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

Weak covalent interactions and anionic polymerisation in cluster environments

Supplementary information

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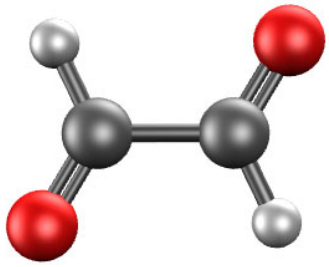
COMPUTATIONAL DETAILS

All structures reported here were optimised using the QChem 5.1 program package, with the Minnesota-06 (M06-2X) functional and Dunning's augmented correlation-consistent basis set of double-zeta quality (aug-cc-pVDZ). The geometry optimisations were carried out under the stated symmetry constraints. In cluster cases, complete explorations of the geometry space were not attempted; hence, the structures shown do not necessarily correspond to global potential minima. See the main article text for details and explanation.

STRUCTURES SHOWN IN FIG. 4 OF THE MAIN ARTICLE

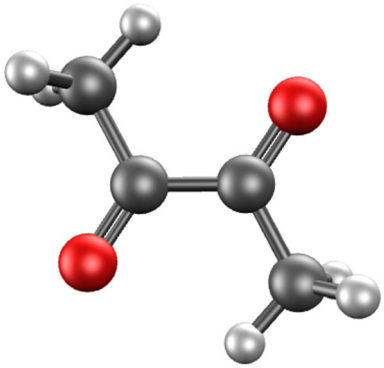
The perspectives and orientations in the following figures are not the same as in main article's Fig. 4.

Glyoxal monomer anion, gl^- (C_{2h} symmetry point group)



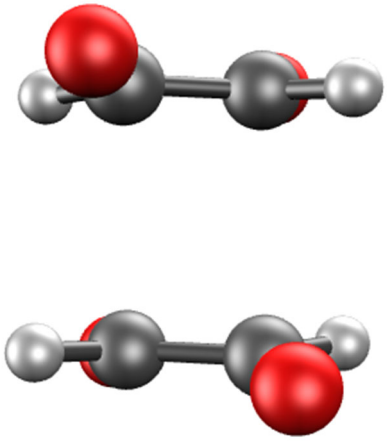
		Coordinates (Angstroms)		
ATOM		X	Y	Z
1	C	0.6149153686	-0.3632781750	0.0000000000
2	C	-0.6149153686	0.3632781750	0.0000000000
3	O	1.7727924620	0.1465066996	0.0000000000
4	H	0.4894421655	-1.4723690303	0.0000000000
5	O	-1.7727924620	-0.1465066996	0.0000000000
6	H	-0.4894421655	1.4723690303	0.0000000000

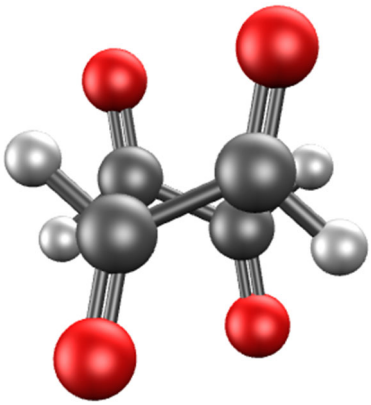
Biacetyl monomer anion, ba^- (C_{2h} symmetry point group)



		Coordinates (Angstroms)		
ATOM		X	Y	Z
1	C	0.6556135688	0.2979035805	-0.0000000000
2	O	0.8652501126	1.5498097028	-0.0000000000
3	C	-0.6556135688	-0.2979035805	-0.0000000000
4	O	-0.8652501126	-1.5498097028	0.0000000000
5	C	-1.8505182437	0.6427949872	-0.0000000000
6	H	-1.5269980317	1.6890705606	-0.0000000000
7	H	-2.4723103480	0.4415730840	-0.8857931777
8	H	-2.4723103480	0.4415730840	0.8857931777
9	C	1.8505182437	-0.6427949872	0.0000000000
10	H	1.5269980317	-1.6890705606	0.0000000000
11	H	2.4723103480	-0.4415730840	-0.8857931777
12	H	2.4723103480	-0.4415730840	0.8857931777

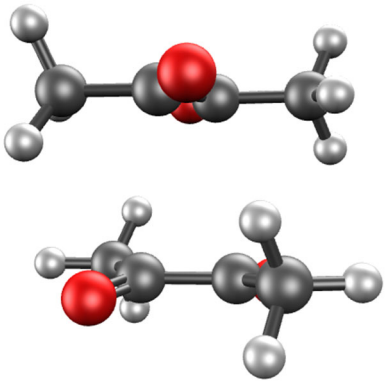
Glyoxal dimer anion, $(gl)_2^-$ (D_2 symmetry point group)

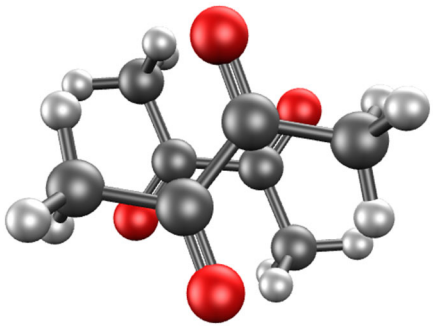




ATOM		Coordinates (Angstroms) X	Y	Z
1	C	-1.3035539624	0.3020213169	0.6768920260
2	C	-1.3035539624	-0.3020213169	-0.6768920260
3	O	-1.4469127028	1.5074895006	0.8784868618
4	H	-1.2522308496	-0.4370903796	1.5050246429
5	O	-1.4469127028	-1.5074895006	-0.8784868618
6	H	-1.2522308496	0.4370903796	-1.5050246429
7	C	1.3035539624	0.3020213169	-0.6768920260
8	C	1.3035539624	-0.3020213169	0.6768920260
9	O	1.4469127028	1.5074895006	-0.8784868618
10	H	1.2522308496	-0.4370903796	-1.5050246429
11	O	1.4469127028	-1.5074895006	0.8784868618
12	H	1.2522308496	0.4370903796	1.5050246429

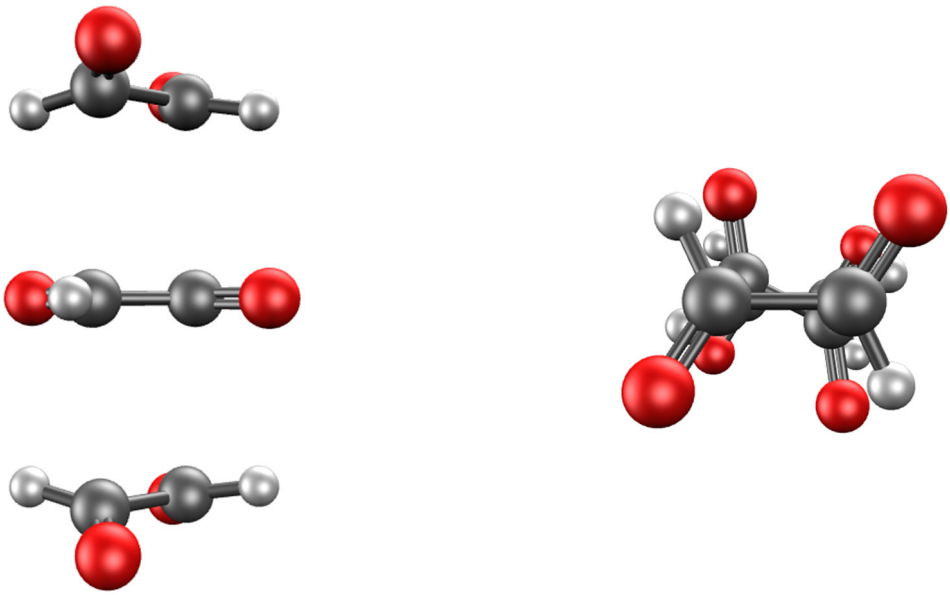
Biacetyl dimer anion, $(ba)_2^-$ (C_2 symmetry point group)





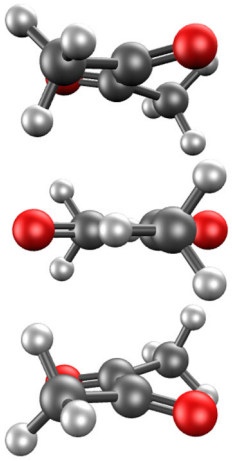
		Coordinates (Angstroms)		
ATOM		X	Y	Z
1	O	-1.7529639130	0.0233125684	1.5167019251
2	C	-0.5850693943	0.4532682360	1.4441634267
3	C	0.5850693943	-0.4532682360	1.4441634267
4	O	1.7529639130	-0.0233125684	1.5167019251
5	C	0.3268152617	-1.9440814486	1.4534363233
6	H	-0.7390076477	-2.1664599950	1.3477113652
7	H	0.8999505452	-2.3978471262	0.6342225228
8	H	0.6964442540	-2.3587838305	2.4016095659
9	C	-0.3268152617	1.9440814486	1.4534363233
10	H	0.7390076477	2.1664599950	1.3477113652
11	H	-0.8999505452	2.3978471262	0.6342225228
12	H	-0.6964442540	2.3587838305	2.4016095659
13	H	1.9518735616	0.9444818494	-0.4681784793
14	C	1.4424647673	1.3263424800	-1.3642348311
15	H	1.3743175231	2.4187950915	-1.3478291856
16	H	2.0226667162	0.9909746143	-2.2342045331
17	C	0.0528585033	0.7534115414	-1.4481752280
18	O	-0.9499318375	1.4422583872	-1.6222605105
19	C	-0.0528585033	-0.7534115414	-1.4481752280
20	O	0.9499318375	-1.4422583872	-1.6222605105
21	C	-1.4424647673	-1.3263424800	-1.3642348311
22	H	-1.3743175231	-2.4187950915	-1.3478291856
23	H	-2.0226667162	-0.9909746143	-2.2342045331
24	H	-1.9518735616	-0.9444818494	-0.4681784793

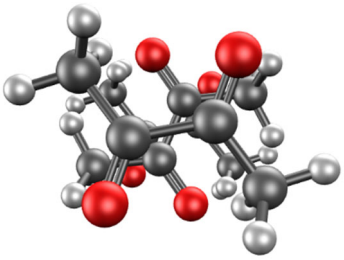
Glyoxal trimer anion, $(gl)_3^-$ (C_{2h} symmetry point group)



ATOM		Coordinates (Angstroms) X	Y	Z
1	C	-0.5886767908	-0.4791577526	2.7994764194
2	C	0.5886767908	0.4791577526	2.7994764194
3	O	-0.4391038375	-1.6414268612	3.1041734970
4	H	-1.5765426418	-0.0220320001	2.5922247054
5	O	0.4391038375	1.6414268612	3.1041734970
6	H	1.5765426418	0.0220320001	2.5922247054
7	C	0.7088075889	0.1659074148	0.0000000000
8	C	-0.7088075889	-0.1659074148	0.0000000000
9	O	1.6302950633	-0.6781177427	0.0000000000
10	H	0.9231623340	1.2571482971	0.0000000000
11	O	-1.6302950633	0.6781177427	0.0000000000
12	H	-0.9231623340	-1.2571482971	0.0000000000
13	C	-0.5886767908	-0.4791577526	-2.7994764194
14	C	0.5886767908	0.4791577526	-2.7994764194
15	O	-0.4391038375	-1.6414268612	-3.1041734970
16	H	-1.5765426418	-0.0220320001	-2.5922247054
17	O	0.4391038375	1.6414268612	-3.1041734970
18	H	1.5765426418	0.0220320001	-2.5922247054

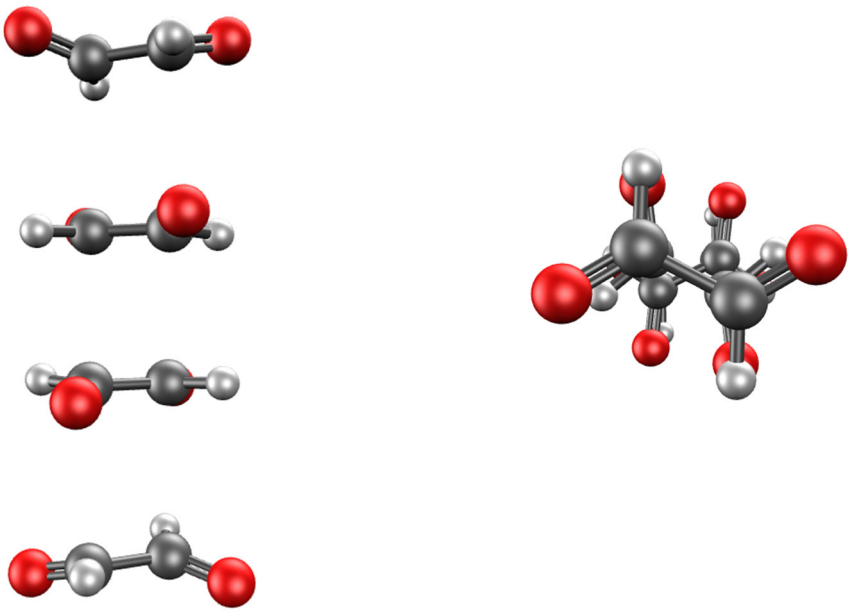
Biacetyl trimer anion, $(ba)_3^-$ (C_{2h} symmetry point group)





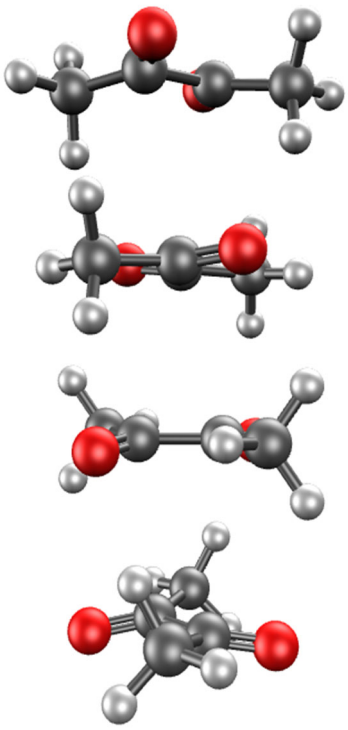
		Coordinates (Angstroms)		
ATOM		X	Y	Z
1	C	-1.0378582818	-1.6598501687	-2.8768399046
2	C	0.1427161510	-0.7554504523	-3.0675485872
3	C	-0.1427161510	0.7554504523	-3.0675485872
4	C	1.0378582818	1.6598501687	-2.8768399046
5	O	1.2752946534	-1.1410911854	-3.2848371056
6	O	-1.2752946534	1.1410911854	-3.2848371056
7	H	-0.7050840327	-2.7002512387	-2.9283060160
8	H	-1.7832643825	-1.4430806457	-3.6517974517
9	H	-1.5081966865	-1.4354180189	-1.9069650177
10	H	0.7050840327	2.7002512387	-2.9283060160
11	H	1.7832643825	1.4430806457	-3.6517974517
12	H	1.5081966865	1.4354180189	-1.9069650177
13	C	0.6761627167	-0.2839023032	0.0000000000
14	C	-0.6761627167	0.2839023032	0.0000000000
15	C	-0.8310547905	1.7907351824	0.0000000000
16	C	0.8310547905	-1.7907351824	0.0000000000
17	O	1.7061666889	0.4379567512	0.0000000000
18	O	-1.7061666889	-0.4379567512	0.0000000000
19	H	0.1381483858	2.2982306366	0.0000000000
20	H	-1.4091451491	2.0838634349	0.8866280203
21	H	-1.4091451491	2.0838634349	-0.8866280203
22	H	-0.1381483858	-2.2982306366	0.0000000000
23	H	1.4091451491	-2.0838634349	0.8866280203
24	H	1.4091451491	-2.0838634349	-0.8866280203
25	C	-1.0378582818	-1.6598501687	2.8768399046
26	C	0.1427161510	-0.7554504523	3.0675485872
27	C	-0.1427161510	0.7554504523	3.0675485872
28	C	1.0378582818	1.6598501687	2.8768399046
29	O	1.2752946534	-1.1410911854	3.2848371056
30	O	-1.2752946534	1.1410911854	3.2848371056
31	H	-0.7050840327	-2.7002512387	2.9283060160
32	H	-1.7832643825	-1.4430806457	3.6517974517
33	H	-1.5081966865	-1.4354180189	1.9069650177
34	H	0.7050840327	2.7002512387	2.9283060160
35	H	1.7832643825	1.4430806457	3.6517974517
36	H	1.5081966865	1.4354180189	1.9069650177

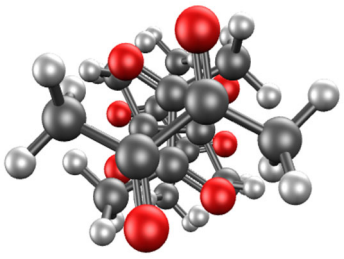
Glyoxal tetramer anion, $(gl)_4^-$ (D_2 symmetry point group)



		Coordinates (Angstroms)		
ATOM		X	Y	Z
1	C	4.2885019711	-0.6752245269	0.3556940144
2	C	4.2885019711	0.6752245269	-0.3556940144
3	O	4.5562265041	-1.6796764506	-0.2554967657
4	H	4.1028068111	-0.6503905203	1.4474579016
5	O	4.5562265041	1.6796764506	0.2554967657
6	H	4.1028068111	0.6503905203	-1.4474579016
7	C	1.2987330496	0.6653675504	-0.3298632480
8	C	1.2987330496	-0.6653675504	0.3298632480
9	O	1.4465423432	0.8073635760	-1.5430298816
10	H	1.2501166566	1.5255709294	0.3696920220
11	O	1.4465423432	-0.8073635760	1.5430298816
12	H	1.2501166566	-1.5255709294	-0.3696920220
13	C	-1.2987330496	-0.6653675504	-0.3298632480
14	C	-1.2987330496	0.6653675504	0.3298632480
15	O	-1.4465423432	-0.8073635760	-1.5430298816
16	H	-1.2501166566	-1.5255709294	0.3696920220
17	O	-1.4465423432	0.8073635760	1.5430298816
18	H	-1.2501166566	1.5255709294	-0.3696920220
19	C	-4.2885019711	0.6752245269	0.3556940144
20	C	-4.2885019711	-0.6752245269	-0.3556940144
21	O	-4.5562265041	1.6796764506	-0.2554967657
22	H	-4.1028068111	0.6503905203	1.4474579016
23	O	-4.5562265041	-1.6796764506	0.2554967657
24	H	-4.1028068111	-0.6503905203	-1.4474579016

Biacetyl tetramer anion, $(ba)_4^-$ (S_4 symmetry point group)





		Coordinates (Angstroms)		
ATOM		X	Y	Z
1	C	0.6146798299	0.4673166116	4.6266392433
2	O	0.4475330712	1.6518952168	4.8247412106
3	C	1.9513536900	-0.1840640331	4.4365188895
4	H	2.7344112593	0.5766870795	4.4817799824
5	H	2.0908984480	-0.9464230947	5.2124285640
6	H	1.9581289684	-0.7093925889	3.4704207716
7	C	-0.6146798299	-0.4673166116	4.6266392433
8	O	-0.4475330712	-1.6518952168	4.8247412106
9	C	-1.9513536900	0.1840640331	4.4365188895
10	H	-2.7344112593	-0.5766870795	4.4817799824
11	H	-2.0908984480	0.9464230947	5.2124285640
12	H	-1.9581289684	0.7093925889	3.4704207716
13	C	0.0189133149	0.7531614990	1.4654441020
14	O	-1.0211748786	1.4119125893	1.5832393580
15	C	-0.0189133149	-0.7531614990	1.4654441020
16	O	1.0211748786	-1.4119125893	1.5832393580
17	C	1.3648939235	1.4304079600	1.4210018306
18	H	2.1793640550	0.7042934134	1.3668255074
19	H	1.3995992892	2.0688407064	0.5299050447
20	H	1.4652439613	2.0627503201	2.3123176634
21	C	-1.3648939235	-1.4304079600	1.4210018306
22	H	-2.1793640550	-0.7042934134	1.3668255074
23	H	-1.3995992892	-2.0688407064	0.5299050447
24	H	-1.4652439613	-2.0627503201	2.3123176634
25	C	0.7531614990	-0.0189133149	-1.4654441020
26	O	1.4119125893	1.0211748786	-1.5832393580
27	C	-0.7531614990	0.0189133149	-1.4654441020

28	O	-1.4119125893	-1.0211748786	-1.5832393580
29	C	1.4304079600	-1.3648939235	-1.4210018306
30	H	0.7042934134	-2.1793640550	-1.3668255074
31	H	2.0627503201	-1.4652439613	-2.3123176634
32	H	2.0688407064	-1.3995992892	-0.5299050447
33	C	-1.4304079600	1.3648939235	-1.4210018306
34	H	-0.7042934134	2.1793640550	-1.3668255074
35	H	-2.0627503201	1.4652439613	-2.3123176634
36	H	-2.0688407064	1.3995992892	-0.5299050447
37	C	0.4673166116	-0.6146798299	-4.6266392433
38	O	1.6518952168	-0.4475330712	-4.8247412106
39	C	-0.1840640331	-1.9513536900	-4.4365188895
40	H	0.5766870795	-2.7344112593	-4.4817799824
41	H	-0.7093925889	-1.9581289684	-3.4704207716
42	H	-0.9464230947	-2.0908984480	-5.2124285640
43	C	-0.4673166116	0.6146798299	-4.6266392433
44	O	-1.6518952168	0.4475330712	-4.8247412106
45	C	0.1840640331	1.9513536900	-4.4365188895
46	H	-0.5766870795	2.7344112593	-4.4817799824
47	H	0.7093925889	1.9581289684	-3.4704207716
48	H	0.9464230947	2.0908984480	-5.2124285640