-179.837
cc16	1.409644
ccc16	123.053
dih16	0.205
cc17	1.389974
ccc17	120.617
dih17	179.910
cc18	1.399164
ccc18	120.344
dih18	0.001
cc19	1.395618
ccc19	119.781
dih19	0.002
cc20	1.407825
ccc20	118.288
dih20	-0.006
hc21	1.097194
hcn21	111.814
dih21	-0.139
hc22	1.093856
hcn22	109.393
dih22	-121.104
hc23	1.093881
hcn23	109.383
dih23	120.813

hc24	1.095778
hcc24	115.648
dih24	-0.213
hc25	1.083578
hcc25	122.151
dih25	0.110
hc26	1.091110
hcc26	114.754
dih26	-179.718
hc27	1.085561
hcc27	119.372
dih27	179.940
hc28	1.086321
hcc28	119.643
dih28	-179.973
hc29	1.086359
hcc29	120.068
dih29	-179.988
hc30	1.086273
hcc30	119.843
dih30	179.981
hc31	1.087431
hcc31	119.198
dih31	179.994

4. Z-matrix coordinates of the 1-oxabuta-1,3-diene complexes

4.1 η^2 olefin cisoid

fe			
c	1 cfe2		
c	1 cfe3	2 cfec3	
c	1 cfe4	3 cfec4	2 dih4
c	1 cfe5	4 cfec5	3 dih5
o	2 oc6	1 ocfe6	5 dih6
o	3 oc7	1 ocfe7	5 dih7
o	4 oc8	1 ocfe8	5 dih8
o	5 oc9	1 ocfe9	2 dih9
o	3 oc10	1 ocfe10	5 dih10
c	10 col1	3 coc11	1 dih11
c	11 cc12	10 cco12	3 dih12
c	12 cc13	11 ccc13	10 dih13
c	13 cc14	12 ccc14	11 dih14
c	14 cc15	13 ccc15	12 dih15
c	15 cc16	14 ccc16	13 dih16
c	16 cc17	15 ccc17	14 dih17
c	17 cc18	16 ccc18	15 dih18
c	18 cc19	17 ccc19	16 dih19
h	11 hc20	12 hcc20	13 dih20
h	12 hc21	13 hcc21	14 dih21
h	13 hc22	14 hcc22	19 dih22
h	15 hc23	14 hcc23	19 dih23

h	16	hc24	15	hcc24	14	dih24
h	17	hc25	18	hcc25	19	dih25
h	18	hc26	19	hcc26	14	dih26
h	19	hc27	18	hcc27	17	dih27
cfe2=		1.818891				
cfe3=		1.838784				
cfec3=		179.103				
cfe4=		1.792269				
cfec4=		89.029				
dih4=		18.155				
cfe5=		1.798679				
cfec5=		112.610				
dih5=		89.626				
oc6=		1.146749				
ocfe6=		178.275				
dih6=		13.877				
oc7=		1.143752				
ocfe7=		175.203				
dih7=		-76.929				
oc8=		1.150931				
ocfe8=		179.202				
dih8=		-57.454				
oc9=		1.151240				
ocfe9=		177.760				
dih9=		-94.476				
oc10=		2.840896				
ocfe10=		95.498				
dih10=		98.233				
oc11=		1.220093				
coc11=		83.524				
dih11=		-16.248				
cc12=		1.478137				
cco12=		125.386				
dih12=		54.280				
cc13=		1.414163				
ccc13=		121.619				
dih13=		4.957				
cc14=		1.479753				
ccc14=		126.700				
dih14=		148.813				
cc15=		1.406909				
ccc15=		118.575				
dih15=		-178.392				
cc16=		1.392052				
ccc16=		121.188				
dih16=		179.031				
cc17=		1.396953				
ccc17=		120.101				
dih17=		-0.330				
cc18=		1.396145				
ccc18=		119.451				
dih18=		-0.466				

cc19= 1.393928
ccc19= 120.412
dih19= 0.481
hc20= 1.111686
hcc20= 114.255
dih20= -174.253
hc21= 1.087393
hcc21= 120.375
dih21= -6.263
hc22= 1.087298
hcc22= 113.554
dih22= 153.511
hc23= 1.087735
hcc23= 119.044
dih23= -179.199
hc24= 1.086678
hcc24= 119.718
dih24= 179.869
hc25= 1.086218
hcc25= 120.259
dih25= 179.941
hc26= 1.086785
hcc26= 119.513
dih26= 179.793
hc27= 1.086011
hcc27= 119.039
dih27= -178.638

4.2 η^2 olefin transoid

fe
c 1 cfe2
c 1 cfe3 2 cfec3
c 1 cfe4 2 cfec4 3 dih4
c 1 cfe5 2 cfec5 3 dih5
o 2 oc6 1 ocfe6 4 dih6
o 3 oc7 1 ocfe7 4 dih7
o 4 oc8 1 ocfe8 5 dih8
o 5 oc9 1 ocfe9 4 dih9
o 1 ofe10 4 ofec10 8 dih10
c 10 co11 1 cofe11 4 dih11
c 11 cc12 10 cco12 1 dih12
c 12 cc13 11 ccc13 10 dih13
c 13 cc14 12 ccc14 11 dih14
c 14 cc15 13 ccc15 12 dih15
c 15 cc16 14 ccc16 13 dih16
c 16 cc17 15 ccc17 14 dih17
c 17 cc18 16 ccc18 15 dih18
c 18 cc19 17 ccc19 16 dih19
h 11 hc20 12 hcc20 13 dih20
h 12 hc21 13 hcc21 14 dih21
h 13 hc22 14 hcc22 19 dih22

h	15	hc23	14	hcc23	19	dih23
h	16	hc24	15	hcc24	14	dih24
h	17	hc25	18	hcc25	19	dih25
h	18	hc26	19	hcc26	14	dih26
h	19	hc27	18	hcc27	17	dih27
cfe2=						1.821120
cfe3=						1.823678
cfec3=						179.353
cfe4=						1.791735
cfec4=						90.396
dih4=						-53.830
cfe5=						1.801429
cfec5=						89.634
dih5=						59.454
oc6=						1.146176
ocfe6=						178.428
dih6=						-95.959
oc7=						1.147752
ocfe7=						176.352
dih7=						23.185
oc8=						1.151028
ocfe8=						179.116
dih8=						-41.172
oc9=						1.149770
ocfe9=						177.981
dih9=						-11.069
ofe10=						3.867704
ofec10=						164.757
dih10=						-175.865
col1=						1.215759
cofe11=						36.496
dih11=						-13.265
cc12=						1.474744
cco12=						124.557
dih12=						-54.658
cc13=						1.414808
ccc13=						121.672
dih13=						-166.255
cc14=						1.480479
ccc14=						126.609
dih14=						148.148
cc15=						1.406660
ccc15=						118.623
dih15=						-178.139
cc16=						1.391874
ccc16=						121.172
dih16=						179.064
cc17=						1.396958
ccc17=						120.088
dih17=						-0.254
cc18=						1.396048
ccc18=						119.442

dih18= -0.493
cc19= 1.393986
ccc19= 120.457
dih19= 0.464
hc20= 1.115278
hcc20= 114.853
dih20= 12.404
hc21= 1.086822
hcc21= 120.679
dih21= -5.881
hc22= 1.089208
hcc22= 112.654
dih22= 154.068
hc23= 1.087902
hcc23= 119.125
dih23= -179.336
hc24= 1.086567
hcc24= 119.703
dih24= 179.895
hc25= 1.086215
hcc25= 120.270
dih25= 179.955
hc26= 1.086566
hcc26= 119.448
dih26= 179.778
hc27= 1.085804
hcc27= 119.064
dih27= -178.602

4.3 η^3 allyl

fe
c 1 cfe2
c 1 cfe3 2 cfec3
c 1 cfe4 2 cfec4 3 dih4
c 1 cfe5 2 cfec5 3 dih5
o 2 oc6 1 ocfe6 4 dih6
o 3 oc7 1 ocfe7 4 dih7
o 4 oc8 1 ocfe8 5 dih8
o 5 oc9 1 ocfe9 4 dih9
o 3 oc10 1 ocfe10 4 dih10
c 10 co11 3 coc11 1 dih11
c 11 cc12 10 cco12 3 dih12
c 12 cc13 11 ccc13 10 dih13
c 13 cc14 12 ccc14 11 dih14
c 14 cc15 13 ccc15 12 dih15
c 15 cc16 14 ccc16 13 dih16
c 16 cc17 15 ccc17 14 dih17
c 17 cc18 16 ccc18 15 dih18
c 18 cc19 17 ccc19 16 dih19
h 11 hc20 12 hcc20 13 dih20

h	12	hc21	13	hcc21	14	dih21
h	13	hc22	14	hcc22	19	dih22
h	15	hc23	14	hcc23	19	dih23
h	16	hc24	15	hcc24	14	dih24
h	17	hc25	18	hcc25	19	dih25
h	18	hc26	19	hcc26	14	dih26
h	19	hc27	18	hcc27	17	dih27
cfe2=		1.840491				
cfe3=		1.983199				
cfec3=		174.580				
cfe4=		1.793851				
cfec4=		95.061				
dih4=		178.011				
cfe5=		1.786507				
cfec5=		94.132				
dih5=		-79.007				
oc6=		1.147439				
ocfe6=		177.920				
dih6=		-98.764				
oc7=		1.196684				
ocfe7=		139.933				
dih7=		19.399				
oc8=		1.146620				
ocfe8=		176.704				
dih8=		99.135				
oc9=		1.149276				
ocfe9=		179.223				
dih9=		18.199				
oc10=		1.405064				
ocfe10=		99.499				
dih10=		-161.088				
oc11=		1.402285				
coc11=		103.303				
dih11=		-0.226				
cc12=		1.403718				
cco12=		119.887				
dih12=		69.905				
cc13=		1.411174				
ccc13=		121.849				
dih13=		-23.757				
cc14=		1.476310				
ccc14=		124.709				
dih14=		-170.948				
cc15=		1.406143				
ccc15=		118.251				
dih15=		-166.274				
cc16=		1.393193				
ccc16=		121.119				
dih16=		-179.977				
cc17=		1.395697				
ccc17=		120.115				
dih17=		-0.219				

cc18= 1.397207
ccc18= 119.477
dih18= -0.050
cc19= 1.392527
ccc19= 120.395
dih19= 0.250
hc20= 1.084688
hcc20= 121.680
dih20= -179.528
hc21= 1.086410
hcc21= 120.466
dih21= -4.782
hc22= 1.085358
hcc22= 114.056
dih22= 169.725
hc23= 1.087520
hcc23= 119.181
dih23= -179.883
hc24= 1.086408
hcc24= 119.665
dih24= 179.831
hc25= 1.086262
hcc25= 120.213
dih25= -179.727
hc26= 1.086589
hcc26= 119.518
dih26= 179.929
hc27= 1.086231
hcc27= 118.767
dih27= 179.610

4.4 η^3 C-acyl

fe
c 1 cfe2
c 1 cfe3 2 cfec3
c 1 cfe4 2 cfec4 3 dih4
c 1 cfe5 2 cfec5 3 dih5
o 2 oc6 1 ocfe6 4 dih6
o 3 oc7 1 ocfe7 4 dih7
o 4 oc8 1 ocfe8 5 dih8
o 5 oc9 1 ocfe9 4 dih9
o 1 ofe10 4 ofec10 8 dih10
c 1 cfe11 4 cfec11 8 dih11
c 11 cc12 1 ccfe12 4 dih12
c 12 cc13 11 ccc13 1 dih13
c 13 cc14 12 ccc14 11 dih14
c 14 cc15 13 ccc15 12 dih15
c 15 cc16 14 ccc16 13 dih16
c 16 cc17 15 ccc17 14 dih17
c 17 cc18 16 ccc18 15 dih18
c 14 cc19 13 ccc19 12 dih19

h	11	hc20	12	hcc20	1	dih20
h	12	hc21	11	hcc21	1	dih21
h	13	hc22	12	hcc22	11	dih22
h	15	hc23	14	hcc23	13	dih23
h	16	hc24	15	hcc24	14	dih24
h	17	hc25	16	hcc25	15	dih25
h	18	hc26	17	hcc26	16	dih26
h	19	hc27	14	hcc27	13	dih27
cfe2=		1.889610				
cfe3=		1.980737				
cfec3=		174.675				
cfe4=		1.799353				
cfec4=		94.889				
dih4=		145.434				
cfe5=		1.781546				
cfec5=		95.374				
dih5=		-116.388				
oc6=		1.144904				
ocfe6=		175.103				
dih6=		-69.574				
oc7=		1.202933				
ocfe7=		133.080				
dih7=		5.902				
oc8=		1.143791				
ocfe8=		177.303				
dih8=		113.424				
oc9=		1.149447				
ocfe9=		179.715				
dih9=		85.883				
ofe10=		2.064441				
ofec10=		98.081				
dih10=		-54.102				
cfe11=		2.153470				
cfec11=		133.146				
dih11=		-60.448				
cc12=		1.400613				
ccfe12=		74.165				
dih12=		143.198				
cc13=		1.531326				
ccc13=		118.765				
dih13=		-77.367				
cc14=		1.529304				
ccc14=		114.231				
dih14=		-175.309				
cc15=		1.400778				
ccc15=		122.093				
dih15=		-139.357				
cc16=		1.396675				
ccc16=		120.582				
dih16=		-178.208				
cc17=		1.393955				
ccc17=		120.524				

dih17= 0.496
cc18= 1.396013
ccc18= 119.360
dih18= 0.369
cc19= 1.403613
ccc19= 119.431
dih19= 43.539
hc20= 1.101207
hcc20= 120.133
dih20= -118.311
hc21= 1.084967
hcc21= 118.500
dih21= 119.454
hc22= 1.102057
hcc22= 109.770
dih22= -53.425
hc23= 1.084020
hcc23= 119.843
dih23= 1.031
hc24= 1.086751
hcc24= 119.333
dih24= -179.644
hc25= 1.086585
hcc25= 120.370
dih25= 179.952
hc26= 1.086827
hcc26= 120.236
dih26= 179.179
hc27= 1.087104
hcc27= 119.993
dih27= -0.766

4.5 η^2 N=C cisoid

fe
c 1 cfe2
c 1 cfe3 2 cfec3
c 1 cfe4 2 cfec4 3 dih4
c 1 cfe5 2 cfec5 3 dih5
o 2 oc6 1 ocfe6 4 dih6
o 3 oc7 1 ocfe7 4 dih7
o 4 oc8 1 ocfe8 5 dih8
o 5 oc9 1 ocfe9 4 dih9
o 1 ofe10 4 ofec10 8 dih10
c 10 co11 1 cofe11 4 dih11
c 11 cc12 10 cco12 1 dih12
c 12 cc13 11 ccc13 10 dih13
c 13 cc14 12 ccc14 11 dih14
c 14 cc15 13 ccc15 12 dih15
c 15 cc16 14 ccc16 13 dih16
c 16 cc17 15 ccc17 14 dih17
c 17 cc18 16 ccc18 15 dih18

c	18	cc19	17	ccc19	16	dih19
h	11	hc20	12	hcc20	13	dih20
h	12	hc21	13	hcc21	14	dih21
h	13	hc22	14	hcc22	19	dih22
h	15	hc23	14	hcc23	19	dih23
h	16	hc24	15	hcc24	14	dih24
h	17	hc25	18	hcc25	19	dih25
h	18	hc26	19	hcc26	14	dih26
h	19	hc27	18	hcc27	17	dih27
cfe2=		1.829856				
cfe3=		1.829956				
cfec3=		175.318				
cfe4=		1.796350				
cfec4=		91.006				
dih4=		118.548				
cfe5=		1.782189				
cfec5=		91.193				
dih5=		-129.299				
oc6=		1.145423				
ocfe6=		178.687				
dih6=		13.793				
oc7=		1.145715				
ocfe7=		177.901				
dih7=		-95.465				
oc8=		1.151170				
ocfe8=		175.507				
dih8=		-2.218				
oc9=		1.153881				
ocfe9=		177.495				
dih9=		-2.920				
ofe10=		2.077757				
ofec10=		107.468				
dih10=		179.337				
col1=		1.278505				
cofe11=		82.368				
dih11=		-179.365				
cc12=		1.463023				
cco12=		123.876				
dih12=		109.560				
cc13=		1.352495				
ccc13=		122.403				
dih13=		9.396				
cc14=		1.460561				
ccc14=		127.839				
dih14=		176.798				
cc15=		1.408066				
ccc15=		118.591				
dih15=		-176.831				
cc16=		1.392832				
ccc16=		121.169				
dih16=		179.732				
cc17=		1.395591				

ccc17= 119.998
dih17= -0.003
cc18= 1.398948
ccc18= 119.629
dih18= 0.153
cc19= 1.390366
ccc19= 120.375
dih19= -0.110
hc20= 1.101256
hcc20= 115.075
dih20= -153.871
hc21= 1.087807
hcc21= 121.846
dih21= 1.241
hc22= 1.089221
hcc22= 115.616
dih22= -178.215
hc23= 1.087352
hcc23= 119.033
dih23= 179.859
hc24= 1.086505
hcc24= 119.795
dih24= 179.991
hc25= 1.086448
hcc25= 120.116
dih25= 179.966
hc26= 1.086636
hcc26= 119.635
dih26= 179.994
hc27= 1.085989
hcc27= 119.275
dih27= 179.775

4.6 η^2 N=C transoid

fe
c 1 cfe2
c 1 cfe3 2 cfec3
c 1 cfe4 2 cfec4 3 dih4
c 1 cfe5 2 cfec5 3 dih5
o 2 oc6 1 ocfe6 5 dih6
o 3 oc7 1 ocfe7 5 dih7
o 4 oc8 1 ocfe8 5 dih8
o 5 oc9 1 ocfe9 4 dih9
o 1 ofe10 5 ofec10 9 dih10
c 10 co11 1 cofe11 5 dih11
c 11 cc12 10 cco12 1 dih12
c 12 cc13 11 ccc13 10 dih13
c 13 cc14 12 ccc14 11 dih14
c 14 cc15 13 ccc15 12 dih15
c 15 cc16 14 ccc16 13 dih16
c 16 cc17 15 ccc17 14 dih17

c	17	cc18	16	ccc18	15	dih18
c	14	cc19	15	ccc19	16	dih19
h	11	hc20	12	hcc20	13	dih20
h	12	hc21	13	hcc21	14	dih21
h	13	hc22	14	hcc22	15	dih22
h	15	hc23	16	hcc23	17	dih23
h	16	hc24	15	hcc24	14	dih24
h	17	hc25	16	hcc25	15	dih25
h	18	hc26	19	hcc26	14	dih26
h	19	hc27	14	hcc27	15	dih27
cfe2=		1.826197				
cfe3=		1.827504				
cfec3=		174.895				
cfe4=		1.782152				
cfec4=		91.386				
dih4=		-123.650				
cfe5=		1.794696				
cfec5=		91.204				
dih5=		123.044				
oc6=		1.146951				
ocfe6=		178.525				
dih6=		57.729				
oc7=		1.146492				
ocfe7=		178.161				
dih7=		-94.866				
oc8=		1.154037				
ocfe8=		177.606				
dih8=		4.572				
oc9=		1.151593				
ocfe9=		175.421				
dih9=		-0.534				
ofe10=		2.079459				
ofec10=		106.811				
dih10=		179.882				
col1=		1.275044				
cofe11=		84.516				
dih11=		178.082				
cc12=		1.455542				
cco12=		123.517				
dih12=		106.065				
cc13=		1.352564				
ccc13=		121.623				
dih13=		168.033				
cc14=		1.460087				
ccc14=		127.950				
dih14=		-178.155				
cc15=		1.409736				
ccc15=		123.143				
dih15=		0.009				
cc16=		1.390268				
ccc16=		120.730				
dih16=		-179.953				

cc17= 1.399016
ccc17= 120.364
dih17= 0.119
cc18= 1.395593
ccc18= 119.680
dih18= -0.074
cc19= 1.408046
ccc19= 118.131
dih19= -0.020
hc20= 1.103147
hcc20= 115.504
dih20= 3.363
hc21= 1.087061
hcc21= 122.068
dih21= -0.740
hc22= 1.091268
hcc22= 114.891
dih22= 179.954
hc23= 1.085898
hcc23= 119.308
dih23= -179.860
hc24= 1.086582
hcc24= 119.644
dih24= -179.928
hc25= 1.086393
hcc25= 120.110
dih25= 179.903
hc26= 1.086527
hcc26= 119.832
dih26= -179.797
hc27= 1.087538
hcc27= 119.087
dih27= 179.967

4.7 σ^2 N cisoid

fe
c 1 cfe2
c 1 cfe3 2 cfec3
c 1 cfe4 3 cfec4 2 dih4
c 1 cfe5 4 cfec5 3 dih5
o 2 oc6 1 ocfe6 5 dih6
o 3 oc7 1 ocfe7 5 dih7
o 4 oc8 1 ocfe8 5 dih8
o 5 oc9 1 ocfe9 2 dih9
o 1 ofe10 5 ofec10 9 dih10
c 10 co11 1 cofe11 5 dih11
c 11 cc12 10 cco12 1 dih12
c 12 cc13 11 ccc13 10 dih13
c 13 cc14 12 ccc14 11 dih14
c 14 cc15 13 ccc15 12 dih15
c 15 cc16 14 ccc16 13 dih16

c	16	cc17	15	ccc17	14	dih17
c	17	cc18	16	ccc18	15	dih18
c	18	cc19	17	ccc19	16	dih19
h	11	hc20	12	hcc20	13	dih20
h	12	hc21	13	hcc21	14	dih21
h	13	hc22	14	hcc22	19	dih22
h	15	hc23	14	hcc23	19	dih23
h	16	hc24	15	hcc24	14	dih24
h	17	hc25	18	hcc25	19	dih25
h	18	hc26	19	hcc26	14	dih26
h	19	hc27	18	hcc27	17	dih27
cfe2=				1.768608		
cfe3=				1.805269		
cfec3=				90.862		
cfe4=				1.805200		
cfec4=				123.574		
dih4=				-91.687		
cfe5=				1.827000		
cfec5=				118.118		
dih5=				176.193		
oc6=				1.153290		
ocfe6=				179.580		
dih6=				176.134		
oc7=				1.156235		
ocfe7=				179.403		
dih7=				-47.294		
oc8=				1.156190		
ocfe8=				179.365		
dih8=				51.524		
oc9=				1.151872		
ocfe9=				179.402		
dih9=				179.606		
ofe10=				2.070689		
ofec10=				85.306		
dih10=				-0.334		
coll1=				1.239983		
cofe11=				144.716		
dih11=				179.689		
cc12=				1.447185		
cco12=				129.821		
dih12=				0.273		
cc13=				1.359074		
ccc13=				124.901		
dih13=				-0.019		
cc14=				1.454802		
ccc14=				127.472		
dih14=				179.815		
cc15=				1.409375		
ccc15=				118.057		
dih15=				-179.734		
cc16=				1.391866		
ccc16=				120.931		

dih16= 179.886
cc17= 1.395902
ccc17= 119.843
dih17= 0.017
cc18= 1.399962
ccc18= 119.997
dih18= 0.010
cc19= 1.389166
ccc19= 120.226
dih19= -0.019
hc20= 1.102557
hcc20= 114.620
dih20= -179.965
hc21= 1.087205
hcc21= 120.978
dih21= -0.108
hc22= 1.086807
hcc22= 115.352
dih22= -179.890
hc23= 1.086913
hcc23= 119.090
dih23= -179.995
hc24= 1.086023
hcc24= 119.907
dih24= -179.983
hc25= 1.086351
hcc25= 119.949
dih25= 179.994
hc26= 1.086281
hcc26= 119.803
dih26= 179.995
hc27= 1.085662
hcc27= 119.404
dih27= -179.994

4.8 σ^2 N transoid

fe
c 1 cfe2
c 1 cfe3 2 cfec3
c 1 cfe4 3 cfec4 2 dih4
c 1 cfe5 4 cfec5 3 dih5
o 2 oc6 1 ocfe6 5 dih6
o 3 oc7 1 ocfe7 5 dih7
o 4 oc8 1 ocfe8 5 dih8
o 5 oc9 1 ocfe9 2 dih9
o 1 ofe10 5 ofec10 9 dih10
c 10 co11 1 cofe11 5 dih11
c 11 cc12 10 cco12 1 dih12
c 12 cc13 11 ccc13 10 dih13
c 13 cc14 12 ccc14 11 dih14
c 14 cc15 13 ccc15 12 dih15

c	15	cc16	14	ccc16	13	dih16
c	16	cc17	15	ccc17	14	dih17
c	17	cc18	16	ccc18	15	dih18
c	14	cc19	15	ccc19	16	dih19
h	11	hc20	12	hcc20	13	dih20
h	12	hc21	13	hcc21	14	dih21
h	13	hc22	14	hcc22	15	dih22
h	15	hc23	16	hcc23	17	dih23
h	16	hc24	15	hcc24	14	dih24
h	17	hc25	16	hcc25	15	dih25
h	18	hc26	19	hcc26	14	dih26
h	19	hc27	14	hcc27	15	dih27
cfe2=				1.770227		
cfe3=				1.804602		
cfec3=				91.174		
cfe4=				1.804522		
cfec4=				122.004		
dih4=				-92.113		
cfe5=				1.822968		
cfec5=				118.851		
dih5=				175.829		
oc6=				1.153349		
ocfe6=				179.899		
dih6=				134.110		
oc7=				1.156684		
ocfe7=				179.329		
dih7=				-83.061		
oc8=				1.156664		
ocfe8=				179.239		
dih8=				84.103		
oc9=				1.152572		
ocfe9=				179.331		
dih9=				-175.800		
ofe10=				2.068557		
ofec10=				85.460		
dih10=				4.173		
col1=				1.240058		
cofe11=				133.340		
dih11=				179.777		
cc12=				1.439975		
cco12=				126.878		
dih12=				0.137		
cc13=				1.357726		
ccc13=				119.440		
dih13=				-179.989		
cc14=				1.454558		
ccc14=				128.094		
dih14=				179.954		
cc15=				1.410487		
ccc15=				122.875		
dih15=				-0.052		
cc16=				1.389266		

ccc16=	120.471
dih16=	-179.927
cc17=	1.399548
ccc17=	120.258
dih17=	-0.006
cc18=	1.396067
ccc18=	120.015
dih18=	-0.009
cc19=	1.408927
ccc19=	118.528
dih19=	0.016
hc20=	1.102822
hcc20=	116.581
dih20=	-0.016
hc21=	1.084743
hcc21=	123.089
dih21=	-0.044
hc22=	1.091323
hcc22=	114.861
dih22=	179.927
hc23=	1.085462
hcc23=	119.475
dih23=	-179.997
hc24=	1.086051
hcc24=	119.744
dih24=	-179.996
hc25=	1.086212
hcc25=	119.941
dih25=	-179.992
hc26=	1.086105
hcc26=	119.987
dih26=	-179.987
hc27=	1.087288
hcc27=	119.228
dih27=	-179.986

End of file