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Supporting Information

Relative Orientation of the Carbonyl Groups Determines the Nature of Orbital Interactions in Carbonyl-Carbonyl Short Contacts

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Computational Methods

To investigate the nature of carbonyl-carbonyl interactions in the different structural motifs we carried out theoretical calculations using Gaussian 09 suite of quantum chemical program.[1] We used Minnesota functional (M05-2X)[2] and Møller-Plesset second-order perturbation theory (MP2) exchange correlational functional in conjunction with 6-311+G(2d,p) basis set for the calculations. We carried out NBO second-order perturbation analysis to evaluate the contribution of electron delocalization to the stabilization of carbonyl-carbonyl interactions. AIM analyses were done with Multiwfn[3] software. To visualize structure and determine the crystallographic parameters, we used Mercury 3.6[4] and Chemcraft[5] graphical visualization software.

CSD analysis

The CSD searches were carried out using CCDC ConQuest[4] software. Molecules for motif I-V were extracted from the CSD version 5.37 updates (Nov 2015). For motif VI a separate search was done using ConQuest CSD version 5.39 updates (Feb 2018). Only single crystals of organic molecules with R-factor $\leq$ 0.05 that are error free and without any disorder and polymeric structures were considered in the search. In addition, "only one matching fragment" option was chosen in the CSD to avoid repetition of the same structure. For motif VI, the terminal H positions were normalised from the advanced options.

Criteria for different structural motifs:

The motifs I-VI were categorized based on the C=O···C=O dihedral angle T, the two C=O···C angles θ_3 and θ_4 and the two molecular planes having the X, C and O atoms. The different parameters for an ideal geometry of a particular motif listed in Table S2. The various structural parameters are shown in Figure S1.

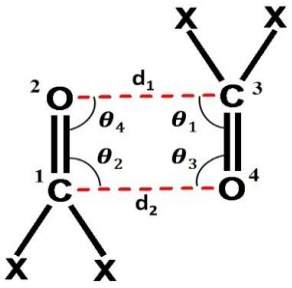


Figure S1: Fragment having C=O···C=O short contact used for the CSD search. Torsion Angle (T) is defined as $C^1=O^2\cdots C^3=O^4$.

Table S1: Statistical data for inter- and intramolecular CO···CO interaction. Molecules were divided based on C=O···C=O torsion angle.

	Total	One-sided	Torsion Angle, T(º)			Reciprocal	Torsion Angle, T(º)		
			|0°±45°|	|90°±45°|	|180°±45°|		|0°±45°|	|90°±45°|	|180°±45°|
Inter-molecular	4237	2897 (68.4%)	1458 (50.3%)	1105 (38.2%)	334 (11.5%)	1340 (31.6%)	1311 (97.8%)	29 (2.2%)	0.0 (0.0%)
Intra-molecular	6221	4749 (76.3%)	112 (2.3%)	2674 (56.3%)	1963 (31.6%)	1472 (23.7%)	110 (7.5%)	1352 (91.8%)	10 (0.7%)

Table S2: Structural parameters for an ideal geometry of each motif type.

Motif	**d_1** Å	**d_2** Å	**T** (º)	**θ_1** (º)	**θ_2** (º)	**θ_3** (º)	**θ_4** (º)
Motif I	≤3.20	>3.20	ND	90	15	75	180
Motif II	≤3.20	≤3.20	0	90	90	90	90
Motif III	≤3.20	>3.20	180	90	50	50	90
Motif IV	≤3.20	>3.20	90	90	70	70	90
Motif V	≤3.20	≤3.20	70	90	90	75	75

A deviation of ±30º of T from the ideal value was considered to club molecules into various structural motif types. ND- not defined as one of the angle is linear.

Table S3. Number of Molecules of each motifs that strictly satisfy the criteria mentioned in Table S2 in intramolecular and intermolecular cases.

	Intramolecular		**Intermolecular**	
	Overall	**≤ 3.0 Å**[a]	**Overall**	**≤ 3.0 Å**[a]
Motif I	15	5	621	220
Motif II	27	4	1243	133
Motif III	1060	656	200	10
Motif IV	1762	1221	400	14
Motif V	1300	194	21	6
Motif VI	-	-	48	15

[a]O···C distances, ($d_{O\cdots C}$).

Motif I (*T-Shaped*)

For the motif I structures, we considered the molecules with one nonbonded O···C short contacts ≤3.20 Å and one of the C=O···C angles (θ_3 or θ_4) between 150°-180°. For motif I, the C=O···C=O dihedral angle is not meaningful as one of the C=O···C angle is linear. For an ideal motif I, the structure will have (θ_3, θ_4) or (θ_4, θ_3) = 180°,75° or 75°, 180°, which is reflected in the θ_3 versus θ_4 shown in Figure S2.

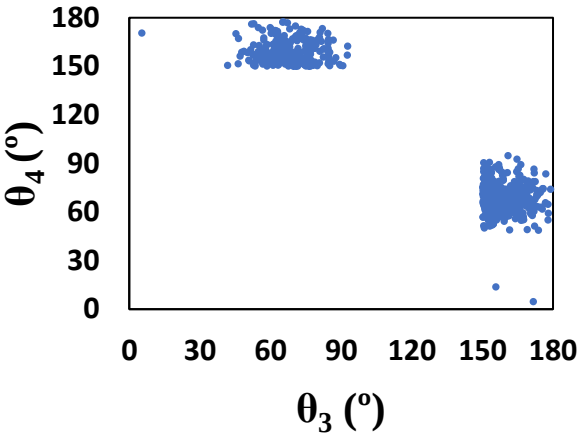


Figure S2: Plot of θ_3 versus θ_4 for molecules that fall under structural motif I.

Motif II (*Antiparallel*)

For the antiparallel motif II, we considered T = 0°±20°, θ_3 and θ_4 ~ 90° and both O···C contacts ≤3.20 Å. For molecules with T = 0°±20°, the plot of θ_3 versus θ_4 is shown in Figure 3. The deviation of the θ_3, θ_4 from the ideal 90º, 90º values indicate sheared antiparallel structures.

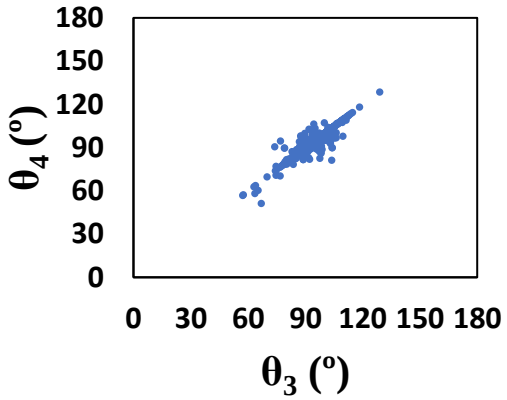


Figure S3: Plot of θ_3 versus θ_4 for molecules with T = 0°±20°.

Motif III (*Parallel*)

For the parallel structure (motif III), one nonbonded O···C ≤ 3.20 Å and |T| lie within the range of 180º±20º. The molecules that contain C=O···C angle within 150º-180º were excluded (motif I). For |T| = 180º±20º, (θ_3, θ_4) ~ (50°, 90°) or (θ_3, θ_4) ~ (90°, 50°) [Figure S4, points within the circles]. A few of the slipped parallel structures were also observed wherein θ_3 and θ_4 deviated slightly from the perfect geometry may be due steric hindrance or packing forces.

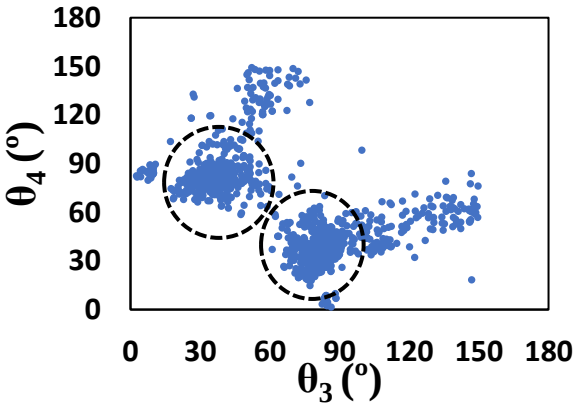


Figure S4: Plot of θ_3 versus θ_4 for molecules with T = 180°±20°.

Motif IV (*L-Shaped*)

For '*L-shaped*' motif IV, one of the nonbonded O···C is ≤ 3.20 Å and |T| lies within the range of 90º±20º. The molecules with C=O···C angle 150º-180º were excluded from this motif as they fall in the motif I category. The θ_3 and θ_4 values of molecules that fall in the structural motif IV category are shown in Figure S5.

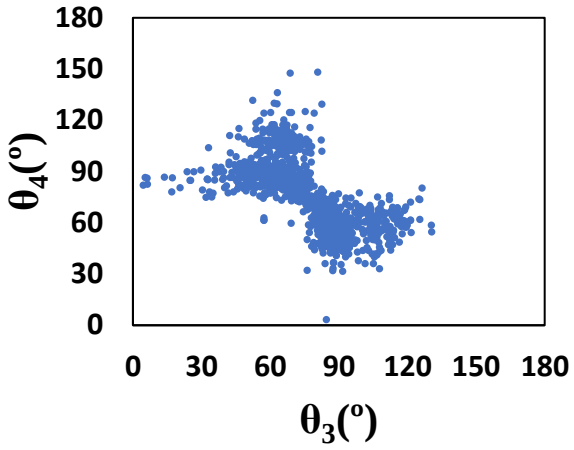


Figure S5: Plot of θ_3 versus θ_4 for molecules with T = 90°±20°.

Motif V (*Reciprocal*)

For motif V, both the non-bonded O···C distances are ≤ 3.20 Å and |T| that lies within the range of 50°-100°. For |T| = 50°-100°, the θ_3 and θ_4 values will both be 75° in an ideal motif V geometry. The plot of θ_3 and θ_4 values for the molecules having motif V geometry is shown in Figure S6.

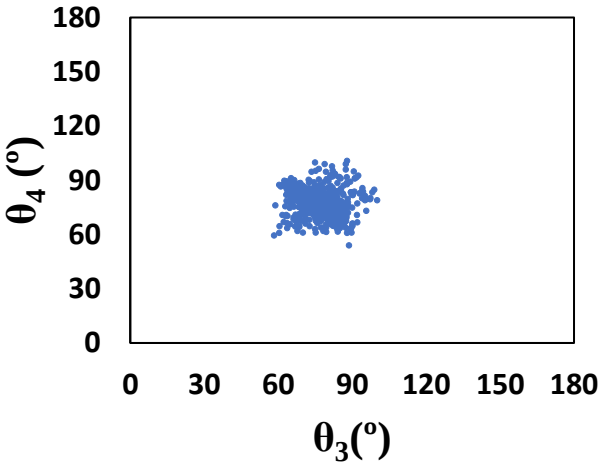


Figure S6: Plot of θ_3 versus θ_4 for molecules with T = 50°-100°

Motif VI: An Unprecedented structural motif

To find unique geometries that resemble the formaldehyde dimer, we carried out three independent CSD search using motifs shown in Figure S7. For the aldehydic, carboxylic and amidic motifs, two planes were considered. Planes having atoms H-C^1=O^2 [motif VI(a)], O-C^1=O^2 [motif VI(b)], N-C^1=O^2 [motif VI(c)] were taken as plane 1 in each case and the plane having atoms X-C^3=O^4 is taken as plane 2. The angle between plane 1 and plane 2 is restricted to 75°-90° during the CSD search (for ideal motif VI angle between plane 1 and 2 should be 90°). We also restricted the distances d_1 and d_3 to $d_1 \leq 3.2$ Å and $d_3 \leq 3.0$ Å during the search (Figure S7).

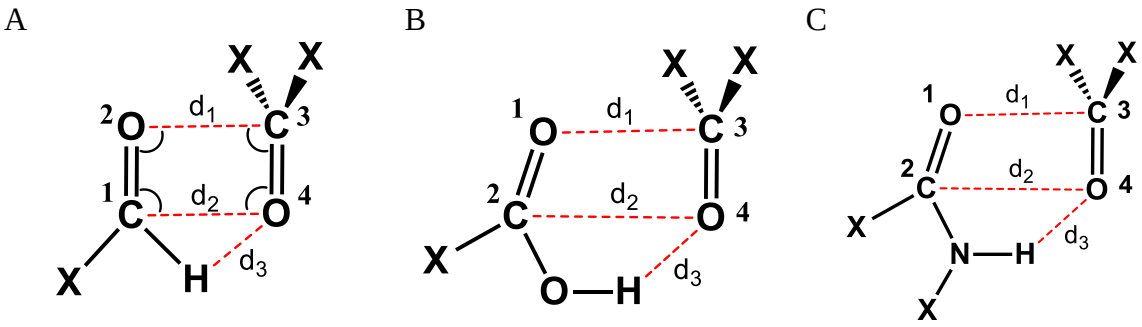


Figure S7: Fragment used search for motif VI in the CSD. Torsion Angle, T is defined as $C^1=O^2\cdots C^3=O^4$.

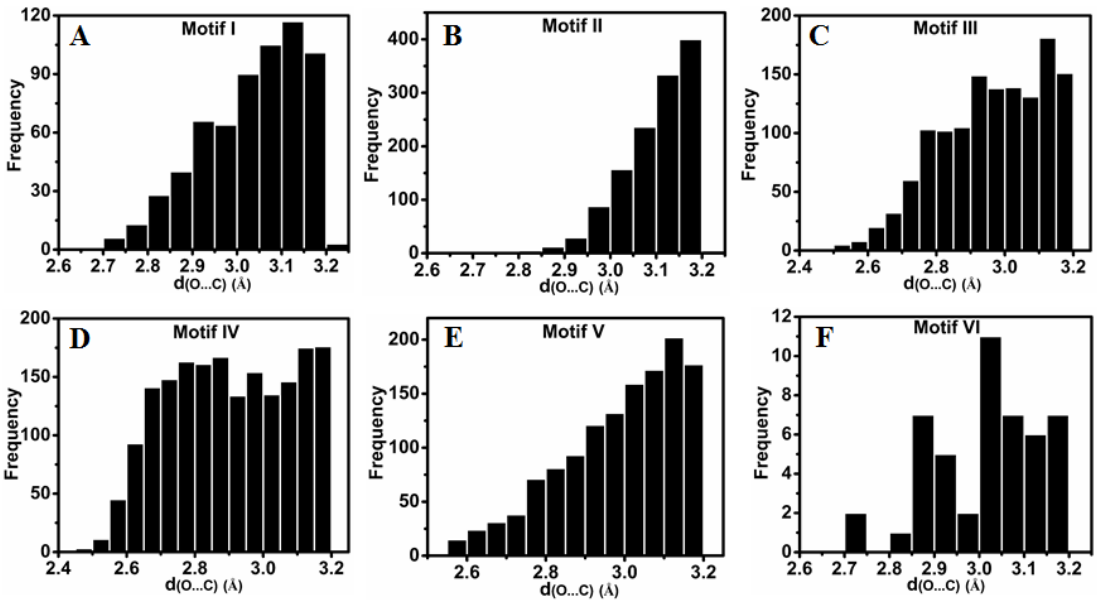


Figure S8: Frequency distribution of O···C distances ($d_{O\cdots C}$) for different structural motifs (I-VI).

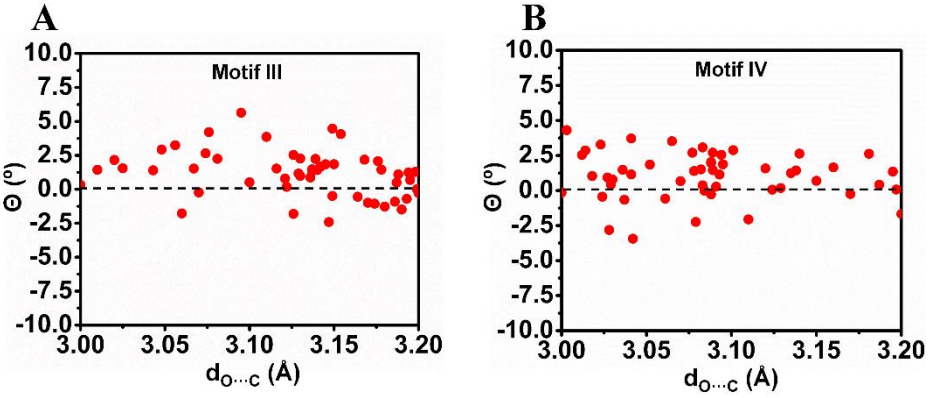


Figure S9: Pyramidality (Θ) of compounds from motif III and motif IV are plotted against the O···C distances [$d_{O\cdots C}$ = 3.0-3.2 Å].

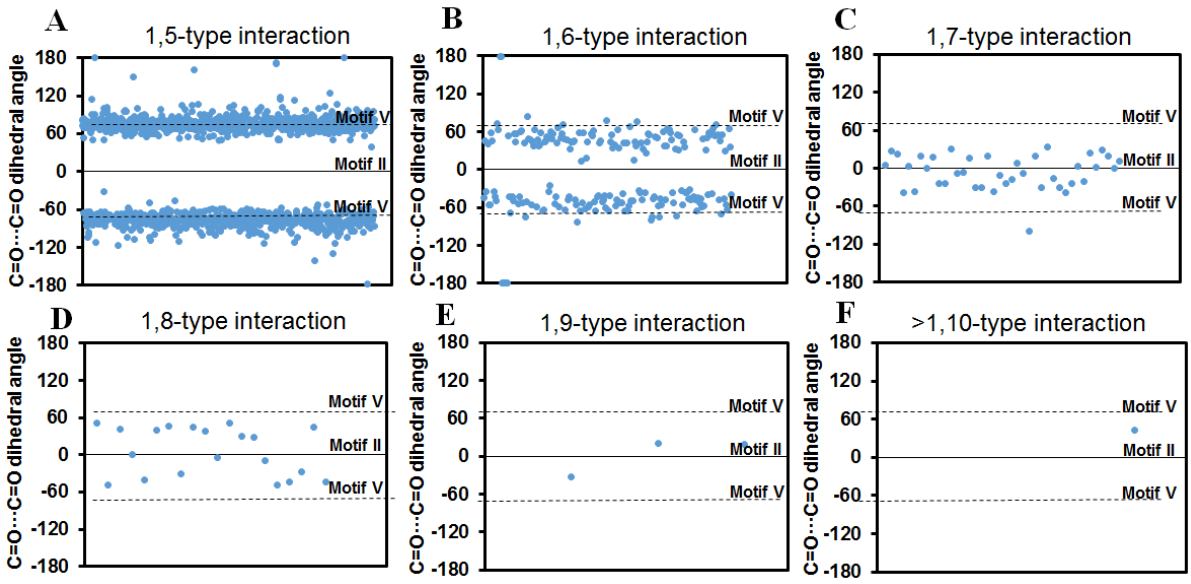


Figure S10. Change in C=O···C=O dihedral angle from intramolecular 1,x-type interactions. Motif V slowly converts to antiparallel motif II with increase in the number of bonds between the two carbonyl groups.

Table S4: Structural parameters and NBO data for different motifs that were retrieved from the CSD. NBO calculations were done in M052X/6-311+G(2d,p) level of theory.

Motifs	Ref. Code	$d_{1(O\cdots C)}$ (Å)	$d_{2(O\cdots C)}$ (Å)	$\theta_{1(O\cdots C=O)}$ (deg)	$\theta_{2(O\cdots C=O)}$ (deg)	$n\rightarrow\pi^*$ (kcal·mol^{-1})		$\pi\rightarrow\pi^*$ (kcal·mol^{-1})	
						$E^1_{(n\rightarrow\pi^*)}$	$E^2_{(n\rightarrow\pi^*)}$	$E^1_{(\pi\rightarrow\pi^*)}$	$E^2_{(\pi\rightarrow\pi^*)}$
Motif I (Intra-molecular)	NALJAL	2.67	3.97	90.9	27.1	2.89	NP	NP	0.11
	DIFSAM	2.73	4.21	93.9	12.8	1.84	NP	0.18	NP
	GIZCOI	2.94	4.22	85.1	18.6	0.83	0.12	0.07	NP
	OBEMUF	3.00	4.27	81.0	8.27	0.45	NP	0.09	NP
	HOFNUM	3.08	4.33	85.3	22.1	0.09	NP	0.09	NP
Motif I (Inter-molecular)	TCBENQ07	2.78	4.43	99.6	2.6	1.62	NP	0.08	NP
	GIHXUS	2.85	4.33	100.6	24.7	1.59	NP	NP	NP
	VAFPID	2.90	4.79	114.5	5.5	0.77	NP	NP	NP
	UKEQEH	2.94	4.34	95.6	25.7	1.00	NP	NP	0.05
	QOPWEY	2.99	4.44	92.8	15.5	1.77	NP	0.13	NP
Motif II (Intra-molecular)	PUXPAB	2.85	2.85	88.0	88.0	0.39	0.50	6.58	2.53
	GOCWIG	2.87	2.87	91.9	91.9	0.33	0.33	0.90	0.90
	NENXOT	2.89	2.93	101.4	98.7	0.15	0.11	1.34	1.3
	ROJTER	3.05	3.05	78.6	78.6	0.29	0.29	0.14	0.14
	ZILQIU	3.10	3.10	117.0	117.0	NP	NP	NP	NP
Motif II (Inter-molecular)	JIFRUL	2.81	2.816	88.5	88.58	0.56	0.97	0.62	0.70
	BADHUL	2.85	2.848	91.8	91.81	NP	NP	NP	2.61
	RIWGAH	2.90	2.90	89.1	89.10	0.31	0.29	0.81	0.66
	ROXRIH	2.95	2.95	84.9	84.91	0.40	0.39	0.58	0.70
	BIVTUV	2.99	2.99	85.9	85.95	0.21	0.21	0.45	0.45
Motif III (Intra-molecular)	IJUTUC	2.56	3.72	103.3	49.1	4.92	NP	0.71	NP
	OSOCOP	2.61	3.78	108.3	52.9	3.77	NP	0.58	NP
	FIKFUA	2.71	3.77	104.9	56.1	2.58	NP	0.61	NP
	LOSNAI	2.80	4.03	101.1	43.2	1.90	NP	0.92	0.06
	VEHYUC	2.89	3.97	109.6	58.3	1.57	NP	0.17	NP
Motif III (Inter-molecular)	NEPTUY	2.82	4.19	94.8	28.82	1.05	NP	0.92	0.11
	NAWLAA	2.95	4.28	95.6	29.56	1.44	NP	0.21	0.02
	OXACDH46	3.03	4.25	101.6	44.21	0.15	NP	0.62	0.05
	REZJAJ	3.09	4.56	111.5	39.13	0.20	NP	0.37	NP
	FOMHAZ13	3.15	4.17	95.0	48.74	0.07	NP	0.28	NP
Motif IV (Intra-molecular)	OROWIC	2.60	3.70	95.0	45.02	4.32	NP	0.16	NP
	YAGXAH	2.82	3.54	106.0	70.89	2.45	NP	0.06	NP
	LIZBIF	2.90	3.55	101.1	70.65	1.74	NP	0.07	NP
	WIMHAC	3.02	3.59	96.2	70.30	0.86	NP	0.07	NP
	WOLGIP	3.10	3.56	94.6	73.65	0.71	NP	NP	NP
Motif V (Intra-molecular)	JIWCUO	2.77	2.75	89.3	89.98	0.86	0.78	1.11	1.45
	XASFUT	2.87	2.86	84.2	84.42	0.73	1.55	0.35	0.12
	KOSZAT	2.90	2.90	92.0	92.06	0.74	0.74	0.40	0.40
	JODGUG	2.92	2.94	82.6	82.16	0.48	0.62	0.10	0.09
	YAHYOX	3.01	3.07	85.0	81.93	0.55	0.20	NP	NP
Motif VI (Inter-molecular)	OJAJEQ	2.87	3.32	101.3	79.3	2.58	NP	NP	NP
	XODSIU	2.88	3.34	102.2	79.7	1.84	NP	NP	NP
	CEGFIF	3.01	3.43	97.4	77.7	1.56	NP	NP	NP
	GESNUP	3.04	3.17	84.7	78.5	1.13	NP	NP	NP
	SAYZIC	3.07	3.31	91.5	79.9	1.16	NP	NP	NP

d_1 = Distance of first donor O to acceptor carbonyl C in Angstrom (Å); d_2 = Distance of second donor O to acceptor carbonyl C in Angstrom (Å); θ_1 = Angle from the first donor O to acceptor C=O in degree (°); θ_2 = Angle from the second donor O to acceptor C=O in degree (°); $E^1_{(n\rightarrow\pi^*)}$ = $n\rightarrow\pi^*$ second order perturbation energy from the first donor carbonyl O lone pair to acceptor carbonyl π^* orbital; $E^2_{(n\rightarrow\pi^*)}$ = $n\rightarrow\pi^*$ second order perturbation energy from the second donor carbonyl O lone pair to acceptor carbonyl π^* orbital; $E^1_{(\pi\rightarrow\pi^*)}$ = $\pi\rightarrow\pi^*$ second order perturbation energy from the first donor carbonyl π orbital to acceptor carbonyl π^* orbital; $E^2_{(\pi\rightarrow\pi^*)}$ = $\pi\rightarrow\pi^*$ second order perturbation energy from the second donor carbonyl π orbital to acceptor carbonyl π^* orbital; NP – not present at 0.05 threshold value.

Table S5. X-ray Structural parameters and NBO analysis for compounds of motif VI retrieved from CSD. NBO calculations were done in M052X/6-311+G(2d,p) level of theories.

Motif	Ref. Code	$d_{1(O\cdots C)}$ (Å)	$d_{3(O\cdots H)}$ (Å)	$\theta_{1(O\cdots C=O)}$ (°)	$\theta_{5(O\cdots H-C)}$ (°)	n→π* (kcal·mol^{-1}) $E^1_{(n\rightarrow\pi^*)}$	n→π* (kcal·mol^{-1}) $E^2_{(n\rightarrow\pi^*)}$	π→π* (kcal·mol^{-1}) $E_{(\pi\rightarrow\pi^*)}$	n→σ* (kcal·mol^{-1}) $E_{(n\rightarrow\sigma^*)}$
Motif VI (Inter-molecular)	OJAJEQ	2.87	2.65	101.3	128.1	2.58	NP	NP	0.23
	XODSIU	2.89	2.68	102.2	128.0	1.84	NP	NP	1.40
	CEGFIF	3.01	2.80	97.4	126.6	1.56	NP	NP	0.04
	GESNUP	3.04	2.53	84.7	126.7	1.13	NP	NP	0.15
	SAYZIC	3.07	2.74	91.5	119.2	1.16	NP	NP	0.05

d_3 = Distance between O and H in Angstrom (Å); θ_5 = Angle formed by O···H-C. $E^1_{(n\rightarrow\pi^*)}$ = n→π* second order perturbation energy from the first donor carbonyl O lone pair to acceptor carbonyl π* orbital; $E^2_{(n\rightarrow\pi^*)}$ = n→π* second order perturbation energy from the second donor carbonyl O lone pair to acceptor carbonyl π* orbital; ; $E_{(\pi\rightarrow\pi^*)}$ = π→π* second order perturbation energy from the donor carbonyl π orbital to acceptor carbonyl π* orbital; $E_{(n\rightarrow\sigma^*)}$ = n→σ* second order perturbation energy from the O lone pair to CH σ* orbital. NP – not present at 0.05 threshold value.

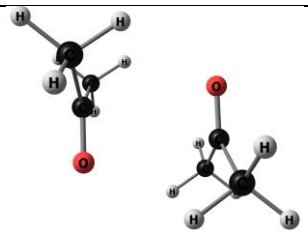
Table S6: Structural data and NBO analysis of molecules from the CSD. Participation of sp-character and p-character oxygen lone pairs in $n\rightarrow\pi^*$ interaction is shown.

Motifs	Ref. Code	$d_{1(O\cdots C)}$ (Å)	$\theta_{1(O\cdots C=O)}$ (deg)	$\theta_{4(C=O\cdots C)}$ (deg)	n→π* (kcal·mol^{-1}) n(sp)→π*	n→π* (kcal·mol^{-1}) n(p)→π*	Θ (deg)	Δ (Å)
Motif I (Intra-molecular)	NALJAL	2.67	90.9	153.7	2.27	0.62	0.31	0.003
	DIFSAM	2.73	93.9	154.6	1.70	0.14	2.3	0.019
	GIZCOI	2.94	85.1	166.1	0.78	0.05	-0.93	-0.008
	OBEMUF	3.00	81.0	167.4	0.42	0.03	-0.98	-0.008
	HOFNUM	3.08	85.3	163.3	0.02	0.07	0.45	0.003
Motif I (Inter-molecular)	TCBENQ07	2.78	99.6	160.8	1.62	0.01	0.64	0.012
	GIHXUS	2.85	100.6	166.9	1.51	0.08	0.34	0.003
	VAFPID	2.90	114.5	169.0	0.77	0.01	1.18	0.01
	UKEQEH	2.94	95.6	163.6	0.93	0.07	0.43	0.004
	QOPWEY	2.99	92.8	163.2	1.77	NP	0.68	0.006
Motif II (Intra-molecular)	PUXPAB	2.85	88.0	91.8	0.80	0.09	0.6(2)	0.005
	GOCWIG	2.87	91.9	88.0	0.66	NP	2.8(2)	0.023
	NENXOT	2.89	101.4	80.2	0.26	NP	1.81(18)	0.015
	ROJTER	3.05	78.6	101.0	0.46	0.12	0.7(3)	0.006
	ZILQIU	3.10	117.0	62.9	0.03	0.04	0.66(15)	0.005
Motif II (Inter-molecular)	JIFRUL	2.81	88.5	91.4	1.12	NP	2.48	0.02
	BADHUL	2.85	91.8	88.1	NP	NP	0.65	0.006
	RIWGAH	2.90	89.1	90.9	0.51	0.09	1.47	0.12
	ROXRIH	2.95	84.9	95.0	0.70	0.09	0.88	0.007
	BIVTUV	2.99	85.9	94.0	0.38	0.04	1.43	0.011
Motif III (Intra-molecular)	IJUTUC	2.56	103.3	92.1	1.01	3.91	4.6(6)	0.038
	OSOCOP	2.61	108.3	89.1	0.24	3.53	3.22(15)	0.027
	FIKFUA	2.71	104.9	85.0	0.40	2.18	4.5(4)	0.037
	LOSNAI	2.80	101.1	100.8	0.79	1.11	3.7(4)	0.033
	VEHYUC	2.89	109.6	86.2	0.25	1.32	4.1(8)	0.032
Motif III (Inter-molecular)	NEPTUY	2.82	94.8	118.1	0.96	0.09	2.83	0.023
	NAWLAA	2.95	95.6	118.7	0.59	0.85	2.92	0.024
	OXACDH46	3.03	101.6	101.5	0.15	NP	0.27	0.002
	REZJAJ	3.09	111.5	111.9	0.17	0.03	-0.06	0
	FOMHAZ13	3.15	95.0	95.0	0.04	0.03	-1.27	-0.009

Motif IV (Intra-molecular)	OROWIC	2.60	95.0	124.6	1.85	2.47	2.0(2)	0.017
	YAGXAH	2.82	106.0	90.4	0.44	2.01	5.28(18)	0.044
	LIZBIF	2.90	101.1	95.5	0.40	1.34	-1.2(2)	-0.001
	WIMHAC	3.02	96.2	94.1	0.18	0.68	0.41(16)	0.004
	WOLGIP	3.10	94.6	92.1	0.12	0.59	0.3(2)	0.002
Motif V (Intra-molecular)	JIWCUO	2.77	89.3	77.7	0.79	0.85	0.7(3)	0.006
	XASFUT	2.87	84.2	83.6	1.11	1.17	1.18(18)	0.01
	KOSZAT	2.90	92.0	77.1	0.32	1.16	1.9(3)	0.015
	JODGUG	2.92	82.6	87.1	0.29	0.81	0.78(16)	0.007
	YAHYOX	3.01	85.0	79.4	0.11	0.64	2.08(19)	0.017
Motif VI (Inter-molecular)	OJAJEQ	2.87	101.3	99.1	0.30	2.28	0.02	0
	XODSIU	2.88	102.2	98.7	0.16	1.68	0.01	0
	CEGFIF	3.01	97.4	101.0	0.26	1.30	-0.04	0
	GESNUP	3.04	84.7	101.6	0.20	0.93	0.08	0
	SAYZIC	3.07	91.5	99.9	0.17	0.99	-0.04	-0.032

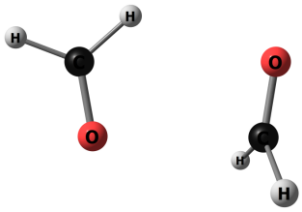
$\theta_{4(C=O\cdots C)}$ = Angle between the C=O···C**;** Θ = pyramidalization of the carbonyl group in degree (º); Δ = pyramidalization of the carbonyl group in angstrom (Å); NP – not present at 0.01 threshold value.

Cartesian Coordinates



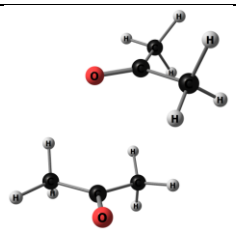
Acetone Dimer
Point Group: C2h
MP2/6-311+G(2d,p)

6	-0.212415	-1.571977	0.000000
8	1.001755	-1.420746	0.000000
6	-1.001755	-1.655039	1.282608
6	-1.001755	-1.655039	-1.282608
1	-0.330931	-1.621281	2.139701
1	-0.330931	-1.621281	-2.139701
1	-1.589032	-2.576652	1.305721
1	-1.699449	-0.814247	1.322959
1	-1.699449	-0.814247	-1.322959
1	-1.589032	-2.576652	-1.305721
6	0.212415	1.571977	0.000000
8	-1.001755	1.420746	0.000000
6	1.001755	1.655039	-1.282608
6	1.001755	1.655039	1.282608
1	0.330931	1.621281	-2.139701
1	0.330931	1.621281	2.139701
1	1.699449	0.814247	-1.322959
1	1.589032	2.576652	-1.305721
1	1.589032	2.576652	1.305721
1	1.699449	0.814247	1.322959



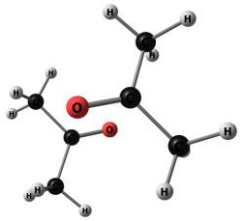
Formaldehyde Dimer
Point Group: Cs
MP2/6-311+G(2d,p)

6	-1.181638	1.184331	0.000000
8	0.000000	1.470196	0.000000
1	-1.956514	1.967845	0.000000
1	-1.517021	0.134721	0.000000
6	1.108516	-1.017994	0.000000
8	0.089337	-1.680452	0.000000
1	1.598785	-0.709271	0.936595
1	1.598785	-0.709271	-0.936595



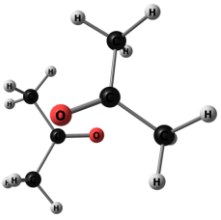
Acetone Dimer optimized at T=90º
MP2/6-311+G(2d,p)

6	-1.800342	0.161547	0.104494
8	-1.955954	1.154531	-0.587195
6	-2.218826	-1.210775	-0.361517
6	-1.191308	0.241089	1.487919
1	-2.812677	-1.130883	-1.270311
1	-2.784257	-1.728263	0.417706
1	-1.317622	-1.794019	-0.568693
1	-0.735459	1.217338	1.646327
1	-0.460295	-0.557462	1.635238
1	-1.983210	0.093743	2.228757
8	0.936946	-0.722233	-1.075445
6	1.670279	-0.107220	-0.316129
6	2.626352	-0.813926	0.615764
6	1.675242	1.402802	-0.281860
1	2.622905	-1.885062	0.420953
1	2.330492	-0.625171	1.651937
1	3.636056	-0.412838	0.494196
1	0.763570	1.790075	-0.735145
1	2.540194	1.758110	-0.850983
1	1.783974	1.774938	0.739115



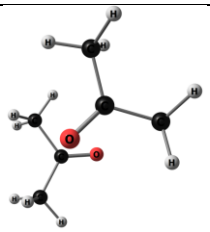
Acetone Dimer
O···C = 3.09 Å
C=O···C=O = 0º
MP2/6-311+G(2d,p)

6	0.632267	-1.454810	0.000000
8	1.592674	-0.696722	0.000000
6	0.000000	-1.934598	1.282608
6	0.000000	-1.934598	-1.282608
1	0.556407	-1.558358	2.139701
1	-0.025191	-3.027131	1.305721
1	-1.032245	-1.576577	1.322958
1	0.556407	-1.558358	-2.139701
1	-1.032245	-1.576577	-1.322958
1	-0.025191	-3.027131	-1.305721
8	-1.592674	0.696722	0.000000
6	-0.632267	1.454810	0.000000
6	0.000000	1.934598	-1.282608
6	0.000000	1.934598	1.282608
1	-0.556407	1.558358	-2.139701
1	1.032245	1.576577	-1.322958
1	0.025191	3.027131	-1.305721
1	-0.556407	1.558358	2.139701
1	0.025191	3.027131	1.305721
1	1.032245	1.576577	1.322958



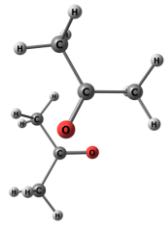
Acetone Dimer
O···C = 3.09 Å
C=O···C=O = 20º
MP2/6-311+G(2d,p)

6	1.559064	-0.030840	0.352998
8	0.979915	-0.239156	1.410169
6	2.058681	-1.159384	-0.513120
6	1.788705	1.366555	-0.168627
1	1.873369	-2.115393	-0.026407
1	3.127533	-1.039886	-0.708643
1	1.535884	-1.126735	-1.472593
1	1.425221	2.102982	0.546269
1	1.264317	1.478564	-1.121547
1	2.852997	1.528001	-0.358367
8	-0.977679	-0.244627	-1.407310
6	-1.560238	-0.029632	-0.353355
6	-1.782843	1.370409	0.164198
6	-2.066634	-1.153311	0.515111
1	-1.385162	2.102348	-0.536887
1	-1.290685	1.473861	1.135032
1	-2.851055	1.546551	0.315657
1	-1.945479	-2.106350	0.002895
1	-3.116308	-0.995763	0.774841
1	-1.488937	-1.160690	1.443644



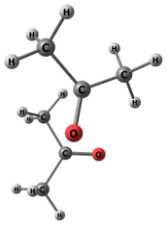
Acetone Dimer
O···C = 3.09 Å
C=O···C=O = 40º
MP2/6-311+G(2d,p)

6	-1.639428	-0.025446	-0.342186
8	-1.194907	-0.712122	-1.250657
6	-2.364255	-0.636122	0.830587
6	-1.463135	1.473989	-0.311600
1	-2.596743	-1.679701	0.625615
1	-3.276585	-0.080667	1.059875
1	-1.706066	-0.575299	1.702275
1	-0.849409	1.801629	-1.149248
1	-1.004112	1.768895	0.634998
1	-2.442558	1.957676	-0.367484
8	0.931831	-0.205615	1.370169
6	1.601613	-0.091428	0.353903
6	2.111215	1.249690	-0.118870
6	1.948232	-1.281684	-0.503651
1	1.700288	2.051676	0.491849
1	1.852599	1.400679	-1.170010
1	3.202833	1.262368	-0.049834
1	1.739160	-2.204643	0.034399
1	2.994649	-1.248282	-0.815388
1	1.325103	-1.246430	-1.402238



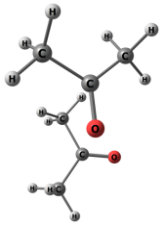
Acetone Dimer
O···C = 3.09 Å
C=O···C=O = 60º
MP2/6-311+G(2d,p)

6	1.695718	0.080433	-0.291622
8	1.509686	1.189754	-0.768542
6	2.418560	-0.113433	1.017347
6	1.197960	-1.174551	-0.972290
1	2.902331	0.813841	1.319212
1	3.152751	-0.919222	0.942208
1	1.680471	-0.400779	1.771649
1	0.537966	-0.920357	-1.800971
1	0.684002	-1.816277	-0.253588
1	2.054816	-1.734621	-1.358949
8	-0.917577	-0.046588	1.360815
6	-1.618301	0.068689	0.366657
6	-2.358789	-1.108732	-0.224189
6	-1.778763	1.391717	-0.338880
1	-2.044810	-2.034779	0.254778
1	-2.193653	-1.162754	-1.303059
1	-3.432530	-0.967481	-0.069320
1	-1.409138	2.198959	0.290662
1	-2.821849	1.562798	-0.614934
1	-1.185551	1.370607	-1.258017



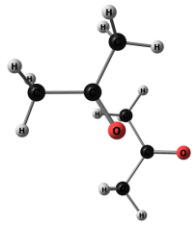
Acetone Dimer
O···C = 3.09 Å
C=O···C=O = 80º
MP2/6-311+G(2d,p)

6	-1.797959	0.167821	0.161985
8	-1.861588	1.307681	-0.271134
6	-2.379130	-1.004756	-0.587164
6	-1.123374	-0.148459	1.479022
1	-3.014490	-0.653593	-1.398327
1	-2.943407	-1.656627	0.084314
1	-1.549587	-1.585227	-1.001047
1	-0.537709	0.704906	1.818705
1	-0.496851	-1.038087	1.386119
1	-1.893499	-0.368620	2.224949
8	0.905728	-0.612962	-1.125044
6	1.670697	-0.078612	-0.337507
6	2.643698	-0.879971	0.494838
6	1.696889	1.421032	-0.161414
1	2.633647	-1.924765	0.188788
1	2.364775	-0.801813	1.549925
1	3.651905	-0.468543	0.399263
1	0.770220	1.857923	-0.531094
1	2.539628	1.820552	-0.734613
1	1.857318	1.693814	0.883881



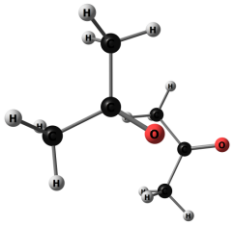
Acetone Dimer
O···C = 3.09 Å
C=O···C=O = 100º
MP2/6-311+G(2d,p)

6	0.000000	0.000000	0.000000
8	0.000000	0.000000	1.220248
6	1.279209	0.000000	-0.799835
6	-1.287085	-0.002989	-0.797032
1	2.125816	0.222082	-0.152532
1	1.227282	0.720445	-1.620025
1	1.406305	-0.995902	-1.233877
1	-2.124909	-0.281252	-0.159459
1	-1.210882	-0.673558	-1.655412
1	-1.459058	1.005343	-1.186935
8	-0.028750	-3.064046	-0.432183
6	-1.184729	-3.364986	-0.681492
6	-1.609983	-3.836255	-2.052561
6	-2.260523	-3.291895	0.376410
1	-0.740654	-3.958789	-2.696425
1	-2.295179	-3.105311	-2.492018
1	-2.156052	-4.780069	-1.975489
1	-1.900810	-2.723876	1.233246
1	-2.510957	-4.308491	0.695030
1	-3.173179	-2.844484	-0.023995



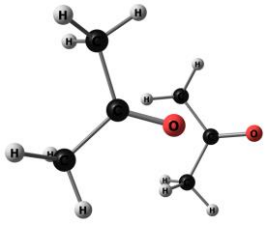
Acetone Dimer
O···C = 3.09 Å
C=O···C=O = 120º
MP2/6-311+G(2d,p)

6	1.972203	-0.148139	0.075704
8	2.427827	-0.964292	-0.708351
6	2.163541	1.336890	-0.111357
6	1.201644	-0.578368	1.306611
1	2.898761	1.524655	-0.891981
1	2.474774	1.807525	0.824990
1	1.203122	1.770053	-0.403626
1	0.805149	-1.583128	1.167105
1	0.400860	0.125928	1.539026
1	1.889315	-0.586546	2.158399
8	-0.859687	0.343007	-1.071102
6	-1.775806	0.072308	-0.312228
6	-2.509046	1.140505	0.466080
6	-2.229793	-1.352253	-0.097789
1	-2.144101	2.127516	0.186905
1	-2.361145	0.980550	1.538094
1	-3.583757	1.073980	0.277935
1	-1.574619	-2.036603	-0.634094
1	-3.256124	-1.467068	-0.457984
1	-2.233812	-1.592237	0.968725



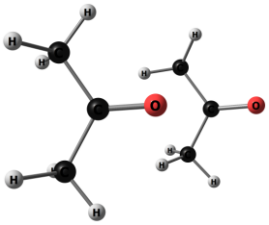
Acetone Dimer
O···C = 3.09 Å
C=O···C=O = 140º
MP2/6-311+G(2d,p)

6	0.000000	0.000000	0.000000
8	0.000000	0.000000	1.219897
8	3.018303	0.000000	-0.682523
6	3.380270	-0.696985	-1.615980
6	-0.043601	1.278892	-0.800851
6	0.006081	-1.292418	-0.789542
1	-0.263492	2.122187	-0.148358
1	-0.789643	1.210017	-1.597064
1	0.934773	1.424990	-1.265864
1	0.433211	-2.094118	-0.188915
1	0.549624	-1.184132	-1.729756
1	-1.029417	-1.549164	-1.035031
6	3.528981	-0.142240	-3.014348
6	3.689954	-2.164520	-1.435348
1	3.370494	0.934890	-3.011310
1	2.800227	-0.620025	-3.676037
1	4.520919	-0.372188	-3.411289
1	3.474424	-2.467972	-0.412391
1	4.744636	-2.347361	-1.659301
1	3.103211	-2.763869	-2.136738



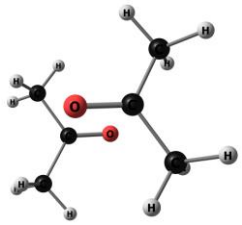
Acetone Dimer
O···C = 3.09 Å
C=O···C=O = 160º
MP2/6-311+G(2d,p)

6	2.006752	-0.072656	0.033507
8	2.651418	-0.415189	-0.943698
8	-0.866601	0.079979	-1.105147
6	-1.787434	0.033495	-0.306551
6	1.830145	1.380360	0.406141
6	1.376185	-1.090511	0.959980
1	2.481020	2.005228	-0.203074
1	2.042866	1.533140	1.467721
1	0.788822	1.659472	0.227750
1	1.209943	-2.025073	0.426652
1	0.441139	-0.721566	1.384734
1	2.066642	-1.273708	1.789563
6	-2.368581	1.284294	0.312905
6	-2.400927	-1.279072	0.122534
1	-1.957438	2.169736	-0.169160
1	-2.129570	1.303816	1.380716
1	-3.458044	1.283359	0.228189
1	-1.824022	-2.110559	-0.278403
1	-3.428589	-1.335692	-0.247885
1	-2.448145	-1.341936	1.212857



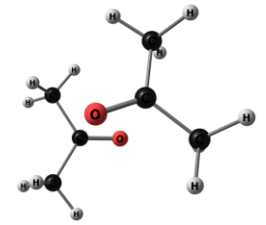
Acetone Dimer
O···C = 3.09 Å
C=O···C=O = 180º
MP2/6-311+G(2d,p)

6	2.008982	-0.020093	0.023915
8	2.673433	-0.077234	-0.997422
8	-0.871541	-0.041879	-1.106616
6	-1.787763	0.007598	-0.302887
6	1.692400	1.295573	0.696880
6	1.498075	-1.270081	0.706487
1	2.257297	2.100837	0.230260
1	1.919807	1.243384	1.765170
1	0.623233	1.494999	0.592890
1	1.423149	-2.081469	-0.015381
1	0.533315	-1.099270	1.186320
1	2.212707	-1.551526	1.486695
6	-2.356724	1.324049	0.176071
6	-2.411347	-1.244375	0.270384
1	-1.895414	2.150576	-0.361898
1	-2.175828	1.434209	1.249476
1	-3.439818	1.343133	0.030387
1	-1.874424	-2.124319	-0.079480
1	-3.458087	-1.306165	-0.040358
1	-2.402818	-1.207511	1.363121



Acetone Dimer
O···C = 3.0 Å
C=O···C=O = 0º
MP2/6-311+G(2d,p)

6	0.553205	-1.462634	0.000000
8	1.519709	-0.712138	0. 000000
6	-0.079259	-1.941325	1.282623
6	-0.079259	-1.941325	-1.282623
1	0.476894	-1.564237	2.139487
1	-0.103715	-3.033927	1.306558
1	-1.110492	-1.583349	1.322313
1	0.476894	-1.564237	-2.139487
1	-1.110492	-1.583349	-1.322313
1	-0.103715	-3.033927	-1.306558
8	-1.519709	0.712138	0.000000
6	-0.553205	1.462634	0.000000
6	0.079259	1.941325	-1.282623
6	0.079259	1.941325	1.282623
1	-0.476894	1.564237	-2.139487
1	1.110492	1.583349	-1.322313
1	0.103715	3.033927	-1.306558
1	-0.476894	1.564237	2.139487
1	0.103715	3.033927	1.306558
1	1.110492	1.583349	1.322313

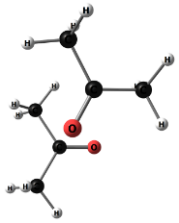


Acetone Dimer
O···C = 3.0 Å
C=O···C=O = 20º
MP2/6-311+G(2d,p)

6	1.560758	-0.035492	0.351779
8	0.978399	-0.246357	1.406662
6	2.061023	-1.162520	-0.515840
6	1.791731	1.362990	-0.166213
1	1.942108	-2.113790	0.000191
1	3.109134	-1.006780	-0.782842
1	1.477240	-1.172352	-1.440531
1	1.382469	2.096713	0.526286
1	1.317850	1.464780	-1.146142
1	2.862859	1.537836	-0.298073
8	-0.978238	-0.237379	-1.406686
6	-1.560824	-0.024650	-0.352277
6	-1.785663	1.374501	0.166630
6	-2.067037	-1.150021	0.514014
1	-1.375503	2.106990	-0.526647
1	-1.308677	1.474121	1.145310
1	-2.855731	1.553244	0.301657
1	-1.949582	-2.101704	-0.001581
1	-3.115487	-0.990980	0.777753
1	-1.486163	-1.161644	1.440509

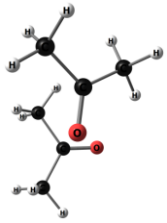
Acetone Dimer
O···C = 3.0 Å
C=O···C=O = 40º
MP2/6-311+G(2d,p)

6	-1.607716	0.012180	-0.313685
8	-1.161604	-0.658921	-1.232767
6	-2.300711	-0.620185	0.866546
6	-1.489544	1.517559	-0.291478
1	-2.474089	-1.677868	0.675991
1	-3.245166	-0.112966	1.078376
1	-1.654956	-0.509555	1.741812
1	-0.889282	1.864594	-1.131067
1	-1.045160	1.839076	0.653362
1	-2.488312	1.959428	-0.352350
8	0.890101	-0.259452	1.325560
6	1.577561	-0.130763	0.322790
6	2.074339	1.219457	-0.136729
6	1.954248	-1.311911	-0.534178
1	1.651766	2.011987	0.478327
1	1.816001	1.374864	-1.187418
1	3.165497	1.244583	-0.064946
1	1.747448	-2.240167	-0.004501
1	3.005022	-1.264282	-0.828880
1	1.344882	-1.278494	-1.442263



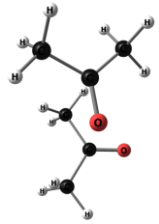
Acetone Dimer
O···C = 3.0 Å
C=O···C=O = 60º
MP2/6-311+G(2d,p)

6	1.663815	0.053291	-0.276474
8	1.478517	1.157397	-0.764220
6	2.356166	-0.127185	1.050805
6	1.220411	-1.211664	-0.976465
1	2.779720	0.818982	1.382948
1	3.137944	-0.887490	0.976896
1	1.618533	-0.472361	1.779865
1	0.578008	-0.971567	-1.823051
1	0.704310	-1.872956	-0.277328
1	2.104279	-1.743947	-1.340870
8	-0.869511	-0.007492	1.329317
6	-1.590267	0.099505	0.347845
6	-2.332353	-1.085186	-0.225914
6	-1.772125	1.418638	-0.359027
1	-2.007657	-2.006682	0.254632
1	-2.180077	-1.145031	-1.306429
1	-3.404824	-0.948329	-0.058903
1	-1.396879	2.230524	0.261080
1	-2.820824	1.581722	-0.618081
1	-1.193887	1.397053	-1.287659



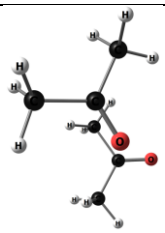
Acetone Dimer
O···C = 3.0 Å
C=O···C=O = 80º
MP2/6-311+G(2d,p)

6	-1.760818	0.149784	0.160226
8	-1.830807	1.291877	-0.263907
6	-2.308351	-1.025024	-0.610559
6	-1.140112	-0.163025	1.504760
1	-2.882938	-0.675078	-1.466325
1	-2.930984	-1.651204	0.033880
1	-1.468004	-1.630907	-0.959045
1	-0.568360	0.691417	1.865325
1	-0.511238	-1.053791	1.444174
1	-1.941825	-0.377389	2.218340
8	0.855003	-0.582990	-1.112771
6	1.637325	-0.056776	-0.335460
6	2.613739	-0.869081	0.481957
6	1.680258	1.441869	-0.157583
1	2.586228	-1.913907	0.177061
1	2.353230	-0.786676	1.541388
1	3.625196	-0.470093	0.369376
1	0.758784	1.889330	-0.527246
1	2.528743	1.833196	-0.727928
1	1.841844	1.710162	0.888782



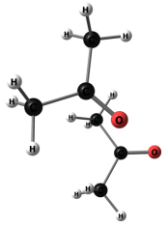
Acetone Dimer
O···C = 3.0 Å
C=O···C=O = 100º
MP2/6-311+G(2d,p)

6	-1.778489	0.183035	0.102201
8	-1.979852	1.157305	-0.603127
6	-2.179324	-1.208467	-0.322194
6	-1.145717	0.307776	1.472197
1	-2.766247	-1.163219	-1.237843
1	-2.750980	-1.700027	0.469674
1	-1.275028	-1.795524	-0.500290
1	-0.693148	1.290851	1.592670
1	-0.408756	-0.481870	1.635929
1	-1.926352	0.181792	2.228935
8	0.851475	-0.563868	-1.132882
6	1.666766	-0.116056	-0.341327
6	2.566678	-1.014857	0.473877
6	1.830618	1.372677	-0.145207
1	2.441213	-2.052535	0.169224
1	2.323297	-0.908731	1.535161
1	3.610259	-0.712107	0.354015
1	0.973637	1.898481	-0.564387
1	2.740108	1.694921	-0.661898
1	1.953753	1.619520	0.911667



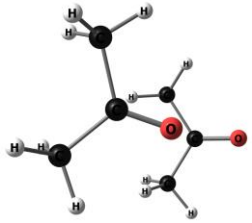
Acetone Dimer
O···C = 3.0 Å
C=O···C=O = 120º
MP2/6-311+G(2d,p)

6	1.916931	-0.142898	0.056435
8	2.335079	-0.953867	-0.751730
6	2.119817	1.342386	-0.119497
6	1.201242	-0.579302	1.318212
1	2.808502	1.530567	-0.941391
1	2.499626	1.789677	0.803084
1	1.152526	1.799000	-0.343391
1	0.799695	-1.583879	1.192338
1	0.410842	0.122966	1.590033
1	1.926101	-0.590408	2.138481
8	-0.825057	0.341968	-1.059992
6	-1.746753	0.069962	-0.306654
6	-2.494005	1.138258	0.457749
6	-2.192664	-1.356294	-0.087887
1	-2.136476	2.126086	0.171915
1	-2.350676	0.989191	1.531977
1	-3.567021	1.060285	0.264360
1	-1.522921	-2.039335	-0.607665
1	-3.211492	-1.481964	-0.465517
1	-2.213992	-1.588114	0.980201



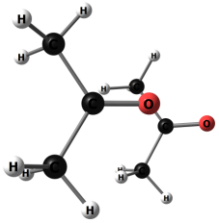
Acetone Dimer
O···C = 3.0 Å
C=O···C=O = 140º
MP2/6-311+G(2d,p)

6	1.922827	-0.101522	0.087492
8	2.421973	-0.793200	-0.782666
6	2.032278	1.404327	0.076331
6	1.197950	-0.717656	1.266580
1	2.729311	1.723016	-0.696840
1	2.356092	1.772276	1.053782
1	1.043981	1.821696	-0.131287
1	0.820360	-1.703107	0.997621
1	0.387749	-0.077055	1.619838
1	1.912622	-0.827263	2.088570
8	-0.824118	0.228308	-1.072468
6	-1.737795	0.172266	-0.264540
6	-2.274133	1.408933	0.420045
6	-2.385178	-1.140314	0.109258
1	-1.785215	2.299367	0.028211
1	-2.102772	1.336712	1.498169
1	-3.354581	1.483622	0.272252
1	-1.874225	-1.962752	-0.388286
1	-3.438038	-1.128098	-0.186348
1	-2.356386	-1.280783	1.193139



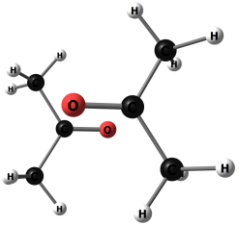
Acetone Dimer
O···C = 3.0 Å
C=O···C=O = 160º
MP2/6-311+G(2d,p)

6	1.923048	-0.085907	0.076941
8	2.467320	-0.608857	-0.879391
6	1.957041	1.407763	0.299701
6	1.220570	-0.912476	1.134003
1	2.625101	1.878531	-0.419499
1	2.279822	1.633359	1.319968
1	0.947424	1.805085	0.172157
1	0.876214	-1.850536	0.701608
1	0.387636	-0.370041	1.584842
1	1.939870	-1.133401	1.929147
8	-0.839680	0.189471	-1.059505
6	-1.727631	0.332117	-0.233827
6	-2.124176	1.696773	0.282647
6	-2.482533	-0.847820	0.332389
1	-1.628517	2.476787	-0.293031
1	-1.840613	1.782062	1.336326
1	-3.208114	1.825509	0.231284
1	-2.035842	-1.778455	-0.012977
1	-3.525689	-0.800319	0.006755
1	-2.484635	-0.812082	1.425015



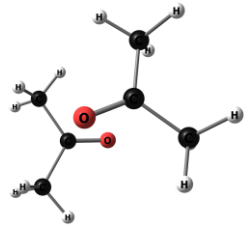
Acetone Dimer
O···C = 3.0 Å
C=O···C=O = 180º
MP2/6-311+G(2d,p)

6	1.936137	-0.015110	0.000062
8	2.552946	-0.074662	-1.048909
8	-0.848124	-0.043653	-1.116663
6	-1.762948	0.006625	-0.309584
6	1.669901	1.299875	0.696361
6	1.446292	-1.263778	0.701423
1	2.190085	2.107295	0.183776
1	1.991189	1.247204	1.740494
1	0.595451	1.496704	0.689866
1	1.307546	-2.063536	-0.023938
1	0.519874	-1.082405	1.248546
1	2.206708	-1.569459	1.427334
6	-2.327336	1.323407	0.173528
6	-2.390772	-1.244990	0.259563
1	-1.848430	2.151027	-0.347107
1	-2.168850	1.421124	1.251587
1	-3.407025	1.353707	0.005188
1	-1.862969	-2.126049	-0.101107
1	-3.440626	-1.297099	-0.042347
1	-2.372400	-1.216463	1.352443



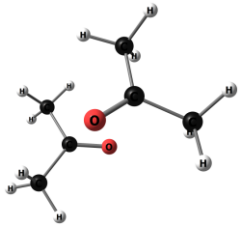
Acetone Dimer
O···C = 2.9 Å
C=O···C=O = 0º
MP2/6-311+G(2d,p)

6	0.464706	-1.467043	0.000000
8	1.442583	-0.731326	0.000000
6	-0.170401	-1.941993	1.282590
6	-0.170401	-1.941993	-1.282590
1	0.386376	-1.565827	2.139472
1	-0.197548	-3.034599	1.307432
1	-1.198984	-1.581214	1.321020
1	0.386376	-1.565827	-2.139472
1	-1.198984	-1.581214	-1.321020
1	-0.197548	-3.034599	-1.307432
8	-1.442583	0.731326	0.000000
6	-0.464706	1.467043	0.000000
6	0.170401	1.941993	-1.282590
6	0.170401	1.941993	1.282590
1	-0.386376	1.565827	-2.139472
1	1.198984	1.581214	-1.321020
1	0.197548	3.034599	-1.307432
1	-0.386376	1.565827	2.139472
1	0.197548	3.034599	1.307432
1	1.198984	1.581214	1.321020



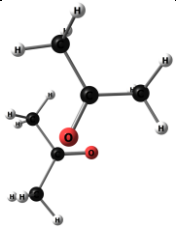
Acetone Dimer
O···C = 2.9 Å
C=O···C=O = 20º
MP2/6-311+G(2d,p)

6	1.548652	-0.050272	0.274452
8	0.996073	-0.260470	1.345274
6	2.047230	-1.175728	-0.595831
6	1.772487	1.348578	-0.245864
1	1.866753	-2.132927	-0.109550
1	3.115591	-1.052875	-0.793178
1	1.522212	-1.143411	-1.553370
1	1.373972	2.081150	0.454276
1	1.285995	1.453401	-1.218502
1	2.842612	1.521953	-0.389089
8	-0.890308	-0.218067	-1.285458
6	-1.528518	-0.009249	-0.263338
6	-1.795044	1.388785	0.237415
6	-2.051773	-1.138125	0.587003
1	-1.383536	2.124023	-0.452100
1	-1.338568	1.504735	1.224320
1	-2.870528	1.548227	0.350516
1	-1.907876	-2.089244	0.077155
1	-3.108766	-0.990096	0.820807
1	-1.495992	-1.142886	1.529021



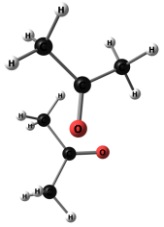
Acetone Dimer
O···C = 2.9 Å
C=O···C=O = 40º
MP2/6-311+G(2d,p)

6	-1.604916	0.002081	-0.275129
8	-1.178011	-0.671136	-1.201634
6	-2.296031	-0.624149	0.909429
6	-1.479005	1.507073	-0.256203
1	-2.444250	-1.688556	0.735980
1	-3.255520	-0.134620	1.095387
1	-1.668192	-0.481576	1.792406
1	-0.876283	1.848189	-1.096589
1	-1.034663	1.830511	0.687566
1	-2.476019	1.952453	-0.322073
8	0.843961	-0.241282	1.259074
6	1.561435	-0.120002	0.276705
6	2.090448	1.224071	-0.163941
6	1.938219	-1.303743	-0.576118
1	1.666889	2.020244	0.445702
1	1.857567	1.388996	-1.219248
1	3.180044	1.231384	-0.068626
1	1.720227	-2.230437	-0.048193
1	2.990906	-1.263850	-0.864639
1	1.333518	-1.266489	-1.487351



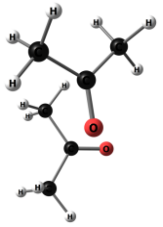
Acetone Dimer
O···C = 2.9 Å
C=O···C=O = 60º
MP2/6-311+G(2d,p)

6	1.652136	0.041621	-0.240284
8	1.471779	1.145970	-0.729068
6	2.341150	-0.141338	1.088364
6	1.219800	-1.222895	-0.948421
1	2.730503	0.812009	1.441125
1	3.150856	-0.870699	1.000411
1	1.615263	-0.528879	1.807127
1	0.576519	-0.982560	-1.794374
1	0.708579	-1.893773	-0.255244
1	2.109044	-1.743789	-1.316374
8	-0.824676	0.005384	1.267726
6	-1.572569	0.112278	0.306835
6	-2.331956	-1.071540	-0.245135
6	-1.767099	1.430389	-0.398271
1	-2.000715	-1.992414	0.232086
1	-2.202470	-1.136462	-1.328428
1	-3.400149	-0.929500	-0.056549
1	-1.384343	2.243302	0.215836
1	-2.818931	1.591974	-0.644918
1	-1.199421	1.408146	-1.333478



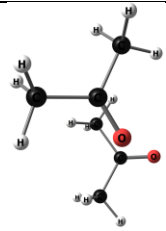
Acetone Dimer
O···C = 2.9 Å
C=O···C=O = 80º
MP2/6-311+G(2d,p)

6	-1.743596	0.122679	0.134990
8	-1.811935	1.263192	-0.293279
6	-2.288873	-1.054954	-0.633110
6	-1.141507	-0.183220	1.489829
1	-2.834819	-0.708553	-1.508835
1	-2.940774	-1.657874	0.004899
1	-1.451876	-1.682402	-0.948664
1	-0.559380	0.666520	1.845124
1	-0.527359	-1.085086	1.449519
1	-1.955054	-0.372040	2.197290
8	0.810825	-0.544390	-1.064988
6	1.617668	-0.027323	-0.306877
6	2.604095	-0.850342	0.487139
6	1.678879	1.470671	-0.129518
1	2.563817	-1.893372	0.177492
1	2.363100	-0.772114	1.551575
1	3.615937	-0.457346	0.358456
1	0.749794	1.925068	-0.470941
1	2.511850	1.855150	-0.726810
1	1.876119	1.737429	0.911153



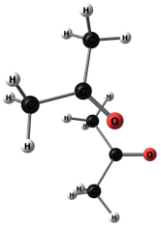
Acetone Dimer
O···C = 2.9 Å
C=O···C=O = 100º
MP2/6-311+G(2d,p)

6	-1.767182	0.153848	0.082786
8	-1.968981	1.127403	-0.623031
6	-2.169962	-1.238140	-0.338549
6	-1.145754	0.281979	1.458015
1	-2.728014	-1.196744	-1.272257
1	-2.774213	-1.710163	0.441221
1	-1.269534	-1.840327	-0.479181
1	-0.679033	1.259200	1.572965
1	-0.423660	-0.517229	1.639121
1	-1.937197	0.178721	2.207010
8	0.802975	-0.516711	-1.081107
6	1.648775	-0.081911	-0.314776
6	2.553243	-0.994678	0.479473
6	1.844091	1.404038	-0.127660
1	2.401844	-2.030626	0.180695
1	2.338204	-0.882205	1.546250
1	3.598709	-0.710892	0.332876
1	0.991899	1.943961	-0.538513
1	2.753400	1.707438	-0.655862
1	1.984301	1.652133	0.926921



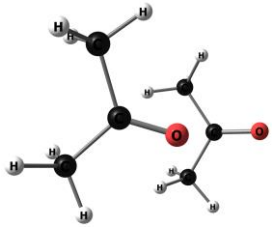
Acetone Dimer
O···C = 2.9 Å
C=O···C=O = 120º
MP2/6-311+G(2d,p)

6	1.891806	-0.116475	0.043350
8	2.281243	-0.932202	-0.774014
6	2.113648	1.366084	-0.134247
6	1.205818	-0.545247	1.324342
1	2.764050	1.546389	-0.988467
1	2.550548	1.797006	0.770907
1	1.146852	1.845542	-0.304139
1	0.782706	-1.541878	1.205802
1	0.436567	0.169363	1.623114
1	1.954926	-0.574329	2.122105
8	-0.779149	0.291928	-1.009838
6	-1.728913	0.034610	-0.286869
6	-2.478067	1.113533	0.460653
6	-2.207566	-1.383881	-0.088100
1	-2.091159	2.095502	0.193379
1	-2.372829	0.954686	1.537876
1	-3.545613	1.059576	0.232013
1	-1.541997	-2.076087	-0.601059
1	-3.222079	-1.487026	-0.483579
1	-2.251485	-1.622813	0.977832



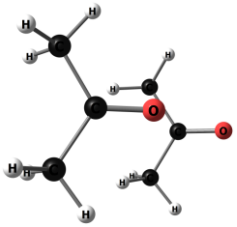
Acetone Dimer
O···C = 2.9 Å
C=O···C=O = 140º
MP2/6-311+G(2d,p)

6	1.885917	-0.078704	0.021014
8	2.381811	-0.695265	-0.905371
8	-0.790581	0.143787	-1.072998
6	-1.724646	0.001102	-0.299745
6	1.950449	1.427400	0.108558
6	1.222898	-0.794812	1.180119
1	2.584631	1.820849	-0.684027
1	2.332803	1.734816	1.086036
1	0.940473	1.829064	0.000234
1	0.870025	-1.773743	0.858905
1	0.404075	-0.208282	1.601114
1	1.969004	-0.931998	1.969402
6	-2.332939	1.170252	0.441124
6	-2.325614	-1.357401	-0.026125
1	-1.867224	2.101906	0.123916
1	-2.196515	1.035794	1.518245
1	-3.409713	1.213499	0.258028
1	-1.773836	-2.124395	-0.566773
1	-3.373451	-1.367077	-0.338969
1	-2.307651	-1.568056	1.046656



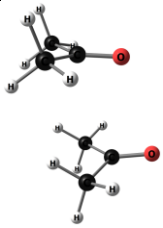
Acetone Dimer
O···C = 2.9 Å
C=O···C=O = 160º
MP2/6-311+G(2d,p)

6	1.883255	-0.121427	0.026481
8	2.454105	-0.484394	-0.986495
8	-0.788479	-0.036446	-1.098070
6	-1.714114	-0.072755	-0.302709
6	1.787726	1.335612	0.414112
6	1.290137	-1.120672	0.998315
1	2.357351	1.946376	-0.284190
1	2.161670	1.479367	1.432024
1	0.739876	1.642712	0.397283
1	1.027142	-2.036479	0.471488
1	0.420568	-0.714526	1.518310
1	2.047491	-1.353493	1.753745
6	-2.271232	1.182378	0.330348
6	-2.357834	-1.376574	0.107578
1	-1.839565	2.065126	-0.138635
1	-2.038792	1.183756	1.399874
1	-3.359980	1.205622	0.239418
1	-1.808289	-2.214956	-0.316685
1	-3.391546	-1.398874	-0.249291
1	-2.391723	-1.459642	1.197149



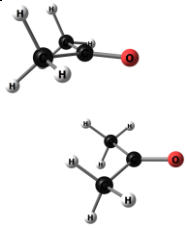
Acetone Dimer
O···C = 2.9 Å
C=O···C=O = 180º
MP2/6-311+G(2d,p)

6	1.863733	-0.028158	-0.042096
8	1.562721	0.027662	1.136865
8	-0.859082	-0.050903	-1.039975
6	-0.967643	-0.104990	-2.255085
6	2.202872	-1.336805	-0.718789
6	1.988934	1.222867	-0.885338
1	2.174683	-2.150140	0.004351
1	3.195574	-1.274710	-1.174476
1	1.485570	-1.532098	-1.518511
1	1.354080	2.006808	-0.476227
1	1.736412	1.035354	-1.930217
1	3.031375	1.555611	-0.850528
6	-1.019741	-1.423913	-2.992812
6	-1.063811	1.143680	-3.101618
1	-0.985927	-2.251378	-2.286027
1	-0.180319	-1.494856	-3.690906
1	-1.935291	-1.482322	-3.587526
1	-0.956360	2.028849	-2.477283
1	-2.032491	1.167574	-3.608753
1	-0.295021	1.136480	-3.879090



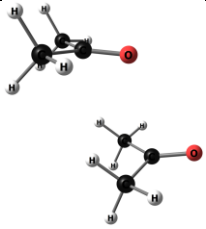
Acetone Dimer
O···C = 3.1 Å
C=O···C = 90º
MP2/6-311+G(2d,p)

6	2.306014	-1.658265	0.000000
8	1.508805	-0.733823	0.000000
6	2.781178	-2.299521	1.286247
6	2.781178	-2.299521	-1.286247
1	2.506413	-1.680278	2.138431
1	2.506413	-1.680278	-2.138431
1	3.858678	-2.476157	1.272793
1	2.297511	-3.276800	1.382731
1	2.297511	-3.276800	-1.382731
1	3.858678	-2.476157	-1.272793
6	3.864561	1.297691	0.000000
8	2.939448	2.090027	0.000000
6	4.499711	0.822500	-1.288526
6	4.499711	0.822500	1.288526
1	3.846488	1.049819	-2.129428
1	3.846488	1.049819	2.129428
1	4.724033	-0.244502	-1.257813
1	5.450515	1.348832	-1.421318
1	5.450515	1.348832	1.421318
1	4.724033	-0.244502	1.257813



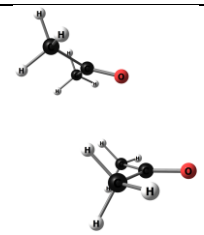
Acetone Dimer
O···C = 3.1 Å
C=O···C = 100º
MP2/6-311+G(2d,p)

6	2.254052	-1.699463	0.000000
8	1.532431	-0.714755	0.000000
6	2.699886	-2.361489	1.285232
6	2.699886	-2.361489	-1.285232
1	2.393866	-1.762796	2.141392
1	2.393866	-1.762796	-2.141392
1	3.782833	-2.508667	1.292876
1	2.242424	-3.353132	1.352469
1	2.242424	-3.353132	-1.352469
1	3.782833	-2.508667	-1.292876
6	3.684149	1.531741	0.000000
8	2.807609	2.377867	0.000000
6	4.282832	1.009501	-1.287277
6	4.282832	1.009501	1.287277
1	3.671050	1.319337	-2.132803
1	3.671050	1.319337	2.132803
1	4.375190	-0.077486	-1.267417
1	5.291572	1.419268	-1.400428
1	5.291572	1.419268	1.400428
1	4.375190	-0.077486	1.267417



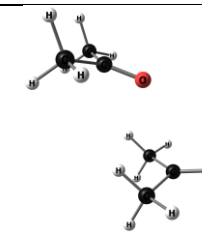
Acetone Dimer
O···C = 3.1 Å
C=O···C = 110º
MP2/6-311+G(2d,p)

6	2.183553	-1.745154	0.000000
8	1.548496	-0.702495	0.000000
6	2.590911	-2.429941	1.285238
6	2.590911	-2.429941	-1.285238
1	2.269320	-1.840602	2.142223
1	2.269320	-1.840602	-2.142223
1	3.674824	-2.572213	1.312621
1	2.136991	-3.423843	1.331044
1	2.136991	-3.423843	-1.331044
1	3.674824	-2.572213	-1.312621
6	3.491564	1.726729	0.000000
8	2.639039	2.597488	0.000000
6	4.070595	1.180734	-1.286244
6	4.070595	1.180734	1.286244
1	3.504219	1.556436	-2.136593
1	3.504219	1.556436	2.136593
1	4.058132	0.089531	-1.282869
1	5.114638	1.497074	-1.373743
1	5.114638	1.497074	1.373743
1	4.058132	0.089531	1.282869



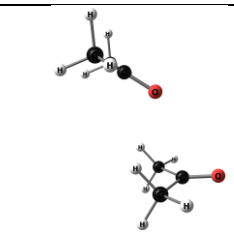
Acetone Dimer
O···C = 3.1 Å
C=O···C = 120º
MP2/6-311+G(2d,p)

6	2.114764	-1.784826	0.000000
8	1.568404	-0.692878	0.000000
6	2.473423	-2.494321	1.285675
6	2.473423	-2.494321	-1.285675
1	2.166604	-1.896040	2.141859
1	2.166604	-1.896040	-2.141859
1	3.551205	-2.676534	1.324285
1	1.982229	-3.470396	1.321704
1	1.982229	-3.470396	-1.321704
1	3.551205	-2.676534	-1.324285
6	3.281630	1.903561	0.000000
8	2.413021	2.758737	0.000000
6	3.867160	1.363243	-1.285534
6	3.867160	1.363243	1.285534
1	3.323782	1.765764	-2.138616
1	3.323782	1.765764	2.138616
1	3.817456	0.273036	-1.295222
1	4.921409	1.648227	-1.353504
1	4.921409	1.648227	1.353504
1	3.817456	0.273036	1.295222



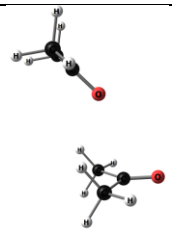
Acetone Dimer
O···C = 3.1 Å
C=O···C = 130º
MP2/6-311+G(2d,p)

6	2.031167	-1.822461	0.000000
8	1.578519	-0.688222	0.000000
6	2.329138	-2.558569	1.285835
6	2.329138	-2.558569	-1.285835
1	2.070299	-1.937438	2.141589
1	2.070299	-1.937438	-2.141589
1	3.388862	-2.825890	1.325642
1	1.761326	-3.492101	1.321310
1	1.761326	-3.492101	-1.321310
1	3.388862	-2.825890	-1.325642
6	3.050609	2.052141	0.000000
8	2.136432	2.858858	0.000000
6	3.662317	1.541052	-1.285028
6	3.662317	1.541052	1.285029
1	3.115962	1.937035	-2.139293
1	3.115962	1.937035	2.139293
1	3.636160	0.450069	-1.302185
1	4.709941	1.851267	-1.341355
1	4.709941	1.851267	1.341355
1	3.636160	0.450069	1.302185



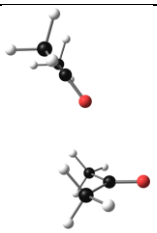
Acetone Dimer
O···C = 3.1 Å
C=O···C = 140º
MP2/6-311+G(2d,p)

6	1.940158	-1.854072	0.000000
8	1.585051	-0.685474	0.000000
6	2.172115	-2.613421	1.285665
6	2.172115	-2.613421	-1.285665
1	1.971749	-1.971129	2.141443
1	1.971749	-1.971129	-2.141443
1	3.203031	-2.975968	1.324243
1	1.521389	-3.491141	1.322028
1	1.521389	-3.491141	-1.322028
1	3.203031	-2.975968	-1.324243
6	2.805371	2.175900	0.000000
8	1.833928	2.913162	0.000000
6	3.451079	1.708534	-1.284658
6	3.451079	1.708534	1.284658
1	2.888741	2.080439	-2.139406
1	2.888741	2.080439	2.139406
1	3.480318	0.617668	-1.306906
1	4.481372	2.072940	-1.333316
1	4.481372	2.072940	1.333316
1	3.480318	0.617668	1.306906



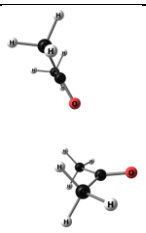
Acetone Dimer
O···C = 3.1 Å
C=O···C = 150º
MP2/6-311+G(2d,p)

6	1.839509	-1.880024	0.000000
8	1.586617	-0.685115	0.000000
6	2.002595	-2.657193	1.285446
6	2.002595	-2.657193	-1.285446
1	1.862180	-1.999381	2.141319
1	1.862180	-1.999381	-2.141319
1	2.996092	-3.112187	1.323292
1	1.274302	-3.471691	1.322017
1	1.274302	-3.471691	-1.322017
1	2.996092	-3.112187	-1.323292
6	2.550476	2.272522	0.000000
8	1.517702	2.921489	0.000000
6	3.234191	1.862346	-1.284204
6	3.234191	1.862346	1.284204
1	2.642278	2.184177	-2.139317
1	2.642278	2.184177	2.139317
1	3.356955	0.777957	-1.304745
1	4.229329	2.314013	-1.332758
1	4.229329	2.314013	1.332758
1	3.356955	0.777957	1.304745



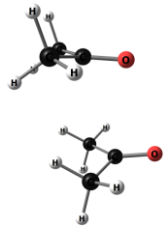
Acetone Dimer
O···C = 3.1 Å
C=O···C = 160º
MP2/6-311+G(2d,p)

6	1.737048	-1.896674	0.000000
8	1.588006	-0.684423	0.000000
6	1.831064	-2.685239	1.285246
6	1.831064	-2.685239	-1.285246
1	1.749046	-2.017820	2.141217
1	1.749046	-2.017820	-2.141217
1	2.780623	-3.225857	1.323055
1	1.033740	-3.432301	1.321386
1	1.033740	-3.432301	-1.321386
1	2.780623	-3.225857	-1.323055
6	2.287289	2.346690	0.000000
8	1.200073	2.900047	0.000000
6	3.004026	1.996868	-1.283805
6	3.004026	1.996868	1.283805
1	2.392066	2.277273	-2.139428
1	2.392066	2.277273	2.139428
1	3.206054	0.924408	-1.307392
1	3.963127	2.520943	-1.327124
1	3.963127	2.520943	1.327124
1	3.206054	0.924408	1.307392



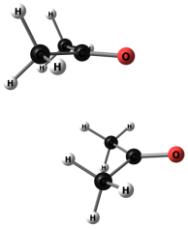
Acetone Dimer
O···C = 3.1 Å
C=O···C = 170º
MP2/6-311+G(2d,p)

6	1.631175	-1.905581	0.000000
8	1.587957	-0.685011	0.000000
6	1.655429	-2.699351	1.285096
6	1.655429	-2.699351	-1.285096
1	1.632234	-2.027413	2.141098
1	1.632234	-2.027413	-2.141098
1	2.553878	-3.321151	1.322945
1	0.795500	-3.373403	1.320857
1	0.795500	-3.373403	-1.320857
1	2.553878	-3.321151	-1.322945
6	2.019383	2.395657	0.000000
8	0.884739	2.844359	0.000000
6	2.765087	2.112579	-1.283504
6	2.765087	2.112579	1.283504
1	2.132603	2.342013	-2.139419
1	2.132603	2.342013	2.139419
1	3.056950	1.060971	-1.308544
1	3.676447	2.715937	-1.324111
1	3.676447	2.715937	1.324111
1	3.056950	1.060971	1.308544



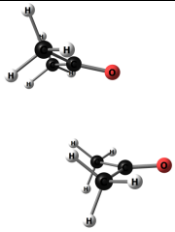
Acetone Dimer
O···C = 3.0 Å
C=O···C = 90º
MP2/6-311+G(2d,p)

6	2.335277	-1.628421	0.000000
8	1.541268	-0.700771	0.000000
6	2.801626	-2.277009	1.285919
6	2.801626	-2.277009	-1.285919
1	2.536774	-1.654730	2.138938
1	2.536774	-1.654730	-2.138938
1	3.875664	-2.472909	1.272976
1	2.300252	-3.245593	1.380795
1	2.300252	-3.245593	-1.380795
1	3.875664	-2.472909	-1.272976
6	3.820402	1.250011	0.000000
8	2.890837	2.036715	0.000000
6	4.464593	0.789029	-1.289461
6	4.464593	0.789029	1.289461
1	3.792548	0.974367	-2.125904
1	3.792548	0.974367	2.125904
1	4.747151	-0.263458	-1.251373
1	5.383563	1.365625	-1.437819
1	5.383563	1.365625	1.437819
1	4.747151	-0.263458	1.251373



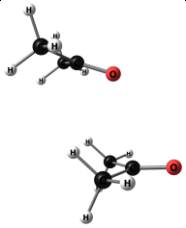
Acetone Dimer
O···C = 3.0 Å
C=O···C = 100º
MP2/6-311+G(2d,p)

6	2.275138	-1.669613	0.000000
8	1.559044	-0.680696	0.000000
6	2.713360	-2.337223	1.285094
6	2.713360	-2.337223	-1.285094
1	2.419518	-1.732657	2.141392
1	2.419518	-1.732657	-2.141392
1	3.793216	-2.504683	1.291024
1	2.237195	-3.320017	1.353798
1	2.237195	-3.320017	-1.353798
1	3.793216	-2.504683	-1.291024
6	3.646428	1.474027	0.000000
8	2.752515	2.301408	0.000000
6	4.260821	0.972207	-1.288262
6	4.260821	0.972207	1.288262
1	3.618363	1.228989	-2.128874
1	3.618363	1.228989	2.128874
1	4.431939	-0.104710	-1.257439
1	5.235822	1.452251	-1.420882
1	5.235822	1.452251	1.420882
1	4.431939	-0.104710	1.257439



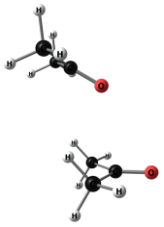
Acetone Dimer
O···C = 3.0 Å
C=O···C = 110º
MP2/6-311+G(2d,p)

6	2.202258	-1.710331	0.000000
8	1.572153	-0.664536	0.000000
6	2.603948	-2.398435	1.285270
6	2.603948	-2.398435	-1.285270
1	2.293823	-1.802608	2.141970
1	2.293823	-1.802608	-2.141970
1	3.685431	-2.558130	1.310057
1	2.134135	-3.384866	1.334030
1	2.134135	-3.384866	-1.334030
1	3.685431	-2.558130	-1.310057
6	3.457259	1.669212	0.000000
8	2.573895	2.508192	0.000000
6	4.060589	1.151200	-1.286951
6	4.060589	1.151200	1.286951
1	3.452292	1.465023	-2.133468
1	3.452292	1.465023	2.133468
1	4.147016	0.063624	-1.269940
1	5.070939	1.558383	-1.395024
1	5.070939	1.558383	1.395024
1	4.147016	0.063624	1.269940



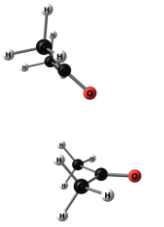
Acetone Dimer
O···C = 3.0 Å
C=O···C = 120º
MP2/6-311+G(2d,p)

6	2.126467	-1.749510	0.000000
8	1.585407	-0.654953	0.000000
6	2.480387	-2.461385	1.285745
6	2.480387	-2.461385	-1.285745
1	2.183129	-1.857984	2.141709
1	2.183129	-1.857984	-2.141709
1	3.555746	-2.657693	1.322077
1	1.976611	-3.431003	1.324309
1	1.976611	-3.431003	-1.324309
1	3.555746	-2.657693	-1.322077
6	3.249769	1.841025	0.000000
8	2.344479	2.656758	0.000000
6	3.863592	1.333499	-1.286001
6	3.863592	1.333499	1.286001
1	3.272987	1.669814	-2.136365
1	3.272987	1.669814	2.136365
1	3.922747	0.243843	-1.280647
1	4.883917	1.719525	-1.374327
1	4.883917	1.719525	1.374327
1	3.922747	0.243843	1.280647



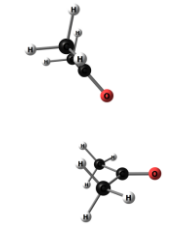
Acetone Dimer
O···C = 3.0 Å
C=O···C = 130º
MP2/6-311+G(2d,p)

6	2.037119	-1.786654	0.000000
8	1.590275	-0.650219	0.000000
6	2.331092	-2.524388	1.285913
6	2.331092	-2.524388	-1.285913
1	2.078041	-1.900607	2.141473
1	2.078040	-1.900606	-2.141473
1	3.388650	-2.800336	1.324808
1	1.755822	-3.453339	1.322555
1	1.755822	-3.453339	-1.322556
1	3.388650	-2.800336	-1.324808
6	3.023367	1.985354	0.000000
8	2.071894	2.747238	0.000000
6	3.663551	1.510796	-1.285419
6	3.663552	1.510796	1.285419
1	3.070685	1.838234	-2.137672
1	3.070685	1.838234	2.137672
1	3.749325	0.422919	-1.287695
1	4.673875	1.924445	-1.361204
1	4.673875	1.924444	1.361204
1	3.749325	0.422919	1.287695



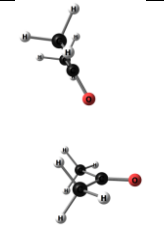
Acetone Dimer
O···C = 3.0 Å
C=O···C = 140º
MP2/6-311+G(2d,p)

6	1.941118	-1.818193	0.000000
8	1.592262	-0.647830	0.000000
6	2.169243	-2.578685	1.285785
6	2.169243	-2.578685	-1.285785
1	1.972521	-1.934936	2.141326
1	1.972521	-1.934936	-2.141326
1	3.198182	-2.946903	1.324318
1	1.513796	-3.452883	1.322554
1	1.513796	-3.452883	-1.322554
1	3.198182	-2.946903	-1.324318
6	2.783792	2.105396	0.000000
8	1.776503	2.792299	0.000000
6	3.456825	1.678428	-1.284958
6	3.456825	1.678428	1.284958
1	2.850667	1.977725	-2.138226
1	2.850667	1.977725	2.138226
1	3.600785	0.596756	-1.292097
1	4.443192	2.147342	-1.352612
1	4.443192	2.147342	1.352612
1	3.600785	0.596756	1.292097



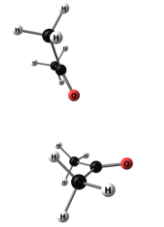
Acetone Dimer
O···C = 3.0 Å
C=O···C = 150º
MP2/6-311+G(2d,p)

6	1.839376	-1.842782	0.000000
8	1.591866	-0.646814	0.000000
6	1.999057	-2.620592	1.285558
6	1.999057	-2.620592	-1.285558
1	1.862101	-1.961744	2.141211
1	1.862101	-1.961744	-2.141211
1	2.990259	-3.080625	1.323288
1	1.266700	-3.431434	1.322620
1	1.266700	-3.431434	-1.322620
1	2.990259	-3.080625	-1.323288
6	2.534214	2.201340	0.000000
8	1.471195	2.798789	0.000000
6	3.240540	1.831153	-1.284378
6	3.240540	1.831153	1.284378
1	2.617856	2.091388	-2.138576
1	2.617856	2.091388	2.138576
1	3.457893	0.761784	-1.294566
1	4.192344	2.367282	-1.345868
1	4.192344	2.367282	1.345868
1	3.457893	0.761784	1.294566



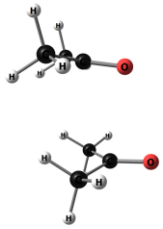
Acetone Dimer
O···C = 3.0 Å
C=O···C = 160º
MP2/6-311+G(2d,p)

6	1.732886	-1.859877	0.000000
8	1.589680	-0.646992	0.000000
6	1.822922	-2.648872	1.285342
6	1.822922	-2.648872	-1.285342
1	1.745356	-1.980639	2.141108
1	1.745356	-1.980639	-2.141108
1	2.769109	-3.195414	1.322842
1	1.020967	-3.390951	1.322127
1	1.020967	-3.390951	-1.322127
1	2.769109	-3.195414	-1.322842
6	2.278119	2.272948	0.000000
8	1.164709	2.770777	0.000000
6	3.014409	1.966326	-1.283982
6	3.014409	1.966326	1.283982
1	2.375241	2.180771	-2.138758
1	2.375241	2.180771	2.138758
1	3.313266	0.916795	-1.296955
1	3.921987	2.574651	-1.340704
1	3.921987	2.574651	1.340704
1	3.313266	0.916795	1.296955



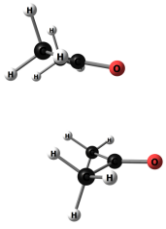
Acetone Dimer
O···C = 3.0 Å
C=O···C = 170º
MP2/6-311+G(2d,p)

6	1.623644	-1.868985	0.000000
8	1.586586	-0.648273	0.000000
6	1.643575	-2.662848	1.285179
6	1.643575	-2.662848	-1.285179
1	1.625169	-1.990504	2.140995
1	1.625169	-1.990504	-2.140995
1	2.537853	-3.290661	1.322709
1	0.779139	-3.331102	1.321570
1	0.779139	-3.331102	-1.321570
1	2.537853	-3.290661	-1.322709
6	2.017653	2.320596	0.000000
8	0.862092	2.711534	0.000000
6	2.778602	2.082256	-1.283808
6	2.778602	2.082256	1.283808
1	2.125077	2.246825	-2.138826
1	2.125077	2.246825	2.138826
1	3.161928	1.060559	-1.299804
1	3.633425	2.762933	-1.336596
1	3.633425	2.762933	1.336596
1	3.161928	1.060559	1.299804



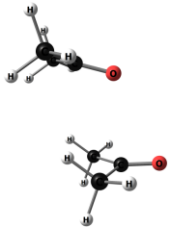
Acetone Dimer
O···C = 2.9 Å
C=O···C = 90º
MP2/6-311+G(2d,p)

6	2.375549	-1.590095	0.000000
8	1.582235	-0.661337	0.000000
6	2.834316	-2.245479	1.285362
6	2.834316	-2.245479	-1.285362
1	2.575457	-1.622874	2.139848
1	2.575457	-1.622874	-2.139848
1	3.905570	-2.455530	1.273946
1	2.319822	-3.207630	1.376414
1	2.319822	-3.207630	-1.376414
1	3.905570	-2.455530	-1.273946
6	3.787330	1.222159	0.000000
8	2.857683	2.008413	0.000000
6	4.438614	0.773245	-1.290426
6	4.438614	0.773245	1.290426
1	3.751914	0.921186	-2.122454
1	3.751914	0.921186	2.122454
1	4.771708	-0.263785	-1.246643
1	5.327059	1.392601	-1.452519
1	5.327059	1.392601	1.452519
1	4.771708	-0.263785	1.246643



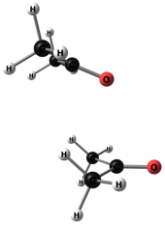
Acetone Dimer
O···C = 2.9 Å
C=O···C = 100º
MP2/6-311+G(2d,p)

6	2.309888	-1.632120	0.000000
8	1.595784	-0.641305	0.000000
6	2.742175	-2.303960	1.284878
6	2.742175	-2.303960	-1.284878
1	2.456947	-1.695821	2.141498
1	2.456947	-1.695821	-2.141498
1	3.819470	-2.486730	1.290114
1	2.252107	-3.279976	1.353850
1	2.252107	-3.279976	-1.353850
1	3.819470	-2.486730	-1.290114
6	3.618248	1.437069	0.000000
8	2.714266	2.253116	0.000000
6	4.243982	0.951671	-1.289291
6	4.243982	0.951671	1.289291
1	3.578444	1.162603	-2.124785
1	3.578444	1.162603	2.124785
1	4.480054	-0.112351	-1.250291
1	5.186502	1.488414	-1.439383
1	5.186502	1.488414	1.439383
1	4.480054	-0.112351	1.250291



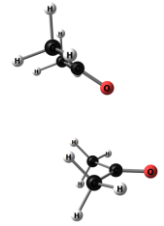
Acetone Dimer
O···C = 2.9 Å
C=O···C = 110º
MP2/6-311+G(2d,p)

6	2.223045	-1.676792	0.000000
8	1.597184	-0.628253	0.000000
6	2.619286	-2.368277	1.285137
6	2.619286	-2.368277	-1.285137
1	2.317902	-1.768304	2.142035
1	2.317902	-1.768304	-2.142035
1	3.698488	-2.542495	1.308568
1	2.136363	-3.348391	1.334980
1	2.136363	-3.348391	-1.334980
1	3.698488	-2.542495	-1.308568
6	3.428802	1.620118	0.000000
8	2.529344	2.441455	0.000000
6	4.046876	1.121430	-1.287849
6	4.046876	1.121430	1.287849
1	3.408432	1.383730	-2.129745
1	3.408432	1.383730	2.129745
1	4.209391	0.043017	-1.259660
1	5.025032	1.596486	-1.415217
1	5.025032	1.596486	1.415217
1	4.209391	0.043017	1.259660



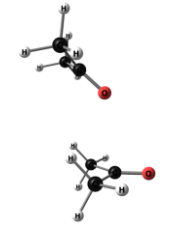
Acetone Dimer
O···C = 2.9 Å
C=O···C = 120º
MP2/6-311+G(2d,p)

6	2.140994	-1.715325	0.000000
8	1.604611	-0.618391	0.000000
6	2.490688	-2.429270	1.285715
6	2.490688	-2.429270	-1.285715
1	2.200296	-1.822489	2.141633
1	2.200296	-1.822489	-2.141633
1	3.564014	-2.636505	1.320835
1	1.977226	-3.393822	1.325583
1	1.977226	-3.393822	-1.325583
1	3.564014	-2.636505	-1.320835
6	3.223819	1.787469	0.000000
8	2.298266	2.579670	0.000000
6	3.855090	1.302623	-1.286615
6	3.855090	1.302623	1.286615
1	3.232375	1.585349	-2.133603
1	3.232375	1.585349	2.133603
1	3.995591	0.220726	-1.269396
1	4.843052	1.761953	-1.393045
1	4.843052	1.761953	1.393045
1	3.995591	0.220726	1.269396



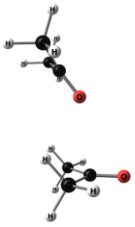
Acetone Dimer
O···C = 2.9 Å
C=O···C = 130º
MP2/6-311+G(2d,p)

6	2.046549	-1.751529	0.000000
8	1.604770	-0.613111	0.000000
6	2.337122	-2.490530	1.285958
6	2.337121	-2.490530	-1.285958
1	2.088164	-1.864914	2.141378
1	2.088163	-1.864913	-2.141378
1	3.393059	-2.772744	1.324429
1	1.756440	-3.416109	1.323218
1	1.756440	-3.416109	-1.323218
1	3.393059	-2.772744	-1.324430
6	3.001429	1.928413	0.000000
8	2.029246	2.663208	0.000000
6	3.659032	1.478703	-1.285854
6	3.659032	1.478702	1.285854
1	3.035736	1.751446	-2.135637
1	3.035736	1.751445	2.135637
1	3.826834	0.400645	-1.276009
1	4.634985	1.965596	-1.378541
1	4.634986	1.965595	1.378541
1	3.826835	0.400645	1.276009



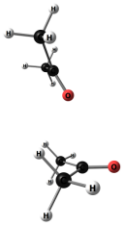
Acetone Dimer
O···C = 2.9 Å
C=O···C = 140º
MP2/6-311+G(2d,p)

6	1.946699	-1.782294	0.000000
8	1.603023	-0.610410	0.000000
6	2.171757	-2.543563	1.285862
6	2.171757	-2.543563	-1.285862
1	1.978112	-1.898615	2.141207
1	1.978112	-1.898615	-2.141207
1	3.199054	-2.916432	1.324308
1	1.512432	-3.414836	1.323030
1	1.512432	-3.414836	-1.323030
1	3.199054	-2.916432	-1.324308
6	2.766592	2.045924	0.000000
8	1.740265	2.703442	0.000000
6	3.455675	1.645458	-1.285260
6	3.455675	1.645458	1.285260
1	2.822623	1.889729	-2.136512
1	2.822623	1.889729	2.136512
1	3.679795	0.577651	-1.280775
1	4.404309	2.184958	-1.368678
1	4.404309	2.184958	1.368678
1	3.679795	0.577651	1.280775



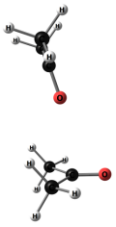
Acetone Dimer
O···C = 2.9 Å
C=O···C = 150º
MP2/6-311+G(2d,p)

6	1.841730	-1.806528	0.000000
8	1.599419	-0.609512	0.000000
6	1.998197	-2.584879	1.285637
6	1.998197	-2.584879	-1.285637
1	1.864513	-1.925120	2.141116
1	1.864513	-1.925120	-2.141116
1	2.987247	-3.049576	1.323233
1	1.262067	-3.392291	1.323116
1	1.262067	-3.392291	-1.323116
1	2.987247	-3.049576	-1.323233
6	2.522295	2.139724	0.000000
8	1.442328	2.705378	0.000000
6	3.242580	1.797990	-1.284745
6	3.242580	1.797990	1.284745
1	2.597442	2.003510	-2.137182
1	2.597442	2.003510	2.137182
1	3.537324	0.747486	-1.284519
1	4.152818	2.400825	-1.360711
1	4.152818	2.400825	1.360711
1	3.537324	0.747486	1.284519



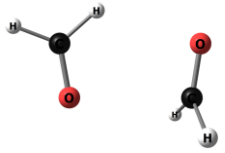
Acetone Dimer
O···C = 2.9 Å
C=O···C = 160º
MP2/6-311+G(2d,p)

6	1.732088	-1.823353	0.000000
8	1.594134	-0.609870	0.000000
6	1.818671	-2.612638	1.285415
6	1.818671	-2.612638	-1.285415
1	1.744922	-1.943753	2.141024
1	1.744922	-1.943753	-2.141024
1	2.761956	-3.164210	1.322646
1	1.012794	-3.350447	1.322733
1	1.012794	-3.350447	-1.322733
1	2.761956	-3.164210	-1.322646
6	2.271823	2.209835	0.000000
8	1.144174	2.673834	0.000000
6	3.019629	1.933038	-1.284316
6	3.019629	1.933038	1.284316
1	2.362949	2.093506	-2.137640
1	2.362949	2.093506	2.137640
1	3.391834	0.907407	-1.287796
1	3.882089	2.602968	-1.354160
1	3.882089	2.602968	1.354160
1	3.391834	0.907407	1.287796



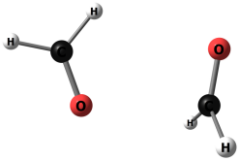
Acetone Dimer
O···C = 2.9 Å
C=O···C = 170º
MP2/6-311+G(2d,p)

6	1.619617	-1.832340	0.000000
8	1.587864	-0.611483	0.000000
6	1.635852	-2.626194	1.285246
6	1.635852	-2.626194	-1.285246
1	1.621538	-1.953531	2.140904
1	1.621538	-1.953531	-2.140904
1	2.526563	-3.259085	1.322497
1	0.767628	-3.289510	1.322184
1	0.767628	-3.289510	-1.322184
1	2.526563	-3.259085	-1.322497
6	2.017022	2.256587	0.000000
8	0.850264	2.611750	0.000000
6	2.787028	2.049012	-1.283950
6	2.787028	2.049012	1.283950
1	2.121208	2.160820	-2.137989
1	2.121208	2.160820	2.137989
1	3.238690	1.055778	-1.290934
1	3.593865	2.785348	-1.348363
1	3.593865	2.785348	1.348363
1	3.238690	1.055778	1.290934



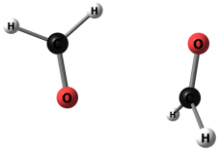
Formaldehyde Dimer
O···C = 2.72 Å
C=O···C = 100º
MP2/6-311+G(2d,p)

6	-1.181638	1.184331	0.000000
8	0.000000	1.470196	0.000000
1	-1.956514	1.967845	0.000000
1	-1.517021	0.134721	0.000000
6	1.108516	-1.017994	0.000000
8	0.089337	-1.680452	0.000000
1	1.598785	-0.709271	0.936595
1	1.598785	-0.709271	-0.936595



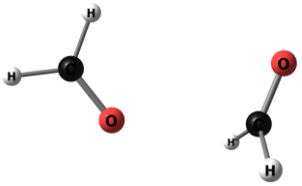
Formaldehyde Dimer
O···C = 2.72 Å
C=O···C = 110º
MP2/6-311+G(2d,p)

6	-1.198149	1.287641	0.000000
8	0.002456	1.470827	0.000000
1	-1.907525	2.131007	0.000000
1	-1.618205	0.267951	0.000000
6	1.309512	-0.919048	0.000000
8	0.363470	-1.681348	0.000000
1	1.765555	-0.560886	0.936641
1	1.765555	-0.560886	-0.936641



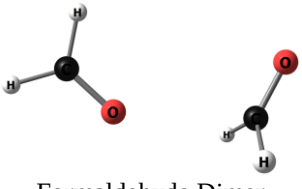
Formaldehyde Dimer
O···C = 2.72 Å
C=O···C = 120º
MP2/6-311+G(2d,p)

6	-1.202532	1.402322	0.000000
8	0.009626	1.472124	0.000000
1	-1.830934	2.307883	0.000000
1	-1.719077	0.428162	0.000000
6	1.504962	-0.804687	0.000000
8	0.705013	-1.718279	0.000000
1	1.893194	-0.372963	0.936346
1	1.893194	-0.372963	-0.936346



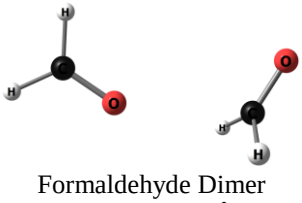
Formaldehyde Dimer
O···C = 2.72 Å
C=O···C = 130º
MP2/6-311+G(2d,p)

6	-1.198808	1.517742	0.000000
8	0.014544	1.474251	0.000000
1	-1.740223	2.477980	0.000000
1	-1.806090	0.597748	0.000000
6	1.689601	-0.673790	0.000000
8	1.064696	-1.714552	0.000000
1	1.995482	-0.179873	0.936133
1	1.995482	-0.179873	-0.936133



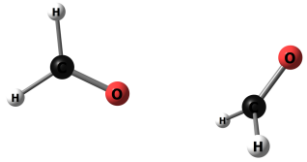
Formaldehyde Dimer
O···C = 2.72 Å
C=O···C = 140º
MP2/6-311+G(2d,p)

6	-1.187993	1.630992	0.000000
8	0.016287	1.476736	0.000000
1	-1.639451	2.636719	0.000000
1	-1.877801	0.771336	0.000000
6	1.863598	-0.525097	0.000000
8	1.412132	-1.651726	0.000000
1	2.086908	0.011477	0.935974
1	2.086908	0.011477	-0.935974



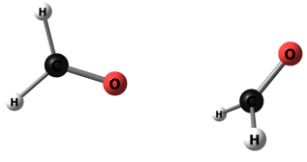
Formaldehyde Dimer
O···C = 2.72 Å
C=O···C = 150º
MP2/6-311+G(2d,p)

6	-1.169634	1.741399	0.000000
8	0.015825	1.479372	0.000000
1	-1.529057	2.783602	0.000000
1	-1.934392	0.947766	0.000000
6	2.025310	-0.359613	0.000000
8	1.736321	-1.538273	0.000000
1	2.170556	0.203129	0.935955
1	2.170556	0.203129	-0.935955



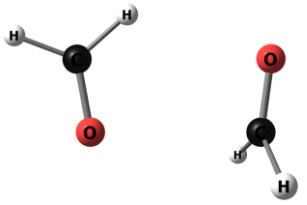
Formaldehyde Dimer
O···C = 2.72 Å
C=O···C = 160º
MP2/6-311+G(2d,p)

6	-1.143452	1.848489	0.000000
8	0.013935	1.481971	0.000000
1	-1.409091	2.918475	0.000000
1	-1.975978	1.126284	0.000000
6	2.172937	-0.178932	0.000000
8	2.032644	-1.384263	0.000000
1	2.246429	0.397519	0.935956
1	2.246429	0.397519	-0.935956



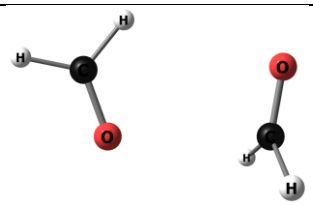
Formaldehyde Dimer
O···C = 2.72 Å
C=O···C = 170º
MP2/6-311+G(2d,p)

6	-1.109784	1.950938	0.000000
8	0.010933	1.484145	0.000000
1	-1.280820	3.040078	0.000000
1	-2.002550	1.304672	0.000000
6	2.305429	0.016091	0.000000
8	2.290559	-1.197211	0.000000
1	2.318306	0.597065	0.935938
1	2.318306	0.597065	-0.935938



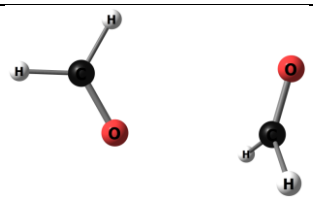
Formaldehyde Dimer
O···C = 2.8 Å
C=O···C = 100º
MP2/6-311+G(2d,p)

6	-1.197822	1.216745	0.000000
8	-0.016929	1.504252	0.000000
1	-1.974878	1.998490	0.000000
1	-1.532088	0.166582	0.000000
6	1.126256	-1.051746	0.000000
8	0.094009	-1.693136	0.000000
1	1.620853	-0.750540	0.936968
1	1.620853	-0.750540	-0.936968



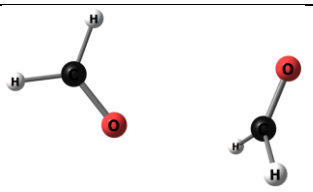
Formaldehyde Dimer
O···C = 2.8 Å
C=O···C = 110º
MP2/6-311+G(2d,p)

6	-1.215430	1.320405	0.000000
8	-0.014819	1.503381	0.000000
1	-1.924998	2.163770	0.000000
1	-1.636214	0.301175	0.000000
6	1.328309	-0.953448	0.000000
8	0.381531	-1.714588	0.000000
1	1.782145	-0.592719	0.936847
1	1.782145	-0.592719	-0.936847



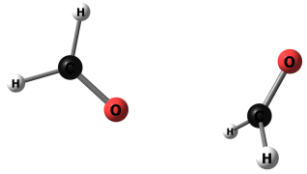
Formaldehyde Dimer
O···C = 2.8 Å
C=O···C = 120º
MP2/6-311+G(2d,p)

6	-1.222699	1.433617	0.000000
8	-0.010552	1.503388	0.000000
1	-1.851011	2.339354	0.000000
1	-1.740287	0.460060	0.000000
6	1.526471	-0.837031	0.000000
8	0.726267	-1.750255	0.000000
1	1.912629	-0.403766	0.936611
1	1.912629	-0.403766	-0.936611



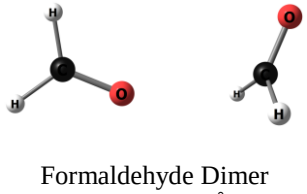
Formaldehyde Dimer
O···C = 2.8 Å
C=O···C = 130º
MP2/6-311+G(2d,p)

6	-1.221384	1.547389	0.000000
8	-0.008090	1.503850	0.000000
1	-1.762770	2.507723	0.000000
1	-1.829316	0.627809	0.000000
6	1.713638	-0.704238	0.000000
8	1.089096	-1.745146	0.000000
1	2.016754	-0.208876	0.936404
1	2.016754	-0.208876	-0.936404



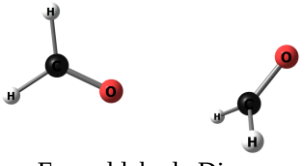
Formaldehyde Dimer
O···C = 2.8 Å
C=O···C = 140º
MP2/6-311+G(2d,p)

6	-1.211474	1.661038	0.000000
8	-0.007531	1.505003	0.000000
1	-1.661646	2.667420	0.000000
1	-1.903086	0.802754	0.000000
6	1.888299	-0.555538	0.000000
8	1.462319	-1.692091	0.000000
1	2.096854	-0.013336	0.936214
1	2.096854	-0.013336	-0.936214



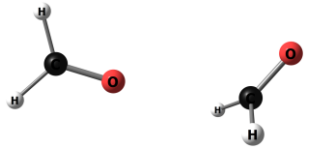
Formaldehyde Dimer
O···C = 2.8 Å
C=O···C = 150º
MP2/6-311+G(2d,p)

6	-1.194894	1.770141	0.000000
8	-0.010152	1.505793	0.000000
1	-1.552545	2.813072	0.000000
1	-1.961865	0.978458	0.000000
6	2.051685	-0.388626	0.000000
8	1.800058	-1.575916	0.000000
1	2.176599	0.178794	0.936154
1	2.176599	0.178794	-0.936154



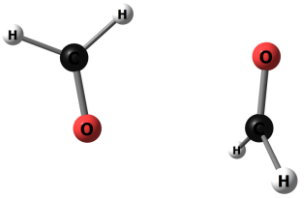
Formaldehyde Dimer
O···C = 2.8 Å
C=O···C = 160º
MP2/6-311+G(2d,p)

6	-1.170380	1.875956	0.000000
8	-0.014114	1.506437	0.000000
1	-1.433383	2.946677	0.000000
1	-2.005270	1.156300	0.000000
6	2.200688	-0.206643	0.000000
8	2.111823	-1.416958	0.000000
1	2.247245	0.372647	0.936039
1	2.247245	0.372647	-0.936039



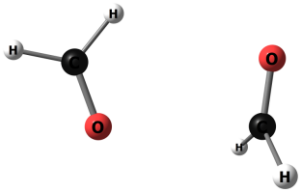
Formaldehyde Dimer
O···C = 2.8 Å
C=O···C = 170º
MP2/6-311+G(2d,p)

6	-1.138163	1.977020	0.000000
8	-0.019154	1.506607	0.000000
1	-1.305868	3.066765	0.000000
1	-2.033448	1.334038	0.000000
6	2.334441	-0.010160	0.000000
8	2.385186	-1.222637	0.000000
1	2.313692	0.570605	0.936012
1	2.313692	0.570605	-0.936012



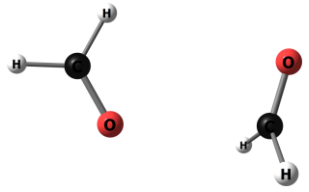
Formaldehyde Dimer
O···C = 2.9 Å
C=O···C = 100º
MP2/6-311+G(2d,p)

6	-1.219712	1.259172	0.000000
8	-0.039933	1.549152	0.000000
1	-1.999825	2.038394	0.000000
1	-1.552818	0.208421	0.000000
6	1.149889	-1.095526	0.000000
8	0.098511	-1.704371	0.000000
1	1.652082	-0.807561	0.937395
1	1.652082	-0.807561	-0.937395



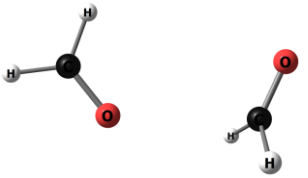
Formaldehyde Dimer
O···C = 2.9 Å
C=O···C = 110º
MP2/6-311+G(2d,p)

6	-1.241252	1.360897	0.000000
8	-0.041223	1.546507	0.000000
1	-1.952980	2.202801	0.000000
1	-1.661888	0.341525	0.000000
6	1.355503	-0.994981	0.000000
8	0.386961	-1.727699	0.000000
1	1.818774	-0.646896	0.937253
1	1.818774	-0.646896	-0.937253



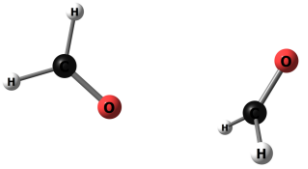
Formaldehyde Dimer
O···C = 2.9 Å
C=O···C = 120º
MP2/6-311+G(2d,p)

6	-1.242943	1.478909	0.000000
8	-0.030884	1.548587	0.000000
1	-1.871333	2.384768	0.000000
1	-1.761944	0.506099	0.000000
6	1.560861	-0.875532	0.000000
8	0.767591	-1.794602	0.000000
1	1.941737	-0.437789	0.936839
1	1.941737	-0.437789	-0.936839



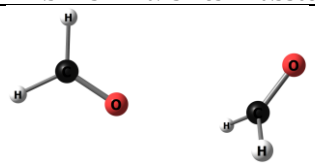
Formaldehyde Dimer
O···C = 2.9 Å
C=O···C = 130º
MP2/6-311+G(2d,p)

6	-1.248866	1.590092	0.000000
8	-0.035746	1.543706	0.000000
1	-1.788149	2.551712	0.000000
1	-1.859885	0.672517	0.000000
6	1.742096	-0.747424	0.000000
8	1.154587	-1.809683	0.000000
1	2.025324	-0.240644	0.936600
1	2.025324	-0.240644	-0.936600



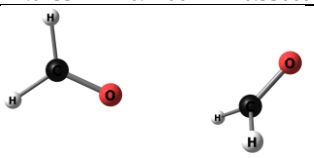
Formaldehyde Dimer
O···C = 2.9 Å
C=O···C = 140º
MP2/6-311+G(2d,p)

6	-1.242168	1.701277	0.000000
8	-0.038670	1.542502	0.000000
1	-1.690217	2.708680	0.000000
1	-1.936295	0.844938	0.000000
6	1.919983	-0.596114	0.000000
8	1.536590	-1.747789	0.000000
1	2.105683	-0.045790	0.936388
1	2.105683	-0.045790	-0.936388



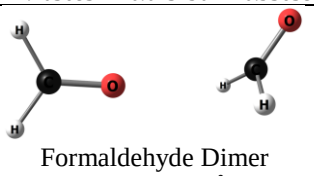
Formaldehyde Dimer
O···C = 2.9 Å
C=O···C = 150º
MP2/6-311+G(2d,p)

6	-1.227854	1.809185	0.000000
8	-0.043939	1.541043	0.000000
1	-1.582088	2.853265	0.000000
1	-1.997558	1.020136	0.000000
6	2.085246	-0.427857	0.000000
8	1.898098	-1.627089	0.000000
1	2.176790	0.145914	0.936234
1	2.176790	0.145914	-0.936234



Formaldehyde Dimer
O···C = 2.9 Å
C=O···C = 160º
MP2/6-311+G(2d,p)

6	-1.205204	1.913885	0.000000
8	-0.050504	1.539447	0.000000
1	-1.463584	2.985710	0.000000
1	-2.043293	1.197920	0.000000
6	2.235784	-0.244619	0.000000
8	2.236656	-1.458351	0.000000
1	2.236999	0.336535	0.936092
1	2.236999	0.336535	-0.936092



Formaldehyde Dimer
O···C = 2.9 Å
C=O···C = 170º
MP2/6-311+G(2d,p)

6	-1.174628	2.013717	0.000000
8	-0.058164	1.537201	0.000000
1	-1.336221	3.104339	0.000000
1	-2.073486	1.375724	0.000000
6	2.370892	-0.046996	0.000000
8	2.536904	-1.249331	0.000000
1	2.292542	0.529095	0.935933
1	2.292542	0.529095	-0.935933

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