Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Material

Theoretical Tools to Distinguish *O*-Ylides from *O*-Ylidic Complexes in Carbene-Solvent Interactions

Sara Gómez*, Albeiro Restrepo, and C. Z. Hadad*

This document contains appendices A0, A1, A2, A3, and A4 that supplement arguments and results of the article.

1 Appendix A0

Natural bond orders for Cc···O interactions in the title clusters

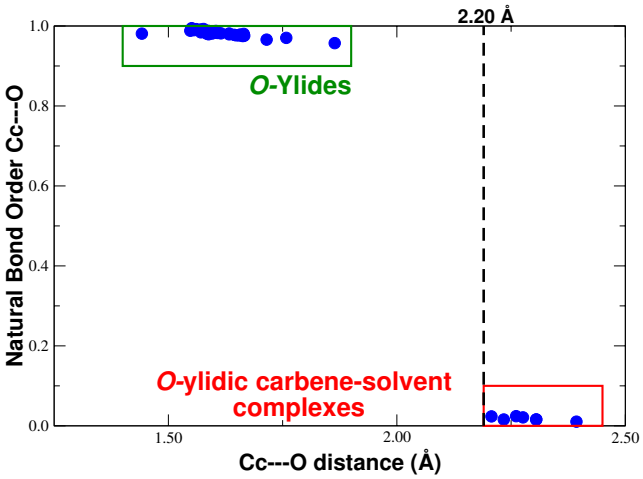


Figure 1: Natural bond orders vs. distances for carbene carbon···oxygen interaction in all FCH···$(MeOH)_3$ equilibrium structures. Bond lengths in Å.

Table 1: Natural Bond Order from Natural Resonance Theory (NRT), Wiberg bond indexes (WBI) and WBI relative values between carbene carbon and the methanol oxygen for *O*-ylides and complexes.

Structure	Cc$\cdots$O Natural Bond Order	Cc$\cdots$O WBI	Relative WBI
1, y_1	0.99	0.63	0.98
2, y_2	0.99	0.63	0.98
3, y_3	0.98	0.57	0.89
4, y_4	0.99	0.62	0.97
5, y_5	0.99	0.59	0.92
6, y_6	0.99	0.62	0.97
7, y_7	0.99	0.58	0.91
8, y_8	0.98	0.54	0.84
9, y_9	0.99	0.60	0.94
10, y_{10}	0.98	0.53	0.83
11, y_{11}	0.98	0.52	0.81
12, y_{12}	0.99	0.64	1.00
13, y_{13}	0.98	0.61	0.95
14, y_{14}	0.98	0.60	0.94
15, y_{15}	0.99	0.58	0.91
16, y_{16}	0.99	0.57	0.89
17, y_{17}	0.98	0.51	0.80
18, y_{18}	0.98	0.58	0.91
19, y_{19}	0.98	0.59	0.92
20, y_{20}	0.98	0.59	0.92
21, y_{21}	0.99	0.59	0.92
22, y_{22}	0.98	0.57	0.89
23, y_{23}	0.98	0.60	0.94
24, y_{24}	0.97	0.47	0.73
25, y_{25}	0.99	0.56	0.88
26, y_{26}	0.99	0.59	0.92
27, y_{27}	0.98	0.54	0.84
31, y_{28}	0.98	0.51	0.80
33, y_{29}	0.98	0.51	0.80
34, y_{30}	0.98	0.56	0.88
35, y_{31}	0.97	0.51	0.80
36, y_{32}	0.98	0.51	0.80
38, y_{33}	0.98	0.54	0.84
41, y_{34}	0.96	0.31	0.48
43, y_{35}	0.98	0.48	0.75
44, y_{36}	0.97	0.40	0.63
28, c_1	0.02	0.09	0.14
29, c_2	0.02	0.09	0.14
30, c_3	-	-	-
32, c_4	0.02	0.11	0.17
37, c_5	0.01	0.07	0.11
39, c_6	0.02	0.12	0.19
40, c_7	0.02	0.10	0.16
42, c_8	0.02	0.10	0.16

2 Appendix A1

Laplacians of electron densities at BCPs for the Cc$\cdots$O interactions

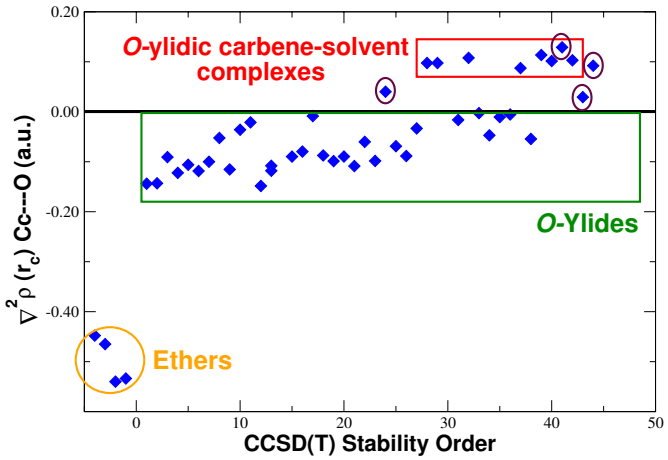


Figure 2: Relationship between the Laplacian of the electron density at carbene carbon-oxygen BCPs and the stability order at CCSD(T) level of theory. Maroon ellipses enclose structures at the borderline between *O*-ylides and *O*-ylidic complexes.

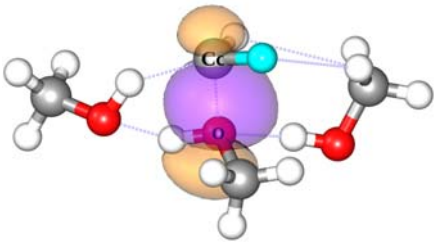
Limit cases: In general, it is difficult to discern if the clusters located at the border of the groups belong to one or other group. However, we were able to distinguish them as ylides, by employing natural charges and orbitals, by comparing with the literature reported Cc–O distances, and by analyzing their Cc–O bond orders. They have been differentiated in all figures by means of ellipses. A summary of the main features for such clusters is offered below.

- **24**, y_{24}: Within limit cases, this is the most stable flourocarbene-(methanol)$_3$ cluster, with a binding energy about 18 kcal/mol. Via NBO analysis, we found that in this aggregate, the C$\cdots$O interaction leads to a σ_{Cc-O} bonding orbital (see the structure at the top panel in Figure 3); so,

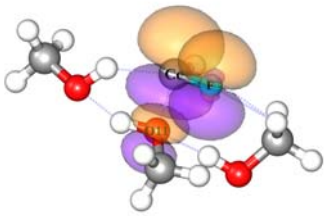
carbene and methanol (that includes O11) constitute a single unit. This situation is also present (but not shown in the figures of this Appendix) for the y_{34}, y_{35} and y_{36} structures.

There is a strong donor $\rightarrow$ acceptor interaction ($E^{(2)}$ =29.40 kcal/mol) which is the result of the interaction between a lone pair of the Fluorine atom in fluorocarbene and the O11–Cc (O11 is the methanol oxygen) antibonding orbital. We denote this interaction as $n_F^{(3)} \rightarrow \sigma^*_{O11-Cc}$ as depicted in middle panel of Figure 3. The interaction between the lone pair of carbene carbon and the O–H antibonding orbital, i.e. $n_{Cc}^{(1)}$ $\rightarrow \sigma^*_{O5-H6}$ (bottom left panel in Figure 3), represents the fact that the hydrogen belonging to O–H is electron acceptor of the σ carbene carbon occupied orbital. It has the largest stabilizing interaction energy among the intermolecular interaction in the cluster: 41.12 kcal/mol. Values for hydrogen bonds among methanol molecules are 35.38 and 3.13 kcal/mol for this aggregate (see the bottom right panel of the Figure 3).

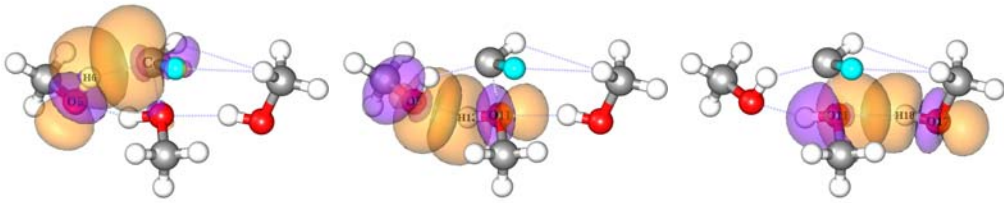
Other useful descriptors indicating that this cluster has *O*-ylide nature are the signs of Δq on carbene carbon and on oxygen atom: $\Delta q(Cc) < 0$ and $\Delta q(O) > 0$, which can be represented as $\mathbf{(FHC^{-}\text{—}\ O^{+}HCH_3)\cdots(2CH_3OH)}$. The WBI for the Cc–O bond in this structure is 0.47 and such value is very close to WBIs for other ylides (see Figure 5 in the paper). Its Cc–O distance is 1.72 Å.



σ_{Cc-O}



$n_F^{(3)} \longrightarrow \sigma^*_{O11-Cc} = \mathbf{29.40}$



$n_{Cc}^{(1)} \longrightarrow \sigma^*_{O5-H6} = \mathbf{41.12}$, $n_{O5}^{(2)} \longrightarrow \sigma^*_{O11-H12} = \mathbf{35.38}$, $n_{O11}^{(1)} \longrightarrow \sigma^*_{O17-H18} = \mathbf{3.13}$

Figure 3: Orbital interactions defining the cluster stabilization for structure labeled as **24**, y_{24} in Figure 2 of the paper. All values in kcal/mol. This cluster constitutes a limit case between *O*-ylides and *O*-ylidic carbene-solvent complexes for the system studied in this work. However, it seems that its ylidic nature has the major contribution, because it exhibits a bonding orbital Cc–O.

- **41**, y_{34}, **43**, y_{35} and **44**, y_{36}: These structures have the same characteristic of the previous case: σ_{Cc-O}, $\Delta q(Cc) < 0$, $\Delta q(O) > 0$, Cc$\cdots$O bond index < 0.5, $\nabla^2\rho(r_c) > 0$. Their $|\mathcal{V}(r_c)|\,/\mathcal{G}(r_c)$ ratios are closer to 2 than to 1, their $\mathcal{H}(\mathbf{r}_c)/\rho(\mathbf{r}_c)$ ratios are well separated (more negative values, stronger interactions) with respect to *O*-ylidic complexes and these three structures are the highest energy aggregates among the 48 minima. Such relative high energies may be a direct result of two factors: on the one hand, in the entire arrangement of these clusters there is a higher proportion of secondary hydrogen bonds (with small contributions to $E(2)$) than primary hydrogen bonds and, on the other hand, the bonding due to this arrangement leads to larger Cc$\cdots$O distances, which are also important in ylidic stabilization.

3 Appendix A2

Complementary QTAIM properties to characterize Cc$\cdots$O interactions

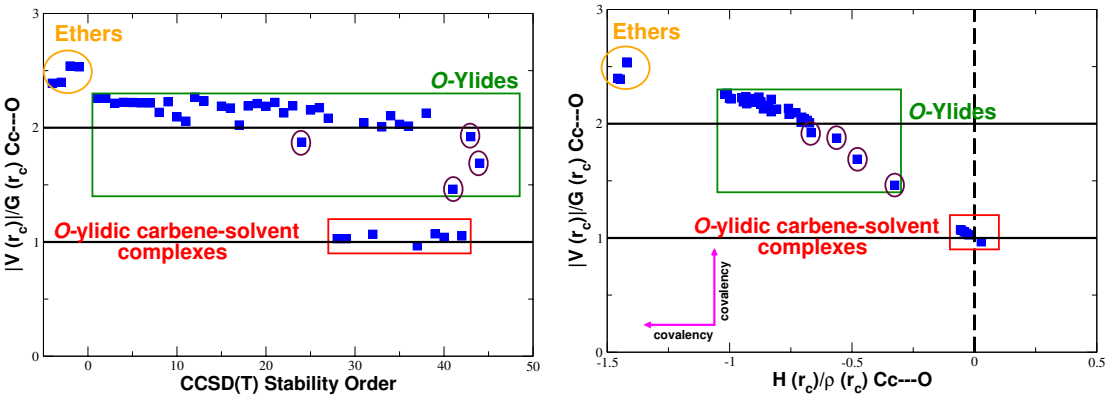


Figure 4: Quantification of the degree of covalency at carbene carbon-oxygen BCPs according to equation 1 in the paper. Boundaries for the considered criteria are shown as solid lines ($|\mathcal{V}(\mathbf{r}_c)|\,/\mathcal{G}(\mathbf{r}_c) = 1, 2$ ratio values) and dashed line ($\mathcal{H}(\mathbf{r}_c)/\rho(\mathbf{r}_c) = 0$). Maroon ellipses enclose structures at the borderline between *O*-ylides and *O*-ylidic complexes.

From the right side of Figure 4 we notice that all Cc$\cdots$O intermolecular interactions have negative total energy densities, except only the hand constructed structure. In the case studied here, the sign and the magnitude of $\mathcal{H}(\mathbf{r}_c)/\rho(\mathbf{r}_c)$ can be considered as good indicators of the strength of the interaction. Thus, ethers and most of the ylides should be classified to have Cc$\cdots$O strong interactions, while complexes are shown to be stabilized by weaker interactions, this seems to be consistent with the covalent character associated to the groups from $|\mathcal{V}(\mathbf{r}_c)|\,/\mathcal{G}(\mathbf{r}_c)$ results.

4 Appendix A3

One of the four mechanisms proposed to describe the chemical transformations when carbenes react with molecules bearing the O–H bond

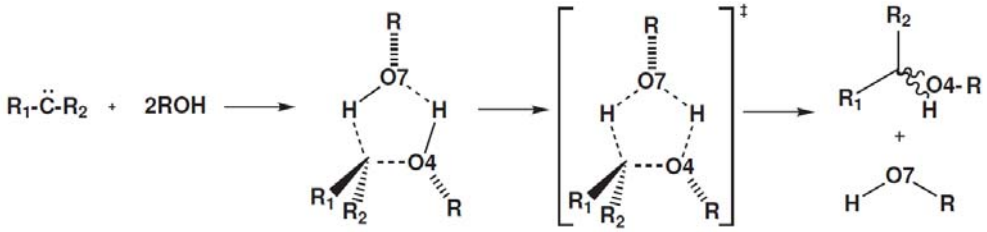


Figure 5: Reaction mechanism for the reaction of substituted singlet carbenes with two alcohol (or water) molecules. This mechanism was independently proposed by Pliego and co-workers, [see Ref. 68 in the paper] and by Marquez and co-workers, [see Ref. 69 in the paper] and features the catalytic action of one water (or alcohol) molecule, an intermediate involving a total of three molecules and a five-member ring early transition state for double proton transfer before alcohol (or ether) formation. It is the reaction channel that affords the highest rate constants [see Refs. 70,71 in the paper].

5 Appendix A4

Optimized geometries at the MP2/6-311++G(d,p) level

Insertion Products (Ethers)			
e_1			
C	1.313067	-0.352417	1.515476
H	2.360672	-0.264694	1.812101
H	0.775019	0.581863	1.701585
H	0.845847	-1.167652	2.067849
O	1.217665	-0.696692	0.125453
H	-0.487981	-1.236201	-0.369194
C	-2.174252	2.403201	-0.059956
H	-3.137466	2.184836	0.416703
H	-1.844873	3.390575	0.267704
H	-2.317661	2.427388	-1.146949
O	-1.173651	1.472215	0.320686
H	1.323588	1.281921	-0.403873
C	-2.081638	-2.346977	-0.110313
H	-1.656984	-3.240845	-0.579010
H	-2.017176	-2.448443	0.979291
H	-3.132317	-2.271527	-0.392264
O	-1.434899	-1.165391	-0.568319
H	-1.468486	0.595615	0.027072
C	1.707969	0.302233	-0.698492
H	1.443655	0.036286	-1.721748
F	3.094486	0.357066	-0.618013
e_2			
C	-1.933792	-2.339784	-0.216341
H	-1.856553	-2.570022	0.852594
H	-2.987543	-2.228392	-0.473429
H	-1.518991	-3.173518	-0.793121
O	-1.289596	-1.113282	-0.539117
H	2.248059	-0.830860	-1.537328
C	1.355584	-0.236408	1.556559
H	2.376164	-0.041879	1.904066
H	0.776618	0.686789	1.501194
H	0.866695	-0.937633	2.231719
O	1.399272	-0.881708	0.270681
H	-0.349040	-1.198557	-0.322522
C	-1.586585	2.398995	-0.214996

H	-1.517901	3.354432	0.308577
H	-0.764542	2.336746	-0.937584
H	-2.539008	2.372763	-0.758668
O	-1.507324	1.373826	0.762762
H	-1.574927	0.530008	0.290353
C	2.193556	-0.216097	-0.639330
H	3.181559	0.005105	-0.220486
F	1.629779	1.002678	-0.990591

e_3

C	2.965026	-1.166590	-0.438964
H	3.470116	-1.132161	0.533905
H	3.139331	-2.147767	-0.883980
H	3.410529	-0.407171	-1.093175
O	1.562885	-0.997684	-0.311590
H	-0.717569	-1.092573	-1.177494
C	0.601892	2.632728	0.280518
H	-0.033126	3.308014	0.863244
H	1.615242	3.035618	0.261866
H	0.218933	2.574134	-0.743313
O	0.673063	1.343690	0.884840
H	1.411542	-0.125033	0.090699
C	-1.330378	-1.566508	1.266506
H	-2.178375	-2.246325	1.120211
H	-0.399572	-2.041492	0.941136
H	-1.262650	-1.300347	2.320535
O	-1.540853	-0.345084	0.554646
H	-0.218137	0.961097	0.874249
C	-1.618854	-0.583913	-0.822730
H	-2.536256	-1.132234	-1.068390
F	-1.687431	0.649396	-1.419404

e_4

C	-1.316137	0.103931	1.778345
H	-2.266097	-0.236367	2.207828
H	-0.535380	-0.646425	1.937708
H	-1.028718	1.043076	2.250103
O	-1.470403	0.380576	0.384754
H	0.073269	1.173683	-0.347803
C	1.343754	2.650460	-0.173814
H	0.777356	3.361305	-0.784634
H	1.156338	2.860350	0.885962
H	2.406802	2.788542	-0.374134
O	1.020238	1.307613	-0.510872
H	1.463924	-0.334873	0.177676

C	2.386656	-2.008281	-0.163742
H	3.398722	-1.647335	0.055432
H	2.304951	-3.037170	0.191099
H	2.238479	-2.000222	-1.250275
O	1.396726	-1.245432	0.508652
H	-1.041418	-1.543828	-0.198226
C	-1.822601	-0.785263	-0.307068
H	-2.803709	-1.145690	0.026022
F	-1.918560	-0.438021	-1.626595

O-Ylides

1, y_1

C	3.061896	-0.960750	0.531687
H	3.813225	-0.194901	0.725164
H	2.691411	-1.348550	1.486139
H	3.523780	-1.774591	-0.034430
O	2.017306	-0.347697	-0.222128
H	1.323826	-1.009548	-0.385460
C	0.366952	2.650224	-0.398670
H	-0.562763	3.216569	-0.336864
H	1.181946	3.258812	0.001017
H	0.572189	2.403797	-1.444500
O	0.200892	1.465295	0.386593
H	0.991107	0.889522	0.253350
C	-2.519160	-0.361229	1.066137
H	-3.410061	-0.885365	0.729459
H	-1.878434	-1.031417	1.640339
H	-2.770646	0.530701	1.641117
O	-1.832936	0.069962	-0.125828
H	-1.010471	0.638817	0.107456
C	-1.509156	-1.110995	-1.077283
H	-1.020533	-0.511532	-1.868129
F	-0.325541	-1.665145	-0.394998

2, y_2

C	-3.118063	-0.676261	-0.276539
H	-3.798765	0.114410	-0.592416
H	-2.767980	-1.221841	-1.158753
H	-3.654564	-1.363315	0.383891
O	-2.035654	-0.051441	0.413089
H	-1.403452	-0.739077	0.682572

C	2.756889	-0.173138	0.272735
H	3.427195	-1.012312	0.104156
H	3.231827	0.774641	0.014970
H	2.404488	-0.172575	1.305242
O	1.646840	-0.362882	-0.625629
H	0.980120	0.412747	-0.559382
C	0.056736	2.634449	0.280054
H	0.984913	3.123741	-0.017870
H	-0.773970	3.325352	0.115968
H	0.106059	2.373328	1.341969
O	-0.097057	1.469723	-0.534165
H	-0.922709	1.006729	-0.254588
C	0.988095	-1.755917	-0.451587
H	0.210463	-1.628360	-1.228549
F	0.195711	-1.512385	0.765384

3, y_3

C	-0.200635	2.335803	0.418281
H	0.668917	2.994255	0.440375
H	-1.101281	2.948555	0.327322
H	-0.239834	1.745564	1.339000
O	-0.065294	1.481212	-0.723671
H	-0.879398	0.921094	-0.759027
C	2.823182	0.173835	0.208799
H	3.554831	-0.633040	0.219849
H	3.176542	0.996010	-0.413779
H	2.617145	0.515320	1.227373
O	1.618140	-0.342832	-0.381104
H	0.977727	0.444990	-0.553141
C	-2.844614	-0.331316	0.558646
H	-3.519006	-1.192640	0.549494
H	-2.218315	-0.368269	1.455262
H	-3.443069	0.580831	0.562641
O	-2.040972	-0.304367	-0.623231
H	-1.451444	-1.073222	-0.574198
C	0.809104	-1.233410	0.685630
H	1.646341	-1.910941	0.936448
F	0.065959	-2.034454	-0.240190

4, y_4

C	-2.634441	0.192634	-0.754589
H	-3.504609	-0.257287	-0.277820
H	-2.878685	1.179695	-1.148793
H	-2.250823	-0.461648	-1.536568
O	-1.640939	0.373184	0.282323

H	-0.805456	0.853275	-0.076040
C	2.216308	-1.489479	0.219374
H	1.460621	-1.230799	0.960683
H	1.847197	-2.336858	-0.361592
H	3.164238	-1.740631	0.703390
O	2.382511	-0.325997	-0.618479
H	2.895638	-0.577206	-1.390336
C	0.922974	2.328297	0.604686
H	0.217650	3.150651	0.727309
H	0.972977	1.748092	1.530238
H	1.907864	2.732599	0.360522
O	0.444057	1.513058	-0.474717
H	1.121408	0.816576	-0.621814
C	-1.096129	-0.873041	1.037227
H	-2.055032	-1.229775	1.454998
F	-0.892255	-1.786567	-0.053043

5, y_5

C	-0.146078	2.655645	0.618470
H	0.772115	3.230427	0.494609
H	-1.002527	3.319182	0.474126
H	-0.177295	2.234349	1.627897
O	-0.145088	1.624143	-0.372672
H	-0.938536	1.054612	-0.232156
C	2.775404	-0.221824	-0.833198
H	3.164450	-1.232749	-0.922319
H	2.754016	0.283621	-1.800224
H	3.367522	0.340374	-0.109197
O	1.416203	-0.344663	-0.381974
H	0.903736	0.536500	-0.394990
C	-2.977568	-0.759032	-0.683542
H	-3.638527	0.071637	-0.932336
H	-2.569836	-1.181964	-1.607178
H	-3.554903	-1.525274	-0.158442
O	-1.943418	-0.241826	0.152570
H	-1.337163	-0.970863	0.371452
C	1.289764	-1.134823	0.979499
H	0.822706	-0.328007	1.581404
F	0.129282	-1.930320	0.659621

6, y_6

C	3.507475	-0.689090	-0.172835
H	2.830080	-1.026846	-0.953253
H	4.485881	-0.455932	-0.598265
H	3.598322	-1.472535	0.582949

O	2.916341	0.499371	0.389084
H	3.451069	0.788364	1.134112
C	-4.029827	-0.484269	0.250751
H	-4.957037	0.070826	0.086934
H	-4.107195	-1.440698	-0.284542
H	-3.947186	-0.698993	1.325362
O	-2.956814	0.302887	-0.218044
H	-2.113877	-0.179520	0.006373
C	-0.121869	1.633183	-0.552086
H	-1.188803	1.776690	-0.400345
H	0.435912	2.560844	-0.423145
H	0.072630	1.186207	-1.527237
O	0.324246	0.723875	0.491697
H	1.319432	0.630644	0.453394
C	-0.356639	-0.678396	0.407329
H	0.085417	-1.101857	1.324062
F	0.418926	-1.281648	-0.625250

7, y_7

C	2.988223	-0.650049	0.536216
H	3.594878	0.169266	0.922648
H	2.525640	-1.181443	1.374022
H	3.633171	-1.338531	-0.016791
O	2.002407	-0.077267	-0.323672
H	1.439531	-0.798807	-0.652368
C	-2.931990	-0.185314	0.347203
H	-3.477597	-1.045820	-0.030804
H	-2.940841	-0.186763	1.438902
H	-3.341582	0.748572	-0.041801
O	-1.586774	-0.306560	-0.146071
H	-1.017399	0.503376	0.095355
C	0.066887	2.750048	-0.373516
H	-0.852555	3.295958	-0.159519
H	0.920794	3.369982	-0.089080
H	0.118353	2.530056	-1.444506
O	0.044385	1.548232	0.401363
H	0.872538	1.045428	0.210988
C	-0.928331	-1.677834	0.309601
H	-0.250594	-1.270997	1.090416
F	-0.008135	-1.841846	-0.785272

8, y_8

C	0.620073	2.197520	0.747974
H	-0.224809	2.854373	0.956211
H	0.767639	1.521919	1.594388

H	1.513299	2.807597	0.589493
O	0.304455	1.462988	-0.441237
H	1.064924	0.872270	-0.629971
C	2.261014	-1.487778	-0.147107
H	1.197128	-1.707841	-0.044916
H	2.754785	-2.284158	-0.710851
H	2.714745	-1.395482	0.843827
O	2.346059	-0.240948	-0.868111
H	3.272521	-0.008395	-0.969080
C	-2.381072	-0.193665	-1.365706
H	-3.288583	-0.766659	-1.177180
H	-2.628906	0.759505	-1.833162
H	-1.692245	-0.774416	-1.983033
O	-1.774584	0.082332	-0.092258
H	-0.939507	0.646591	-0.257771
C	-1.159027	-1.295629	0.532213
H	-2.128478	-1.690165	0.893371
F	-0.603987	-0.732534	1.704141

9, y_9

C	-0.184249	2.094110	0.763436
H	0.708125	2.719582	0.810124
H	-1.067740	2.729591	0.858055
H	-0.162157	1.361013	1.574339
O	-0.180462	1.440178	-0.512280
H	-1.044498	0.988351	-0.599813
C	-2.664676	-1.095867	0.109175
H	-1.842410	-1.150341	0.820108
H	-3.617015	-1.210346	0.633632
H	-2.547655	-1.893142	-0.629378
O	-2.584315	0.199760	-0.511137
H	-3.240279	0.243553	-1.211711
C	2.876420	0.097367	-0.182862
H	3.583482	-0.708901	-0.360322
H	3.177456	1.011546	-0.697340
H	2.761379	0.265720	0.889259
O	1.624043	-0.331023	-0.749063
H	0.925199	0.408265	-0.663948
C	1.113976	-1.661742	-0.087658
H	0.237223	-1.790652	-0.752188
F	0.489548	-1.116529	1.099608

10, y_{10}

C	0.329121	1.737989	1.282209
H	-0.616296	2.190381	1.577476

H	0.468289	0.817110	1.852865
H	1.144914	2.440087	1.475698
O	0.246622	1.459841	-0.124960
H	1.112383	1.102713	-0.403180
C	2.732201	-1.075727	-0.251641
H	1.730975	-1.432306	-0.017140
H	3.198049	-1.746456	-0.978429
H	3.328570	-1.049377	0.664776
O	2.576858	0.241402	-0.805965
H	3.447733	0.609255	-0.975274
C	-2.757625	0.379936	-0.983349
H	-3.458973	-0.392139	-1.298658
H	-3.144948	0.905009	-0.106524
H	-2.563977	1.070161	-1.804588
O	-1.523416	-0.272188	-0.645652
H	-0.825696	0.444353	-0.461179
C	-1.668355	-0.999662	0.821112
H	-2.343300	-1.803714	0.464554
F	-0.410032	-1.649193	0.823581

11, y_{11}

C	-1.463185	2.166767	-0.699458
H	-0.811281	3.040601	-0.723104
H	-1.374177	1.621626	-1.643884
H	-2.496333	2.497432	-0.564024
O	-1.048366	1.355392	0.403771
H	-1.591065	0.539481	0.386965
C	-1.735209	-2.138120	-0.078998
H	-0.757441	-1.830828	-0.455930
H	-1.606203	-2.715388	0.841620
H	-2.254805	-2.745281	-0.825382
O	-2.471653	-0.925261	0.179739
H	-3.295853	-1.153391	0.616786
C	1.727406	0.056014	1.561590
H	2.780624	-0.211737	1.534435
H	1.533153	0.774073	2.359139
H	1.117156	-0.844003	1.672845
O	1.414414	0.690341	0.307553
H	0.445863	0.980881	0.357995
C	1.366459	-0.428741	-0.909098
H	1.328510	0.336674	-1.710576
F	2.717097	-0.798826	-0.913290

12, y_{12}

C	-0.116657	1.764250	-0.528031

H	-1.109208	1.808632	-0.085203
H	0.282560	2.760795	-0.712975
H	-0.140641	1.167610	-1.438764
O	0.757024	1.140879	0.456378
H	1.695800	0.942409	0.125350
C	3.311383	-0.988361	-0.680092
H	3.916688	-0.472072	-1.426443
H	3.911882	-1.780230	-0.223337
H	2.438125	-1.436510	-1.166705
O	2.920941	-0.029714	0.303324
H	2.230223	-0.458984	0.895281
C	-3.988604	-0.699570	-0.028183
H	-4.857490	-0.042496	-0.079168
H	-4.126842	-1.514436	-0.748080
H	-3.931145	-1.123898	0.980864
O	-2.848874	0.090100	-0.336326
H	-2.074817	-0.482370	-0.285630
C	0.387026	-0.219953	1.093893
H	-0.477686	0.086717	1.698309
F	-0.216563	-0.911499	-0.007336

13, y_{13}

C	2.900961	-0.065073	0.535374
H	3.200679	-1.106260	0.640408
H	3.387549	0.394849	-0.327503
H	3.125778	0.490048	1.446600
O	1.468222	-0.059243	0.356983
H	1.062725	0.882206	0.262855
C	-1.001885	2.418695	0.025674
H	-0.720561	3.284440	0.625975
H	-1.636859	2.751351	-0.800030
H	-1.537169	1.692797	0.642130
O	0.209896	1.849248	-0.489314
H	0.008559	1.019386	-1.008036
C	-2.775791	-0.869869	-0.137322
H	-3.622526	-0.203566	0.038984
H	-2.306650	-0.606507	-1.092673
H	-3.152361	-1.897164	-0.203086
O	-1.877704	-0.703603	0.951193
H	-1.107404	-1.242541	0.740080
C	0.850571	-0.745785	-0.913821
H	1.769008	-1.073078	-1.428175
F	0.364754	-1.944998	-0.349761

14, y_{14}

C	-3.338250	-0.564972	0.876800
H	-3.682844	-0.047818	1.773339
H	-4.207057	-0.926254	0.319105
H	-2.720480	-1.420978	1.170697
O	-2.595537	0.364871	0.090011
H	-2.122444	-0.138144	-0.660413
C	0.397870	1.917571	-0.322543
H	1.432593	1.742127	-0.609519
H	-0.179037	2.363136	-1.136073
H	0.339701	2.539882	0.570667
O	-0.157141	0.621117	0.016916
H	-1.124403	0.704504	0.340212
C	2.930827	-0.272963	1.226035
H	3.724750	0.419234	1.510969
H	1.994285	0.047779	1.698435
H	3.189270	-1.269815	1.600579
O	2.841648	-0.246115	-0.191377
H	2.142792	-0.864860	-0.432832
C	-0.416500	-0.368012	-1.197808
H	0.234960	0.095766	-1.954173
F	0.313609	-1.492588	-0.778922

15, y_{15}

C	2.494256	-1.371704	0.524963
H	1.479956	-1.662467	0.254900
H	3.177834	-2.188895	0.280365
H	2.531298	-1.162827	1.597592
O	2.803389	-0.200485	-0.246589
H	3.693484	0.084050	-0.023854
C	0.315782	2.304611	-0.011150
H	-0.740072	2.565184	-0.048540
H	0.588952	2.113266	1.030005
H	0.914708	3.126688	-0.412049
O	0.492819	1.129135	-0.814129
H	1.399267	0.796500	-0.675880
C	-2.096504	-1.009753	-1.297299
H	-2.597836	-1.939173	-1.038833
H	-2.788898	-0.171425	-1.210242
H	-1.657349	-1.055127	-2.294942
O	-1.020962	-0.856259	-0.351331
H	-0.476212	-0.024363	-0.563451
C	-1.558370	-0.808287	1.141155
H	-0.558247	-0.720239	1.612925
F	-2.011093	0.552277	1.182488

16, y_{16}

C	3.104477	-0.904266	0.452428
H	3.814417	-0.077663	0.436144
H	2.646099	-0.966880	1.444051
H	3.639526	-1.833461	0.237277
O	2.128533	-0.628031	-0.556165
H	1.476268	-1.336955	-0.537030
C	-2.280697	-0.968445	-1.116298
H	-2.598586	-1.982936	-0.889225
H	-3.004541	-0.250975	-0.728135
H	-2.120710	-0.827750	-2.186116
O	-1.012413	-0.786774	-0.454611
H	-0.630301	0.137532	-0.647570
C	0.215525	2.427153	0.069461
H	-0.787038	2.849075	0.021341
H	0.393723	2.061790	1.083857
H	0.947150	3.195846	-0.191977
O	0.266911	1.354530	-0.882061
H	1.124090	0.898589	-0.796418
C	-1.136256	-1.013150	1.118538
H	-0.060935	-0.838526	1.332493
F	-1.702412	0.245196	1.491026

17, y_{17}

C	-1.519095	-0.953941	1.252243
H	-2.571301	-0.817065	1.488222
H	-1.192937	-1.956526	1.533587
H	-0.922124	-0.182302	1.744830
O	-1.381813	-0.822809	-0.174977
H	-0.407243	-0.964535	-0.382788
C	1.891878	-2.206626	-0.185700
H	1.339187	-3.105193	-0.462698
H	2.869274	-2.233326	-0.676441
H	2.031712	-2.189660	0.900362
O	1.133937	-1.084013	-0.631139
H	1.597371	-0.268085	-0.349644
C	1.535216	2.371225	0.185931
H	0.490740	2.061423	0.113651
H	1.682262	3.010598	1.060774
H	1.814876	2.914062	-0.721529
O	2.312996	1.162021	0.316932
H	3.243143	1.396064	0.265763
C	-1.606100	0.762700	-0.619871
H	-1.635780	0.528635	-1.702105
F	-2.963504	0.880463	-0.299348

18, y_{18}

C	-3.321404	-0.629187	-0.783426
H	-3.141959	-0.159835	-1.749506
H	-2.738682	-1.549450	-0.709873
H	-4.388062	-0.835542	-0.676071
O	-2.894993	0.321697	0.213665
H	-3.069884	-0.065641	1.077496
C	0.191314	1.982443	0.001607
H	1.246023	1.914886	-0.256892
H	-0.350878	2.627999	-0.689044
H	0.064151	2.324778	1.031620
O	-0.351740	0.647817	-0.145371
H	-1.341662	0.637549	0.002122
C	3.712673	-0.716073	-0.495717
H	4.590331	-0.306001	-1.001707
H	4.061712	-1.353262	0.328213
H	3.168791	-1.348519	-1.210694
O	2.926220	0.363395	-0.036360
H	2.104973	-0.022706	0.372605
C	0.331331	-0.382101	0.864622
H	-0.227684	-0.111602	1.784677
F	-0.321838	-1.549602	0.435452

19, y_{19}

C	0.179952	1.933144	-0.021472
H	1.267689	1.918760	-0.049410
H	-0.229642	2.644588	-0.737997
H	-0.181060	2.144849	0.988259
O	-0.254553	0.614952	-0.435167
H	-1.250397	0.544369	-0.490411
C	-3.753616	-0.067064	0.412340
H	-4.056824	0.978713	0.441908
H	-4.609386	-0.677513	0.114787
H	-3.406585	-0.374605	1.402918
O	-2.703826	-0.165489	-0.558519
H	-2.400208	-1.082110	-0.590831
C	3.873627	-0.561217	-0.166684
H	4.805574	-0.045660	-0.411223
H	4.095315	-1.324631	0.591190
H	3.515095	-1.070093	-1.071702
O	2.951058	0.400574	0.302479
H	2.092635	-0.070050	0.471814
C	0.262269	-0.520892	0.551316
H	-0.462436	-0.372334	1.377723

F	-0.277178	-1.635379	-0.128931

20, y_{20}

C	-0.223434	1.421849	1.262887
H	-1.167615	1.814347	0.891018
H	-0.320084	1.123328	2.306340
H	0.588049	2.133532	1.120325
O	0.038838	0.212628	0.496359
H	0.874535	-0.293807	0.774894
C	-3.654889	-0.918838	-0.486147
H	-4.646662	-0.470981	-0.418514
H	-3.275348	-0.778097	-1.504653
H	-3.742170	-1.992090	-0.283612
O	-2.838833	-0.262744	0.477305
H	-1.956450	-0.638823	0.409032
C	3.366156	-0.932016	0.129101
H	3.825012	-1.043246	1.112436
H	3.863629	-1.607591	-0.572501
H	3.490973	0.099852	-0.216444
O	1.984740	-1.272506	0.252508
H	1.522180	-1.022453	-0.605556
C	0.294250	0.305927	-1.064465
H	-0.713289	0.618072	-1.377827
F	1.054087	1.486377	-1.165840

21, y_{21}

C	1.191516	2.148690	-0.011349
H	0.252655	1.899680	-0.502191
H	1.024522	2.204978	1.065673
H	1.566133	3.100514	-0.394471
O	2.122877	1.091858	-0.330650
H	2.958887	1.282298	0.104936
C	0.375559	-1.479290	-1.432877
H	0.011330	-2.502614	-1.417966
H	-0.453980	-0.771541	-1.413783
H	1.031271	-1.302476	-2.286506
O	1.181115	-1.327229	-0.238222
H	1.562145	-0.399040	-0.214678
C	-3.249579	0.331430	-0.182069
H	-3.779930	0.790822	-1.017629
H	-3.320001	-0.758591	-0.275904
H	-3.739404	0.635979	0.749924
O	-1.902600	0.778989	-0.239820
H	-1.426913	0.355178	0.487645
C	0.395857	-1.676520	1.083453

H	1.283827	-1.771811	1.731528
F	-0.051311	-0.339799	1.456667

22, y_{22}

C	-1.531236	-0.484341	-1.464891
H	-1.027257	0.366938	-1.912771
H	-0.801931	-1.196153	-1.079022
H	-2.241346	-0.937909	-2.155770
O	-2.319548	0.073178	-0.356677
H	-2.846659	-0.639640	0.042527
C	1.964415	-1.886161	0.547172
H	1.954067	-2.978055	0.559654
H	2.999305	-1.553156	0.697309
H	1.351052	-1.521639	1.380289
O	1.451083	-1.466411	-0.706363
H	1.445506	-0.491350	-0.687864
C	1.801229	2.269143	0.046934
H	2.726657	2.341121	-0.528322
H	1.290077	3.238389	-0.000025
H	2.057358	2.059627	1.093381
O	1.010313	1.237980	-0.518968
H	0.148733	1.184722	-0.004407
C	-1.418291	0.725833	0.793716
H	-2.234900	1.257216	1.304431
F	-1.205794	-0.403881	1.601007

23, y_{23}

C	1.915496	-0.264853	1.314023
H	2.931845	-0.440710	0.965942
H	1.923813	0.191177	2.304653
H	1.330358	-1.182206	1.307605
O	1.341391	0.709218	0.400523
H	0.384579	0.905453	0.600733
C	-2.119660	-1.824850	-0.049715
H	-2.744569	-2.131036	0.791230
H	-2.404383	-0.808179	-0.344096
H	-2.310564	-2.505607	-0.887717
O	-0.770787	-1.886419	0.384512
H	-0.216955	-1.625769	-0.362327
C	-1.511684	2.230779	-0.485281
H	-0.876974	1.889837	-1.302248
H	-2.566860	2.068984	-0.720522
H	-1.327178	3.292302	-0.299609
O	-1.132098	1.434948	0.656277
H	-1.577740	1.773109	1.437513

C	1.449387	0.524081	-1.153828
H	2.550307	0.566638	-1.222166
F	1.221672	-0.894101	-1.283408

24, y_{24}

C	-3.572059	-0.760887	-0.697782
H	-3.977890	-1.644838	-0.204636
H	-4.383193	-0.047265	-0.870129
H	-3.144279	-1.055827	-1.662560
O	-2.584314	-0.198637	0.161444
H	-2.110024	0.548317	-0.312320
C	0.185904	0.124779	1.773583
H	1.198771	0.516010	1.786719
H	-0.533342	0.890904	2.067011
H	0.109503	-0.755408	2.411145
O	-0.095388	-0.306772	0.413471
H	-1.056540	-0.606598	0.406942
C	3.244638	-0.352461	-0.825879
H	4.316736	-0.350464	-0.625939
H	3.088093	-0.648613	-1.869963
H	2.860205	0.663902	-0.683187
O	2.655855	-1.275808	0.082413
H	1.703869	-1.228021	-0.048241
C	-0.330895	0.989136	-0.685238
H	0.254863	0.519601	-1.494093
F	0.522054	1.938293	-0.171941

25, y_{25}

C	3.019444	-1.078933	0.408715
H	3.870307	-0.413443	0.559540
H	2.558358	-1.286990	1.380904
H	3.385259	-2.018769	-0.019406
O	2.120981	-0.410823	-0.469864
H	1.351000	-0.978265	-0.576550
C	0.669579	2.490589	-0.141801
H	1.275115	2.259602	-1.015027
H	0.468190	3.563528	-0.097256
H	1.205349	2.163859	0.751532
O	-0.564364	1.766824	-0.292903
H	-1.082001	1.845962	0.518851
C	-1.815892	-1.145313	-1.363143
H	-1.927763	-2.220632	-1.251615
H	-2.735848	-0.637857	-1.071004
H	-1.519725	-0.873605	-2.377061
O	-0.744804	-0.758315	-0.473685

H	-0.606473	0.247294	-0.511065
C	-1.081473	-1.150216	1.045087
H	-0.111255	-0.806395	1.454391
F	-1.930551	-0.035839	1.383582

26, y_{26}

C	2.569543	-0.567314	0.706137
H	2.535092	-1.623326	0.967593
H	3.337062	-0.382618	-0.049019
H	2.744028	0.039930	1.595680
O	1.267725	-0.233050	0.182211
H	1.138733	0.752292	0.019574
C	-2.826985	-0.539798	-0.097989
H	-3.562666	0.249338	0.073482
H	-2.344304	-0.381604	-1.068761
H	-3.352656	-1.501656	-0.117914
O	-1.885141	-0.475025	0.964949
H	-1.188739	-1.098359	0.727951
C	-0.641297	2.414820	-0.132328
H	-1.010948	1.781861	0.672186
H	-0.881209	3.462827	0.059305
H	-1.082744	2.078545	-1.072113
O	0.796095	2.243283	-0.164407
H	1.120429	2.637950	-0.979652
C	0.688271	-0.982010	-1.075127
H	1.623227	-1.440510	-1.450706
F	0.084230	-2.090058	-0.404865

27, y_{27}

C	2.936233	-0.432318	-1.185235
H	3.658958	-1.250085	-1.167031
H	1.960900	-0.828183	-1.494229
H	3.265823	0.303831	-1.927690
O	2.890025	0.116479	0.122143
H	2.246710	0.835630	0.092348
C	-3.415503	0.455749	-0.457553
H	-2.945347	1.042762	0.329249
H	-3.388014	1.020522	-1.392550
H	-4.446208	0.203189	-0.197711
O	-2.626298	-0.749907	-0.568361
H	-2.896797	-1.223932	-1.359424
C	0.200369	-1.502464	1.107822
H	1.257320	-1.365504	1.327291
H	-0.405912	-1.468870	2.016185
H	0.033480	-2.440512	0.575862

O	-0.174900	-0.417985	0.229073
H	-1.095342	-0.576422	-0.113920
C	-0.294485	1.044019	0.945783
H	0.378319	0.814358	1.793759
F	0.567312	1.772735	0.087791

31, y_{28}

C	-0.023827	-0.217068	1.671567
H	1.007515	0.062322	1.867053
H	-0.717866	0.504008	2.107548
H	-0.213237	-1.230091	2.027323
O	-0.195500	-0.216706	0.233298
H	-1.092042	-0.602055	0.045499
C	-3.540584	0.071597	-0.461273
H	-3.034402	0.974206	-0.119831
H	-3.710020	0.141124	-1.538571
H	-4.490982	-0.054353	0.062310
O	-2.653693	-1.022860	-0.151430
H	-2.979687	-1.821707	-0.574398
C	2.941820	-1.107310	-0.862345
H	3.553579	-1.979327	-0.625231
H	1.909735	-1.436843	-1.031913
H	3.325608	-0.657048	-1.785800
O	3.034316	-0.218686	0.239655
H	2.480689	0.541266	0.027895
C	-0.362527	1.327272	-0.344487
H	-0.371055	1.004118	-1.406317
F	0.973543	1.752606	-0.183170

33, y_{29}

C	-0.280664	1.837969	0.478246
H	-1.357974	1.813252	0.625332
H	0.250330	1.975653	1.423538
H	-0.008123	2.613753	-0.237801
O	0.084382	0.558906	-0.084920
H	1.029307	0.613414	-0.387451
C	3.312660	-0.452702	-0.033773
H	2.817953	-0.541338	0.931806
H	3.219000	-1.400874	-0.567891
H	4.364989	-0.185796	0.090268
O	2.616716	0.600563	-0.736947
H	2.928931	0.616798	-1.645836
C	-2.885711	-0.740042	-0.768521
H	-1.938243	-0.554271	-1.270279
H	-2.755716	-1.599863	-0.104327

H	-3.653274	-0.966339	-1.516934
O	-3.200336	0.449825	-0.040387
H	-4.009341	0.278241	0.447508
C	0.182806	-0.573577	1.132370
H	-0.889882	-0.503868	1.397008
F	0.224601	-1.718111	0.318128

34, y_{30}

C	1.238079	2.353896	-0.125658
H	0.617025	1.988989	-0.943595
H	0.788511	3.257651	0.294883
H	2.251744	2.568186	-0.475251
O	1.263025	1.288650	0.846188
H	1.670050	1.618614	1.651536
C	-1.401623	-1.093000	1.381290
H	-2.456165	-1.275718	1.182496
H	-0.779090	-1.928484	1.063341
H	-1.252638	-0.869263	2.439746
O	-1.054149	0.083857	0.618222
H	-0.127941	0.397957	0.779812
C	1.931556	-1.223780	-1.061448
H	1.148798	-0.556381	-1.422028
H	2.825902	-0.634076	-0.834031
H	2.164479	-1.956353	-1.842088
O	1.415679	-1.859220	0.112959
H	2.087424	-2.471125	0.423250
C	-1.267887	0.087595	-0.972384
H	-1.310925	-1.011138	-1.118326
F	-2.624929	0.446287	-1.016610

35, y_{31}

C	3.338436	-0.602517	0.938975
H	2.271335	-0.800793	1.039089
H	3.851215	-1.540500	0.699973
H	3.723266	-0.213458	1.888391
O	3.479196	0.352946	-0.115604
H	4.415284	0.542789	-0.210181
C	-2.992917	-0.346847	1.119429
H	-2.012530	-0.644510	1.487621
H	-3.652860	-0.080443	1.948581
H	-3.412011	-1.173062	0.542482
O	-2.771645	0.805358	0.277364
H	-3.581377	0.983527	-0.208836
C	0.397879	1.592284	-0.249459
H	1.430062	1.360664	-0.505558

H	0.107953	2.566726	-0.643879
H	0.263664	1.547045	0.832972
O	-0.436221	0.596234	-0.882109
H	-1.356344	0.706036	-0.521267
C	-0.014842	-0.909806	-0.316042
H	0.829050	-1.034841	-1.021302
F	-1.046521	-1.628240	-0.946968

36, y_{32}

C	-2.162935	1.750922	-0.021909
H	-2.330415	0.853480	-0.615469
H	-2.902591	1.795177	0.781262
H	-2.243352	2.636875	-0.655836
O	-0.829751	1.638825	0.515872
H	-0.680224	2.363500	1.130745
C	2.782208	0.443384	-0.885454
H	3.743388	0.212812	-0.424071
H	2.314508	-0.488277	-1.221241
H	2.960885	1.090880	-1.750936
O	1.997293	1.099355	0.109657
H	1.146329	1.314304	-0.285181
C	0.626914	-1.612167	1.478975
H	0.560623	-2.671255	1.245794
H	1.603581	-1.215062	1.205822
H	0.412772	-1.423992	2.532594
O	-0.406812	-0.976702	0.700808
H	-0.409825	0.000711	0.825892
C	-0.347508	-1.400873	-0.890129
H	-0.109772	-0.383379	-1.273539
F	-1.727091	-1.473910	-1.132826

38, y_{33}

C	2.279608	-0.632498	0.982817
H	1.280084	-0.463990	1.378910
H	2.453089	-1.712571	0.933005
H	3.017361	-0.177495	1.652419
O	2.316132	-0.036141	-0.318777
H	3.206444	-0.153921	-0.659547
C	0.064167	2.433591	-0.004587
H	1.074527	2.045813	-0.117614
H	0.046603	3.502015	-0.232200
H	-0.287157	2.252750	1.014079
O	-0.746060	1.709898	-0.953748
H	-1.658367	1.992222	-0.833022
C	-0.410332	-1.753481	-1.410482

H	-0.373622	-2.733779	-0.940824
H	-1.265380	-1.698591	-2.089662
H	0.518688	-1.523417	-1.931810
O	-0.548699	-0.803861	-0.344648
H	-0.566491	0.133239	-0.690769
C	-1.831761	-1.102286	0.589457
H	-2.580614	-0.528992	-0.005482
F	-1.516250	-0.173823	1.612963

41, y_{34}

C	0.655813	2.236683	-0.828055
H	-0.136908	1.495488	-0.905316
H	0.266431	3.109362	-0.297229
H	0.982994	2.524729	-1.831972
O	1.721226	1.621596	-0.091755
H	2.446158	2.249053	-0.034631
C	-1.420239	-1.775411	-0.966916
H	-0.332473	-1.765712	-0.925100
H	-1.831105	-2.456341	-0.217787
H	-1.765061	-2.041207	-1.967422
O	-1.840269	-0.421151	-0.667675
H	-2.802744	-0.392537	-0.730251
C	2.198235	-1.689776	0.864534
H	2.053536	-2.771202	0.830589
H	3.263373	-1.491245	1.034006
H	1.626223	-1.288098	1.709603
O	1.753099	-1.161689	-0.375607
H	1.846889	-0.198623	-0.318870
C	-1.655683	-0.126094	1.163924
H	-0.553735	-0.198646	1.055574
F	-1.867198	1.226947	1.142020

43, y_{35}

C	-2.496632	-1.602615	0.290417
H	-1.625055	-1.432511	0.920519
H	-3.335738	-1.933171	0.909900
H	-2.250434	-2.378351	-0.440862
O	-2.797566	-0.356489	-0.353380
H	-3.540630	-0.498387	-0.944997
C	2.372922	0.894454	-0.511470
H	1.524616	1.188557	-1.125184
H	2.918559	1.769324	-0.155656
H	3.031127	0.198604	-1.030598
O	1.773818	0.235367	0.643687
H	2.443361	0.043391	1.312945

C	-0.864817	2.208717	0.574999
H	-0.028830	2.907394	0.655420
H	-1.797949	2.779098	0.653788
H	-0.807162	1.502274	1.411004
O	-0.750693	1.551264	-0.677848
H	-1.462866	0.894921	-0.701093
C	1.036488	-1.240298	0.421125
H	0.384514	-0.872471	-0.391549
F	2.050472	-1.907929	-0.291525

44, y_{36}

C	0.173566	-1.120386	-1.619803
H	-0.259803	-0.142815	-1.431419
H	0.672621	-1.150054	-2.589785
H	-0.594266	-1.891346	-1.546127
O	1.171683	-1.314317	-0.582439
H	1.634984	-2.145926	-0.738553
C	1.824869	2.048598	-0.544423
H	1.519925	2.764201	-1.309745
H	2.560517	2.532186	0.108273
H	2.297154	1.187338	-1.031492
O	0.653959	1.671565	0.166033
H	0.924807	1.021534	0.825688
C	-2.689721	0.946873	0.417304
H	-1.718437	1.416463	0.266689
H	-3.472702	1.615850	0.043795
H	-2.839329	0.781734	1.489938
O	-2.667734	-0.287716	-0.304847
H	-3.519056	-0.711174	-0.171244
C	0.522049	-1.654049	1.015664
H	-0.434197	-1.145104	0.793330
F	1.219993	-0.668372	1.716469

O-ylidic carbene-solvent complexes

28, c_1

C	0.381517	2.567960	-0.515472
H	1.359466	3.042475	-0.428381
H	-0.235275	3.163565	-1.196727
H	-0.092213	2.541534	0.470857
O	0.595908	1.255187	-1.027479
H	-0.264866	0.814876	-1.091806

C	3.077130	-0.890050	0.561988
H	3.333556	-1.821463	1.069518
H	3.621639	-0.851641	-0.389429
H	3.407878	-0.053320	1.189705
O	1.672660	-0.882169	0.367608
H	1.445681	-0.054102	-0.087967
C	-1.128893	-1.826947	-1.242654
H	-0.076631	-1.879475	-0.967304
H	-1.688913	-2.588961	-0.694302
H	-1.245164	-1.974736	-2.319183
O	-1.578414	-0.511388	-0.860988
H	-2.523460	-0.460067	-1.037471
C	-1.777947	-0.585172	1.434383
H	-0.712621	-0.896101	1.378625
F	-1.684573	0.725513	1.649030

29, c_2

C	-3.081161	-0.882836	0.567412
H	-3.338232	-1.813054	1.076809
H	-3.410096	-0.044617	1.194116
H	-3.626737	-0.845306	-0.383441
O	-1.676917	-0.877159	0.371403
H	-1.449159	-0.050554	-0.086431
C	-0.378222	2.566994	-0.516008
H	-1.354962	3.044204	-0.429991
H	0.094232	2.539255	0.470904
H	0.241002	3.160940	-1.196478
O	-0.595652	1.254802	-1.028265
H	0.264258	0.812942	-1.093597
C	1.119700	-1.831704	-1.240012
H	0.068856	-1.880869	-0.958698
H	1.229351	-1.981880	-2.316920
H	1.680785	-2.594076	-0.693292
O	1.574986	-0.516533	-0.863663
H	2.519321	-0.468622	-1.044890
C	1.779950	-0.586931	1.431396
H	0.711279	-0.886678	1.378281
F	1.701019	0.725145	1.643456

32, c_4

C	1.443750	-1.402932	-1.167251
H	0.417489	-1.565920	-0.842044
H	1.513245	-1.552246	-2.247082
H	2.118668	-2.080205	-0.639390
O	1.769299	-0.031883	-0.835557

H	2.664154	0.136458	-1.150106
C	-2.577775	-1.096152	0.663658
H	-3.485413	-0.482202	0.606614
H	-2.872639	-2.120215	0.898850
H	-1.948041	-0.721856	1.480820
O	-1.879984	-1.126935	-0.570143
H	-1.620999	-0.213712	-0.768927
C	-0.733903	2.394770	0.020157
H	-1.755620	2.775872	0.036395
H	-0.492063	1.991702	1.010092
H	-0.057444	3.226254	-0.206112
O	-0.675951	1.387627	-0.984087
H	0.232528	1.054222	-1.013788
C	2.123148	0.035219	1.369370
H	2.017415	1.138571	1.240475
F	0.892277	-0.333626	1.710766

37, c_5

C	0.000812	-0.976520	0.008298
H	0.001147	-1.816971	-0.705136
F	0.000793	-1.556838	1.205261
C	2.962755	0.114583	-0.411024
H	2.338911	0.738443	-1.048023
H	3.974316	0.061672	-0.825406
H	2.997820	0.562111	0.587528
O	2.353414	-1.180928	-0.378999
H	2.865026	-1.729322	0.222735
C	-2.962692	0.112448	-0.410521
H	-2.338700	0.738091	-1.045629
H	-3.973644	0.059048	-0.826325
H	-2.999627	0.558284	0.588727
O	-2.351914	-1.182431	-0.379788
H	-2.863286	-1.732170	0.220916
C	-0.001708	2.569475	0.721686
H	0.887970	2.327450	1.319925
H	-0.003059	3.645818	0.536312
H	-0.890455	2.325295	1.320432
O	-0.001276	1.913686	-0.529573
H	-0.000351	0.951250	-0.337153

39, c_6

C	2.187331	-1.235027	-0.993273
H	3.271434	-1.351975	-1.045935
H	1.728708	-2.009718	-1.620632
H	1.917390	-0.251388	-1.395088

O	1.814542	-1.365844	0.369379
H	0.853666	-1.272230	0.398509
C	1.740748	2.015343	0.493866
H	2.281345	1.131725	0.831332
H	2.323871	2.517517	-0.285987
H	1.609420	2.700469	1.338985
O	0.487060	1.547969	-0.005167
H	-0.016156	2.311798	-0.299559
C	-1.428744	-0.496544	1.688169
H	-0.773483	0.370037	1.731558
H	-2.471419	-0.169334	1.655246
H	-1.263170	-1.139450	2.556499
O	-1.076268	-1.190593	0.478834
H	-1.636333	-1.970754	0.403583
C	-1.865023	-0.328321	-1.393353
H	-0.798624	-0.117770	-1.613828
F	-2.292800	0.842901	-0.907946

40, c_7

C	-2.480741	-1.297895	-0.125321
H	-3.406252	-1.158468	-0.686710
H	-2.538446	-2.263188	0.393100
H	-2.397508	-0.496049	0.617626
O	-1.412475	-1.262724	-1.062088
H	-0.599509	-1.421908	-0.565655
C	-1.068654	2.129461	-0.405090
H	-1.130916	1.201157	-0.971829
H	-1.937409	2.751039	-0.647197
H	-0.152412	2.660306	-0.682848
O	-1.060277	1.763261	0.978864
H	-1.051849	2.577446	1.488009
C	1.061633	-0.791897	1.644541
H	0.373346	0.049122	1.579937
H	0.716205	-1.502065	2.400657
H	2.060924	-0.429909	1.900599
O	1.068024	-1.409618	0.343818
H	1.708139	-2.128678	0.354626
C	2.266765	-0.212055	-1.176129
H	1.327966	-0.251509	-1.771177
F	2.176836	0.968852	-0.569100

42, c_8

C	-1.621542	-0.491547	1.769082
H	-1.788501	0.548396	1.494261
H	-2.532322	-1.070978	1.599247

H	-1.324318	-0.547756	2.819128
O	-0.561622	-0.975127	0.921167
H	-0.354086	-1.872316	1.206031
C	0.480860	2.262471	0.020205
H	0.756434	3.276482	0.312790
H	0.774810	1.579190	0.827179
H	1.032202	1.996861	-0.888451
O	-0.923845	2.259234	-0.187089
H	-1.152277	1.427861	-0.611209
C	3.196673	-0.382002	0.088078
H	3.999965	-0.837443	-0.491879
H	3.226111	0.702409	-0.071419
H	3.375836	-0.588670	1.149989
O	1.979223	-0.952604	-0.367988
H	1.262712	-0.574382	0.153535
C	-1.392878	-1.622934	-1.079635
H	-0.322221	-1.751590	-1.348552
F	-1.653675	-0.392891	-1.540640

Hydrogen bonded carbene-solvent complex

30, c_3			
C	-2.921171	0.711830	0.689473
H	-3.800935	0.099735	0.485549
H	-2.535656	0.452015	1.682285
H	-3.220189	1.765706	0.690330
O	-1.969003	0.443851	-0.331638
H	-1.162231	0.951923	-0.123562
C	0.854672	2.739966	-0.604023
H	0.048249	3.451069	-0.786031
H	1.702144	3.276251	-0.164607
H	1.160297	2.303763	-1.561274
O	0.352825	1.749039	0.288162
H	1.060856	1.095941	0.438362
C	-0.253796	-2.369781	0.025389
H	-0.046948	-3.433838	0.162577
H	0.605952	-1.926185	-0.505285
H	-0.329090	-1.901546	1.017289
O	-1.444577	-2.249127	-0.713106
H	-1.682678	-1.305661	-0.688703
C	2.344481	-0.477020	0.686699
H	2.304746	-1.345477	1.381482
F	3.359601	-0.740419	-0.084554