Electronic Supporting Information

Unveiling the reactivity of CO_2 with carbanions: a theoretical analysis of the carboxylation step

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A. GENERAL INFORMATION

DFT calculations were performed on 28 small organic molecules, containing C-H moieties (neutral organic molecule is eventually indicated as R_i-H). For every molecule considered, geometry optimization and calculation of Gibbs free energy were performed on carbanion $\mathbf{R_i^-}$ (negative charge, singlet states), carboxylated carbanion $\mathbf{R_i\text{-}COO^-}$ (negative charge, singlet states), transition state of the carboxylation step of the carbanion **R_i-TS** (negative charge, singlet state). When different $\mathbf{R_i^-}$ conformer-geometries can be optimised, the correspondence of $\mathbf{R_i\text{-}COO^-}$ and **R_i-TS** structures was carefully evaluated.
All calculations were performed with Gaussian16 software at the C_3P facility of the University of Padova; Gauss View 6 software was used as a graphical interface to build the input and interpret the output.
For all molecules, geometry optimisations and frequency calculations were done, using the density functional theory (DFT) method:

- b3lyp/6-311g(d,p)//b3lyp/6-311g(d,p): B3LYP functional and Pople 6-311g(d,p) basis set;
- ωb97xd/def2tzvp//ωb97xd/def2tzvp: ωB97XD long-range-corrected functional, which includes empirical dispersion and with def2tzvp Ahlrichs' triple-zeta basis set.

Single point calculations (SPE) were evaluated with:

- ωb97xd/aug-cc-pvtz//ωb97xd/def2tzvp: ωB97XD using aug-cc-pvtz basis set which is including diffuse functions) from optimised geometries at the ωB97XD/def2tzvp level;
- b2plypd/aug-cc-pvtz//ωb97XD/def2tzvp: double hybrid b2plypd functional, with the aug-cc-pvtz basis set from optimised geometries at the ωb97XD/def2tzvp level.

A correction of +1.90 kcalmol^{-1} to the computed free energy and enthalpy values was applied to convert the standard state from 1 atm to a 1 M solution.[1,2]
The self-consistent reaction field (SCRF) was used with DFT energies, optimizations, and frequency calculations to model systems in acetonitrile solution, at. For all calculations a pruned (99,590) integration grid was used (keyword: Integral=UltraFine, the default choice in Gaussian16).
All the structures were optimised including a continuum solvation model for acetonitrile (or dimethylsulfoxide, DMSO) using the integral equation formalism variant (IEFPCM).

Stationary points on the potential energy surface were determined to be minima (no vibrational modes with imaginary frequency) and the actual nature of calculated transition states was confirmed by analysis of frequencies (only one mode with imaginary vibrational

frequency) and the reliability of the transition states was corroborated by intrinsic reaction coordinate (IRC) computation.

Entropy corrections through the Truhlar model were also evaluated,[3] using *GoodVibes* as Python program.[4] Low frequencies vibrations (lower than the selected cut-off value) in the rigid-rotor harmonic oscillator (RRHO) are uniformly shifted up to the cut-off value of 50.0 or 100.0 wavenumber.

The command expressed in all computed jobs in this work was:

- To obtain the optimized molecular structure and local minimum of energy: # opt freq b3lyp/6-311g(d,p) scrf=(solvent=acetonitrile) or # opt freq=noraman wb97xd scrf=(solvent=acetonitrile) def2tzvp
- To obtain the scan of the energy while breaking a C-COO bond: opt=modredundant b3lyp/6-311g(d,p) scrf=(solvent=acetonitrile) or # opt=modredundant wb97xd/def2tzvp scrf=(solvent=acetonitrile). Scans were done with an amplitude of 0.1 and 0.01 Å. # opt=modredundant pm3 scrf=(solvent=acetonitrile)
- To obtain the optimized molecular structure of a transition state and local maximum of energy: # opt=(calcfc,ts,noeigen) freq=noraman b3lyp/6-311g(d,p) scrf=(solvent=acetonitrile) or # opt=(calcfc,ts,noeigen) freq=noraman wb97xd/def2tzvp scrf=(solvent=acetonitrile)
- To obtain intrinsic reaction coordinate (IRC) profile: # irc=(calcfc,recorrect=never,maxpoints=20) wb97xd scrf=(solvent=acetonitrile) def2tzvp

B. CONFORMATIONAL ANALYSIS

For anions R_{23}^- , R_{24}^- and R_{25}^- and for the dianion of chalcone R_{27}^{2-}, an initial conformational analysis was performed at semiempirical pm3 level including a solvation model for acetonitrile. The conformational search considered the full rotation of two dihedral angles involving the groups in proximity of the anion site (16 steps of 24° for each dihedral angle, for a total of 256 points). The conformational analysis on R_{23}^-, R_{24}^- and R_{25}^- provided 4 main conformers for R_{23}^- , three conformers for R_{24}^- and four conformers for R_{25}^-, see the images in Figures S1-S3. In the case of R_{27}^{2-}, the two most stable conformers are represented in Figure S4.

The command expressed to obtain the scan of the energy while rotating the dihedral angles is # opt=modredundant pm3 scrf=(solvent=acetonitrile).

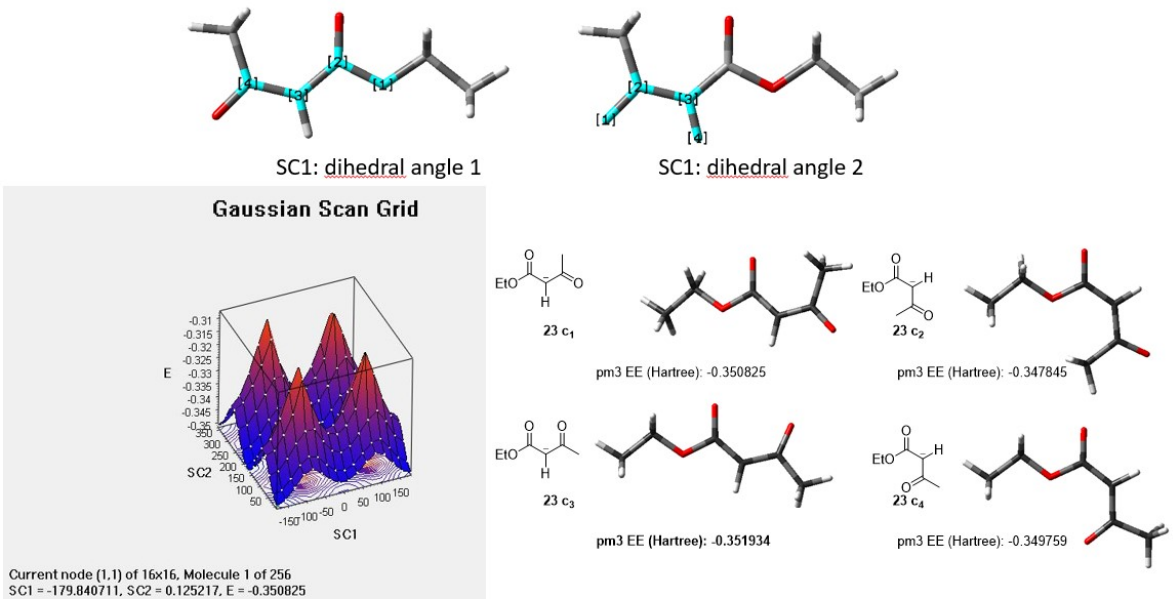


Figure S1. Conformational analysis for anion R_{23}^- with representation of the two dihedral angles scanned (pm3, CH_3CN, 16 steps of 24° for each angle, for a total of 256 conformers), energy map and representation of the most stable four conformers.

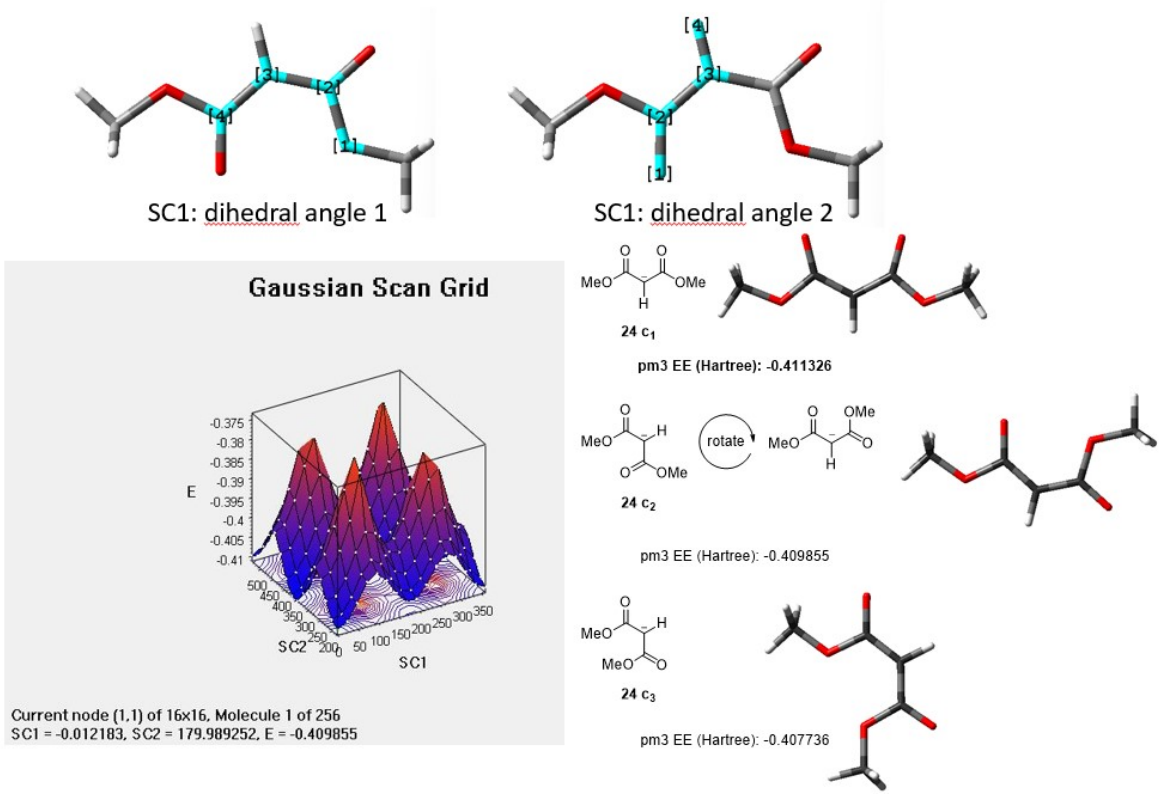


Figure S2. Conformational analysis for anion R_{24}^- with representation of the two dihedral angles scanned (pm3, CH_3CN, 16 steps of 24° for each angle, for a total of 256 conformers), energy map and representation of the most stable three conformers.

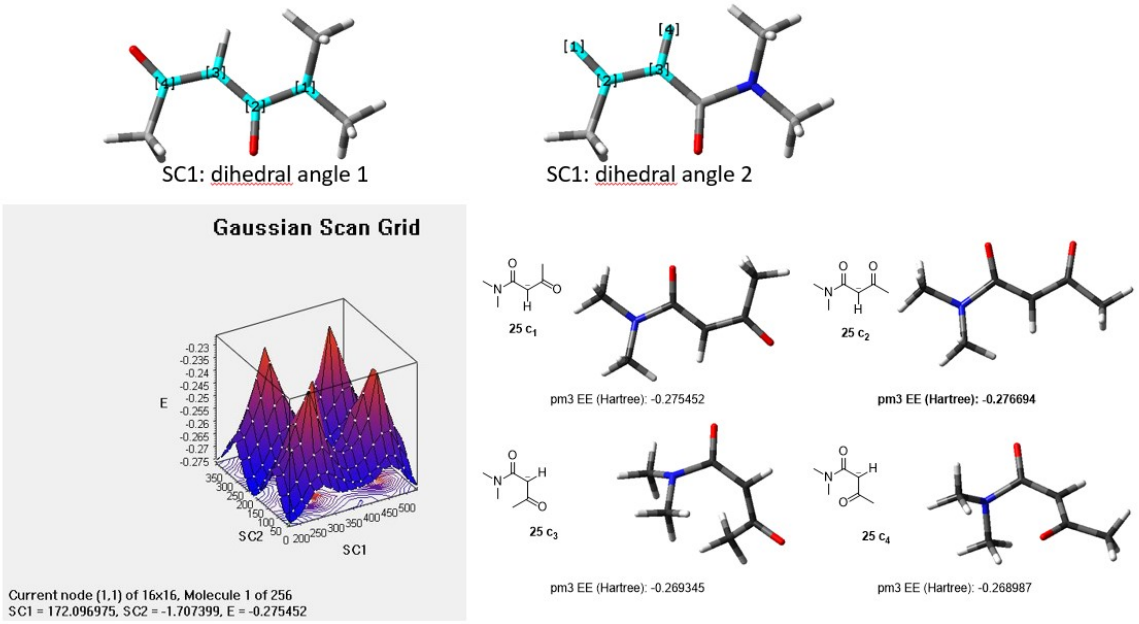


Figure S3. Conformational analysis for anion R_{25}^- with representation of the two dihedral angles scanned (pm3, CH_3CN, 16 steps of 24° for each angle, for a total of 256 conformers), energy map and representation of the most stable four conformers.

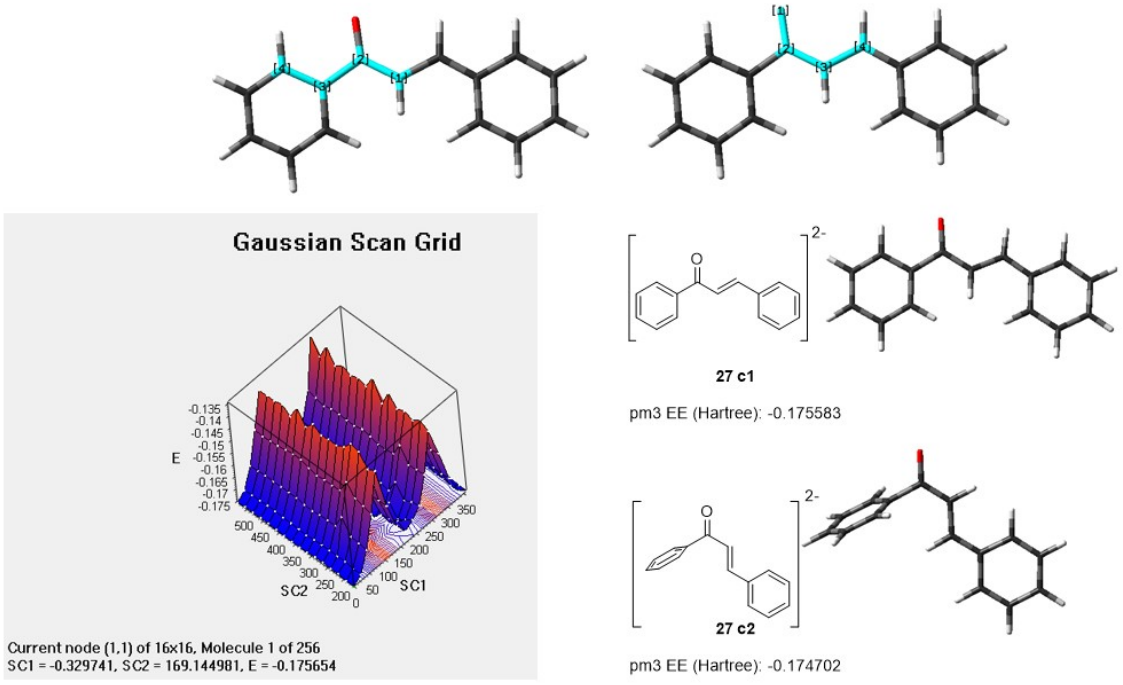


Figure S4. Conformational analysis for anion R_{27}^{2-} with representation of the two dihedral angles scanned (pm3, CH_3CN, 16 steps of 24° for each angle, for a total of 256 conformers), energy map and representation of the most stable two conformers.

For R_{23}^- , R_{24}^- and R_{25}^-, DFT optimisations of the anions at ωb97xd/aug-cc-pvtz//ωb97xd/def2tzvp level were performed on the different conformers to evaluate their relative stability. Then, for the two most stable conformers of each carbanion, calculations were executed also on the corresponding carboxylated species and transition state, to evaluate the impact of the conformational difference on the thermodynamic and activation free energy barrier of the carboxylation step. The results are represented in Table S1, showing that the initial conformation of the carbanions has a minor impact on the calculated ΔG^0 and $\Delta G^{\ddagger}$.

Table S1. Calculated relative free energies between conformers of R_{23}^-, R_{24}^- and R_{25}^- and respective ΔG^0 and $\Delta G^{\ddagger}$ for the carboxylation step for the most stable ones (ωb97XD/aug-cc-pvtz//ωb97XD/def2tzvp). Attention was paid in maintaining the conformational motif when optimising the product and the transition state of the corresponding conformer See the images of the corresponding conformers in Figure S1, S2 and S3. See geometries and x,y,z coordinates in **Section N.2**.

	Relative free energy	**Carboxylation step**	
Carbanion conformers	**(kcalmol^{-1})**	**ΔG^0 (kcalmol^{-1})**	**$\Delta G^{\ddagger}$ (kcalmol^{-1})**
R_{23}^- c_1 (reported in the main text)	**0.00**	4.54	13.87
R_{23}^- c_2	1.41		
R_{23}^- c_3	**0.60**	3.80	14.13
R_{23}^- c_4	1.37		
R_{24}^- c_1 (reported in the main text)	**0.00**	4.25	13.69
R_{24}^- c_2	**1.23**	2.11	13.53
R_{24}^- c_3	2.12		
R_{25}^- c_1 (reported in the main text)	**0.00**	-2.29	12.59
R_{25}^- c_2	**0.17**	-1.55	11.94
R_{25}^- c_3	3.32		
R_{25}^- c_4	1.77		

C. FUNCTIONALS AND BASIS SET COMBINATIONS

To select the best performing level of theory that we employ in the main text analysis, comparation of different functionals and basis set was done taking advantage of the availability of an experimental $\Delta G^{\ddagger}$ value of 10.0 kcal·mol^{-1} for the carboxylation of the indenide anion $\mathbf{R_2}^-$ from a bimolecular rate constant of 2.09±0.07 10^5 $M^{-1}s^{-1}$ (in dimethylsulfoxide at 20°C),[1]. Computed energies for this selected carboxylation reaction are

shown in the Table S2. ωb97XD/aug-cc-pvtz//ωb97XD/def2tzvp level (calculated $\Delta G^{\ddagger}$ = 11.9 kcalmol^{-1} for carboxylation of $\mathbf{R_2^-}$) was chosen as the level of theory among the ones tested.

Table S2. $\Delta G^{\ddagger}$ for indenide anion R_2^- obtained with different levels of theory, solvent IEFPCM (DMSO).

level of theory	$\Delta G^{\ddagger}$ (kcal/mol)
b3lyp/g-311g(d,p)//b3lyp/g-311g(d,p)	12.8
ωb97xd/def2tzvp//ωb97xd/def2tzvp	12.6
ωb97xd/aug-cc-pvtz//ωb97xd/def2tzvp	**11.9**
b2plypd/aug-cc-pvtz//ωb97xd/def2tzvp	15.2
ωb97xd/def2tzvp//ωb97xd/def2tzvp with Truhlar entropy correction (cut-off of 100 cm^{-1})	13.7
ωb97xd/def2tzvp//ωb97xd/def2tzvp with Truhlar entropy correction (cut-off of 50 cm^{-1})	13.1
IEFPCM(DMSO)/B3LYP-D3/6-311+G(d,p)[1]	7.9
Experimental (dmso, 20°C)[1]	10.0

D. $\Delta G^{\ddagger}$ AND EXPERIMENTAL pK_{AH}

Table S3. Computed $\Delta G^{\ddagger}$ (ωb97xd/aug-cc-pvtz//ωb97xd/def2tzvp, IEFPCM(CH_3CN)) and experimental pK_{aH} of carbanions $\mathbf{R_i^-}$.

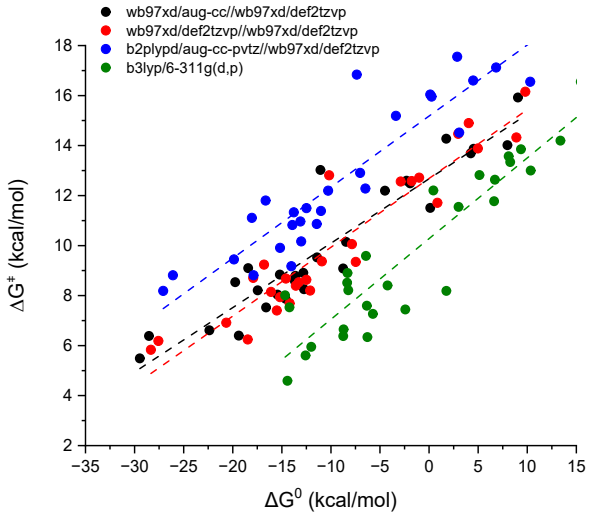
i	species	pK_{aH} (DMSO; H_2O)	ΔG (kcal/mol)
1	cyclopentadiene_anion	18.00	14.27
2	indene_anion	20.10	12.19
3	malonitrile_anion	11.10	14.02
4	acetylene_anion	24.00	7.52
5	phenylacethylene_anion	28.80	8.21
6	diphenylmethane_anion	32.20	6.61
7	pCNtoluene_anion	30.80	8.53
8	pCOPhtoluene_anion	26.90	9.09
9	pNO2toluene_anion	20.40	13.02
10	acetone_anion	26.50	8.90
11	dimethylpentanone_anion	28.30	8.04
12	cyclobutanone_anion	25.10	7.88
13	cyclohexanone_anion	26.40	8.79
14	acetophenone_anion	24.70	8.26
15	pCNacetophenone_anion	22.00	10.15
16	pNMe2acetophenone_anion	27.50	8.84
17	Benzoylacetonitrile_anion	10.20	15.92
18	Phbenzylketone_anion	14.20	12.49
19	2-Facetophenone_anion	21.60	8.59
20	phepropanone_anion	24.40	9.53
21	acetic acid tert-butyl ester_anion	30.30	6.40
22	^{t}BuPhenylacetate_anion	23.60	9.08
23	Etacetoacetate_anion	14.20	13.87
24	diMemalonate_anion	15.70	13.69
25	diMeacetoacetamid_anion	18.20	12.59
26	3-oxo-3-pyrrolidin-1-yl-propionitrile_anion	17.20	11.50

E. Gibbs Energy Tables and correlations with different levels of calculations

The plot of $\Delta G^{\ddagger}$ vs ΔG^{0} values show a fair linear trend according to eq. 2 in the manuscript also with different combinations of functionals and basis sets. The Figure S1 highlight the linear trends of the collected energy data (reported in Table S3-6).

The data plot of $\Delta G^{\ddagger}$ vs ΔG^{0} for ωb97xd/aug-cc-pvtz//ωb97xd/def2tzvp (Figure 1 in the manuscript and Figure S5, black dots) values show a fair linear trend with a slope of α = 0.26±0.02 and an intercept of $\Delta G_0^{\ddagger}$ = 12.7±0.3 kcalmol^{-1}

Similar slopes (α) of 0.28±0.02 are obtained with ωb97xd/def2tzvp//ωb97xd/def2tzvp (red dots) and b2plypd/aug-cc-pvtz//ωb97xd/def2tzvp (blue dots) although there is a major change in the intercept value ($\Delta G_0^{\ddagger}$) of 15.2±0.3 kcalmol^{-1} in the case of the double hybrid functional (/aug-cc-pvtz//ωb97xd/def2tzvp). Comparable behaviour is obtained at b3lyp/g-311g(d,p)//b3lyp/g-311g(d,p) (green dots) level of theory confirming that not so dissimilar results can be obtained using less demanding computational cost.



Equation	y = a + b*x
Plot	DeltaG#
Weight	No Weighting
Intercept	12,68526 ± 0,26781
Slope	0,2753 ± 0,01943
Residual Sum of Squares	27,16677
Pearson's r	0,94093
R-Square (COD)	0,88534
Adj. R-Square	0,88093

Equation	y = a + b*x
Plot	DeltaG#
Weight	No Weighting
Intercept	10,27737 ± 0,24653
Slope	0,32285 ± 0,02698
Residual Sum of Squares	42,34387
Pearson's r	0,91998
R-Square (COD)	0,84636
Adj. R-Square	0,84045

Equation	y = a + b*x
Plot	DeltaG#
Weight	No Weighting
Intercept	15,18141 ± 0,30755
Slope	0,28446 ± 0,02331
Residual Sum of Squares	40,07003
Pearson's r	0,92268
R-Square (COD)	0,85134
Adj. R-Square	0,84562

Figure S5. Calculated $\Delta G^{\ddagger}$ vs ΔG^{0} data for ωb97xd/def2tzvp//ωb97xd/def2tzvp (red dots), ωb97xd/aug-cc-pvtz//ωb97xd/def2tzvp (black dots), b2plypd/aug-cc-pvtz//ωb97xd/def2tzvp (blue dots) and b3lyp/g-311g(d,p)//b3lyp/g-311g(d,p) (green dots), all with IEFPCM(CH_3CN). Linear fitting equations can be derived considering the values of slope as α parameter and the value of intercept as $\Delta G_0^{\ddagger}$ (following eq. 2 in the manuscript) for each levels of calculation.

Table S4. Gibbs Energies, Enthalpic and Entropic contributions obtained at ωb97XD/aug-cc-pvtz//ωb97XD/def2tzvp level, IEFPCM(CH_3CN).

i	wb97XD/aug-cc-pvtz//wb97xd/def2tzvp species	charge	mult.	wb97xd/def2tzvp Gibbs (hartree)	wb97xd/def2tzvp Enthalpy (hartree)	Electronic Energy wb97xD def2tzvp	Electronic Energy wb97xD aug-cc-pvtz	CORRECTED: +1,90 kcal/mol; Gibbs (kcal/mol)	Enthalpy (hartree)	CORRECTED: +1,90 kcal/mol; Enthalpy (kcal/mol)	ΔG°	$\Delta G^{\bullet}$	ΔH°	$\Delta H^{\bullet}$	$T\Delta S^{\circ}$	$T\Delta S^{\bullet}$
	CO_2	0	1	-188.617485	-188.592598	-188.607960	-188.600842	-118352.92	-188.585480	-118337.30						
1	cyclopentadiene_anion	-1	1	-193.560277	-193.529044	-193.613560	-193.612604	-121458.43	-193.528088	-121438.83	1.753	14.275	-8.654	3.839	-10.407	-10.436
	cyclopentadiene_COO	-1	1	-382.170002	-382.130467	-382.233410	-382.227275	-239809.60	-382.124332	-239784.79						
	cyclopentadiene_COO_TS	-1	1	-382.151681	-382.112192	-382.212510	-382.204741	-239797.07	-382.104423	-239772.29						
2	indene_anion	-1	1	-347.166230	-347.128857	-347.263500	-347.259035	-217845.44	-347.124392	-217821.99	-4.488	12.192	-15.140	2.012	-10.652	-10.181
	indene_COO	-1	1	-535.785294	-535.740009	-535.893630	-535.884593	-336202.84	-535.730972	-336174.43						
	indene_COO_TS	-1	1	-535.760670	-535.714634	-535.865060	-535.854065	-336186.16	-535.703639	-336157.28						
3	malonitrile_anion	-1	1	-224.514966	-224.481943	-224.519270	-224.514868	-140880.63	-224.477541	-140859.91	7.982	14.015	-2.732	3.956	-10.713	-10.060
	malonitrile_COO	-1	1	-413.115246	-413.074409	-413.129440	-413.119378	-259225.57	-413.064347	-259199.94						
	malonitrile_COO_TS	-1	1	-413.106598	-413.064719	-413.117580	-413.106551	-259219.54	-413.053690	-259193.26						
4	acetylene_anion	-1	1	-76.825328	-76.802405	-76.821080	-76.821545	-48207.02	-76.802870	-48192.64	-16.596	7.523	-26.329	-0.328	-9.733	-7.851
	acetylene_COO	-1	1	-265.464498	-265.432198	-265.468310	-265.463392	-166576.54	-265.427280	-166556.27						
	acetylene_COO_TS	-1	1	-265.427988	-265.392690	-265.426360	-265.419515	-166552.42	-265.385845	-166530.27						
5	phenylacethylene_anion	-1	1	-307.813196	-307.775762	-307.881470	-307.877679	-193151.46	-307.771971	-193127.97	-17.461	8.209	-27.171	-0.220	-9.710	-8.429
	phenylacetylene_COO	-1	1	-496.453310	-496.406463	-496.529930	-496.521190	-311521.83	-496.397723	-311492.44						
	phenylacetylene_COO_TS	-1	1	-496.414670	-496.365782	-496.486840	-496.475832	-311496.16	-496.354774	-311465.49						
6	diphenylmethane_anion	-1	1	-501.928287	-501.880882	-502.088450	-502.081850	-314958.78	-501.874282	-314929.03	-22.382	6.611	-32.518	-2.734	-10.136	-9.345
	diphenylmethane_COO	-1	1	-690.575659	-690.519520	-690.746860	-690.735896	-433334.08	-690.508556	-433298.85						
	diphenylmethane_COO_TS	-1	1	-690.531730	-690.474330	-690.697600	-690.684361	-433305.08	-690.461091	-433269.06						
7	pCNtoluene_anion	-1	1	-363.208897	-363.168689	-363.290370	-363.284933	-227911.76	-363.163252	-227886.53	-19.744	8.535	-30.159	-1.089	-10.415	-9.624
	pCNtoluene_COO	-1	1	-551.851904	-551.803406	-551.944760	-551.935120	-346284.42	-551.793766	-346253.99						
	pCNtoluene_COO_TS	-1	1	-551.809478	-551.759720	-551.896980	-551.884701	-346256.14	-551.747441	-346224.92						
8	pCOPhtoluene_anion	-1	1	-615.272522	-615.220511	-615.439900	-615.430371	-386081.53	-615.210982	-386048.90	-18.423	9.09	-28.887	-0.105	-10.464	-9.200
	pCOPhtoluene_COO	-1	1	-803.913754	-803.853532	-804.092670	-804.078608	-504452.87	-803.839470	-504415.08						
	pCOPhtoluene_COO_TS	-1	1	-803.872256	-803.810019	-804.044770	-804.028353	-504425.36	-803.793602	-504386.30						
9	pNO2toluene_anion	-1	1	-475.501742	-475.459439	-475.586160	-475.577511	-298374.58	-475.450790	-298348.03	-11.069	13.024	-20.962	3.095	-9.893	-9.929
	pNO2toluene_COO	-1	1	-664.132416	-664.080992	-664.227050	-664.212706	-416738.57	-664.066648	-416706.30						
	pNO2toluene_COO_TS	-1	1	-664.095783	-664.044416	-664.186660	-664.170555	-416714.47	-664.028311	-416682.24						
10	acetone_anion	-1	1	-192.615488	-192.583402	-192.660010	-192.659942	-120866.12	-192.583334	-120845.99	-12.806	8.904	-22.901	-0.618	-10.095	-9.522
	acetone_COO	-1	1	-381.249859	-381.208973	-381.304510	-381.297818	-239231.85	-381.202281	-239206.19						
	acetone_COO_TS	-1	1	-381.216194	-381.174396	-381.266540	-381.258915	-239210.14	-381.166771	-239183.91						
11	dimethylpentanone_anion	-1	1	-349.762574	-349.716322	-349.911320	-349.909960	-219476.62	-349.714962	-219447.60	-15.442	8.038	-28.440	-2.856	-12.998	-10.894
	dimethylpentanone_COO	-1	1	-538.401217	-538.350792	-538.565400	-538.557345	-337844.98	-538.342737	-337813.34						
	dimethylpentanone_COO_TS	-1	1	-538.364384	-538.310606	-538.521520	-538.512880	-337821.50	-538.301966	-337787.75						
12	cyclobutanone_anion	-1	1	-230.683917	-230.651406	-230.734980	-230.733551	-144753.58	-230.649977	-144733.17	-14.620	7.875	-25.090	-2.216	-10.470	-10.092
	cyclobutanone_COO	-1	1	-419.320992	-419.280279	-419.382350	-419.374484	-263121.11	-419.272413	-263095.56						
	cyclobutanone_COO_TS	-1	1	-419.286123	-419.244807	-419.343950	-419.335104	-263098.62	-419.235961	-263072.69						
13	cyclohexanone_anion	-1	1	-309.291258	-309.254072	-309.399050	-309.397410	-194080.30	-309.252432	-194056.97	-13.622	8.788	-24.639	-1.579	-11.017	-10.368
	cyclohexanone_COO	-1	1	-497.926870	-497.882353	-498.046410	-498.038206	-312446.84	-497.874149	-312418.91						
	cyclohexanone_COO_TS	-1	1	-497.892122	-497.846571	-498.007290	-497.998120	-312424.43	-497.837401	-312395.85						
14	acetophenone_anion	-1	1	-384.303018	-384.264859	-384.397680	-384.393004	-241149.00	-384.260183	-241125.05	-12.745	8.255	-21.511	-0.150	-8.766	-8.405
	acetophenone_COO	-1	1	-572.936777	-572.887700	-573.040440	-573.029655	-359514.66	-572.876915	-359483.86						
	acetophenone_COO_TS	-1	1	-572.904409	-572.854758	-573.004100	-572.992217	-359493.66	-572.842875	-359462.50						
15	pCNacetophenone_anion	-1	1	-476.558307	-476.513412	-476.647660	-476.640296	-299038.39	-476.506048	-299010.22	-8.453	10.147	-18.701	0.216	-10.248	-9.931
	pCNacetophenone_COO	-1	1	-665.185271	-665.131821	-665.284930	-665.271413	-417399.76	-665.118304	-417366.22						
	pCNacetophenone_COO_TS	-1	1	-665.156741	-665.102785	-665.252580	-665.237952	-417381.16	-665.088157	-417347.30						
16	pNMe2acetophenone_anion	-1	1	-518.214269	-518.163503	-518.374780	-518.369133	-325178.99	-518.157856	-325147.13	-15.202	8.839	-25.379	-1.164	-10.178	-10.003
	pNMe2acetophenone_COO	-1	1	-706.851964	-706.792530	-707.022970	-707.011194	-443547.10	-706.780754	-443509.81						
	pNMe2acetophenone_COO_TS	-1	1	-706.814893	-706.755181	-706.981920	-706.968903	-443523.06	-706.742164	-443485.59						
17	Benzoylacetonitrile_anion	-1	1	-476.586084	-476.540736	-476.675910	-476.667475	-299055.15	-476.532301	-299026.69	9.058	15.920	-1.530	5.359	-10.588	-10.561
	Benzoylacetonitrile_COO	-1	1	-665.184916	-665.131554	-665.284470	-665.270108	-417399.01	-665.117192	-417365.52						
	Benzoylacetonitrile_COO_TS	-1	1	-665.174798	-665.121393	-665.272190	-665.257009	-417392.15	-665.106212	-417358.63						
18	Phbenzylketone_anion	-1	1	-615.296022	-615.243510	-615.463880	-615.454480	-386096.36	-615.234110	-386063.41	-1.932	12.487	-12.766	1.601	-10.835	-10.886
	Phbenzylketone_COO	-1	1	-803.912086	-803.851953	-804.091060	-804.076015	-504451.21	-803.836908	-504413.48						
	Phbenzylketone_COO_TS	-1	1	-803.890214	-803.830163	-804.066460	-804.050308	-504436.79	-803.814011	-504399.11						
19	2-Facetophenone_anion	-1	1	-483.560058	-483.517030	-483.644000	-483.635192	-303431.15	-483.508222	-303404.15	-13.684	8.593	-24.354	-1.648	-10.670	-10.241
	2-Facetophenone_COO	-1	1	-672.196134	-672.145223	-672.291020	-672.275283	-421797.75	-672.129486	-421765.81						
	2-Facetophenone_COO_TS	-1	1	-672.161141	-672.109546	-672.251820	-672.235576	-421775.48	-672.093302	-421743.10						
20	phepropanone_anion	-1	1	-423.593386	-423.548703	-423.712120	-423.707267	-265803.97	-423.543850	-265775.93	-11.411	9.529	-22.990	-1.228	-11.579	-10.756
	phepropanone_COO	-1	1	-612.225246	-612.174128	-612.356580	-612.345391	-384168.30	-612.162939	-384136.22						
	phepropanone_COO_TS	-1	1	-612.192917	-612.140488	-612.319670	-612.307440	-384147.36	-612.128258	-384114.46						
21	acetic acid tert-butyl ester_anion	-1	1	-385.722142	-385.678231	-385.848670	-385.844244	-242039.67	-385.673805	-242012.12	-19.385	6.398	-30.391	-2.605	-11.006	-9.003
	acetic acid tert-butyl ester_COO	-1	1	-574.366031	-574.314772	-574.504990	-574.494907	-360411.97	-574.304689	-360379.81						
	acetic acid tert-butyl ester_COO_TS	-1	1	-574.326647	-574.272196	-574.457830	-574.446044	-360386.19	-574.260410	-360352.02						
22	^{t}BuPhenylacetate_anion	-1	1	-616.715646	-616.659625	-616.916700	-616.907445	-386987.28	-616.650370	-386952.13	-8.752	9.083	-20.088	-1.113	-11.336	-10.196
	^{t}BuPhenylacetate_COO	-1	1	-805.342001	-805.279158	-805.555710	-805.541387	-505348.95	-805.264835	-505309.51						
	^{t}BuPhenylacetate_COO_TS	-1	1	-805.315209	-805.250549	-805.523420	-805.507467	-505331.11	-805.234596	-505290.54						
23_c1	Etacetoacetate_anion	-1	1	-459.799940	-459.753001	-459.907660	-459.900098	-288522.23	-459.745439	-288492.78	4.539	13.872	-6.165	3.648	-10.703	-10.223
	Etacetoacetate_COO	-1	1	-648.406475	-648.351706	-648.524550	-648.510559	-406870.61	-648.337715	-406836.24						
	Etacetoacetate_COO_TS	-1	1	-648.392276	-648.336742	-648.507110	-648.492445	-406861.28	-648.322077	-406826.43						
23_c2	Etacetoacetate_anion	-1	1	-459.797446	-459.750532	-459.9054354	-459.8981248	-288520.82	-459.743221	-288491.38						
23_c3	Etacetoacetate_anion	-1	1	-459.799123	-459.751909	-459.906663	-459.898967	-288521.63	-459.744213	-288492.01	3.799	14.126	-6.721	3.856	-10.520	-10.270
	Etacetoacetate_COO	-1	1	-648.406483	-648.351147	-648.523890	-648.510119	-406870.75	-648.337376	-406836.03						
	Etacetoacetate_COO_TS	-1	1	-648.390983	-648.335248	-648.505559	-648.490831	-406860.42	-648.320520	-406825.45						
23_c4	Etacetoacetate_anion	-1	1	-459.797893	-459.750261	-459.905116	-459.897413	-288520.86	-459.742558	-288490.97						
24_c1	diMeMalonate_anion	-1	1	-495.740274	-495.693686	-495.825001	-495.814703	-311073.42	-495.683388	-311044.18	4.247	13.688	-8.035	3.334	-12.282	-10.354
	diMemalonate_COO	-1	1	-684.346748	-684.294845	-684.443664	-684.427464	-429422.09	-684.278645	-429389.52						
	diMemalonate_COO_TS	-1	1	-684.332700	-684.277725	-684.424695	-684.407498	-429412.65	-684.260528	-429378.15						
24_c2	diMemalonate_anion	-1	1	-495.738251	-495.691933	-495.823280	-495.813046	-311072.19	-495.681699	-311043.12	2.109	13.526	-8.578	3.185	-10.688	-10.341
	diMemalonate_COO	-1	1	-684.348298	-684.294125	-684.443920	-684.427617	-429423.00	-684.277822	-429389.00						
	diMemalonate_COO_TS	-1	1	-684.330987	-684.276261	-684.423240	-684.406055	-429411.58	-684.259076	-429377.24						
24_c3	diMemalonate_anion	-1	1	-495.73673	-495.689859	-495.821135	-495.8110086	-311071.30	-495.679733	-311041.89						
25_c1	diMeacetoacetamid_anion	-1	1	-439.899292	-439.851955	-440.019140	-440.013257	-276035.44	-439.846072	-276005.73	-2.291	12.595	-12.172	1.856	-9.881	-10.739
	diMeacetoacetamid_COO	-1	1	-628.516573	-628.460095	-628.645490	-628.633317	-394390.64	-628.447922	-394355.20						
	diMeacetoacetamid_COO_TS	-1	1	-628.493704	-628.438593	-628.621590	-628.608564	-394375.76	-628.425567	-394341.18						
25_c2	diMeacetoacetamid_anion	-1	1	-439.899001	-439.850608	-440.017721	-440.011850	-276035.26	-439.844737	-276004.89	-1.550	11.944	-12.429	2.393	-10.880	-9.551
	diMeacetoacetamid_COO	-1	1	-628.514941	-628.458999	-628.644389	-628.632387	-394389.73	-628.446997	-394354.62						
	diMeacetoacetamid_COO_TS	-1	1	-628.494449	-628.436389	-628.619204	-628.606191	-394376.23	-628.423376	-394339.80						
25_c3	diMeacetoacetamid_anion	-1	1	-439.893480	-439.847603	-440.014815	-440.009455	-276032.12	-439.842243	-276003.33						
25_c4	diMeacetoacetamid_anion	-1	1	-439.896412	-439.849731	-440.017011	-440.011186	-276033.67	-439.843906	-276004.37						
26	3-oxo-3-pyrrolidin-1-yl-propionitrile_anion	-1	1	-456.921803	-456.875961	-457.040510	-457.033322	-286716.41	-456.868773	-286687.64	0.124	11.504	-10.916	1.204	-11.040	-10.301
	3-oxo-3-pyrrolidin-1-yl-propionitrile_COO	-1	1	-645.534911	-645.481775	-645.664760	-645.651606	-405069.20	-645.468621	-405035.86						
	3-oxo-3-pyrrolidin-1-yl-propionitrile_COO_TS	-1	1	-645.517597	-645.463283	-645.643650	-645.629675	-405057.82	-645.449308	-405023.74						
27	calcone_DA	-2	1	-654.037138	-653.981641	-654.216510	-654.209673	-410408.39	-653.974804	-410373.57	-28.527	6.384	-39.053	-3.970	-10.526	-10.355
	calcone_COO	-2	1	-842.695530	-842.631921	-842.887170	-842.874741	-528789.84	-842.619492	-528749.92						
	calcone_COO_TS	-2	1	-842.641737	-842.577854	-842.828460	-842.814190	-528754.92	-842.563584	-528714.84						
28	flavone_DA	-2	1	-728.077459	-728.023297	-728.240500	-728.229840	-456867.01	-728.012637	-456833.02	-29.463	5.488	-41.608	-5.142	-12.145	-10.630
	flavone_COO	-2	1	-916.737075	-916.677381	-916.914670	-916.898686	-575249.39	-916.661397	-575211.93						
	flavone_COO_TS	-2	1	-916.682622	-916.620513	-916.853400	-916.836172	-575214.43	-916.603285	-575175.46						

Table S5. Gibbs Energies, Enthalpic and Entropic contributions at ωb97XD/def2tzvp//ωb97XD/def2tzvp level, IEFPCM(CH_3CN).

i	wb97xd/def2tzvp species	charge	mult.	Gibbs (hartree)	**CORRECTED** + 1,90 (kcal/mol) Gibbs (kcal/mol)	Enthalpy (hartree)	**CORRECTED** + 1,90 (kcal/mol) Enthalpy (kcal/mol)	ΔG^0	ΔG^*	ΔH^0	ΔH^*	$T\Delta S^0$	$T\Delta S^*$
	CO_2	0	1	-188.617485	-118357.38	-188.592598	-118341.77						
1	cyclopentadiene_anion	-1	1	-193.560277	-121459.03	-193.529044	-121439.43	2.969	14.466	-7.438	4.030	-10.407	-10.436
	cyclopentadiene_COO	-1	1	-382.170002	-239813.45	-382.130467	-239788.64						
	cyclopentadiene_COO_TS	-1	1	-382.151681	-239801.95	-382.112192	-239777.17						
2	indene_anion	-1	1	-347.166230	-217848.24	-347.128857	-217824.79	-2.891	12.561	-13.543	2.380	-10.652	-10.181
	indene_COO	-1	1	-535.785294	-336208.52	-535.740009	-336180.10						
	indene_COO_TS	-1	1	-535.760670	-336193.06	-535.714634	-336164.18						
3	malonitrile_anion	-1	1	-224.514966	-140883.40	-224.481943	-140862.67	8.896	14.323	-1.817	4.263	-10.713	-10.060
	malonitrile_COO	-1	1	-413.115246	-259231.88	-413.074409	-259206.26						
	malonitrile_COO_TS	-1	1	-413.106598	-259226.46	-413.064719	-259200.18						
4	acetylene_anion	-1	1	-76.825328	-48206.73	-76.802405	-48192.35	-15.508	7.403	-25.240	-0.449	-9.733	-7.851
	acetylene_COO	-1	1	-265.464498	-166579.62	-265.432198	-166559.35						
	acetylene_COO_TS	-1	1	-265.427988	-166556.71	-265.392690	-166534.56						
5	phenylacethylene_anion	-1	1	-307.813196	-193153.84	-307.775762	-193130.35	-16.100	8.147	-25.810	-0.282	-9.710	-8.429
	phenylacetylene_COO	-1	1	-496.453310	-311527.32	-496.406463	-311497.92						
	phenylacetylene_COO_TS	-1	1	-496.414670	-311503.07	-496.365782	-311472.39						
6	diphenylmethane_anion	-1	1	-501.928287	-314962.92	-501.880882	-314933.17	-20.654	6.911	-30.791	-2.433	-10.136	-9.345
	diphenylmethane_COO	-1	1	-690.575659	-433340.96	-690.519520	-433305.73						
	diphenylmethane_COO_TS	-1	1	-690.531730	-433313.39	-690.474330	-433277.37						
7	pCNtoluene_anion	-1	1	-363.208897	-227915.17	-363.168689	-227889.94	-17.915	8.707	-28.330	-0.917	-10.415	-9.624
	pCNtoluene_COO	-1	1	-551.851904	-346290.47	-551.803406	-346260.03						
	pCNtoluene_COO_TS	-1	1	-551.809478	-346263.84	-551.759720	-346232.62						
8	pCOPhtoluene_anion	-1	1	-615.272522	-386087.51	-615.220511	-386054.88	-16.801	9.239	-27.266	0.039	-10.464	-9.200
	pCOPhtoluene_COO	-1	1	-803.913754	-504461.70	-803.853532	-504423.91						
	pCOPhtoluene_COO_TS	-1	1	-803.872256	-504435.66	-803.810019	-504396.60						
9	pNO2toluene_anion	-1	1	-475.501742	-298380.01	-475.459439	-298353.46	-10.176	12.811	-20.070	2.882	-9.893	-9.929
	pNO2toluene_COO	-1	1	-664.132416	-416747.57	-664.080992	-416715.30						
	pNO2toluene_COO_TS	-1	1	-664.095783	-416724.58	-664.044416	-416692.35						
10	acetone_anion	-1	1	-192.615488	-120866.17	-192.583402	-120846.03	-12.496	8.629	-22.591	-0.893	-10.095	-9.522
	acetone_COO	-1	1	-381.249859	-239236.05	-381.208973	-239210.39						
	acetone_COO_TS	-1	1	-381.216194	-239214.92	-381.174396	-239188.69						
11	dimethylpentanone_anion	-1	1	-349.762574	-219477.47	-349.716322	-219448.45	-15.177	7.936	-28.175	-2.958	-12.998	-10.894
	dimethylpentanone_COO	-1	1	-538.401217	-337850.03	-538.350792	-337818.39						
	dimethylpentanone_COO_TS	-1	1	-538.364384	-337826.92	-538.310606	-337793.17						
12	cyclobutanone_anion	-1	1	-230.683917	-144754.47	-230.651406	-144734.07	-14.193	7.688	-24.663	-2.404	-10.470	-10.092
	cyclobutanone_COO	-1	1	-419.320992	-263126.05	-419.280279	-263100.50						
	cyclobutanone_COO_TS	-1	1	-419.286123	-263104.17	-419.244807	-263078.24						
13	cyclohexanone_anion	-1	1	-309.291258	-194081.33	-309.254072	-194058.00	-13.275	8.530	-24.291	-1.838	-11.017	-10.368
	cyclohexanone_COO	-1	1	-497.926870	-312451.99	-497.882353	-312424.06						
	cyclohexanone_COO_TS	-1	1	-497.892122	-312430.19	-497.846571	-312401.60						
14	acetophenone_anion	-1	1	-384.303018	-241151.93	-384.264859	-241127.99	-12.112	8.199	-20.878	-0.206	-8.766	-8.405
	acetophenone_COO	-1	1	-572.936777	-359521.43	-572.887700	-359490.63						
	acetophenone_COO_TS	-1	1	-572.904409	-359501.12	-572.854758	-359469.96						
15	pCNacetophenone_anion	-1	1	-476.558307	-299043.01	-476.513412	-299014.84	-7.848	10.055	-18.097	0.124	-10.248	-9.931
	pCNacetophenone_COO	-1	1	-665.185271	-417408.24	-665.131821	-417374.70						
	pCNacetophenone_COO_TS	-1	1	-665.156741	-417390.34	-665.102785	-417356.48						
16	pNMe2acetophenone_anion	-1	1	-518.214269	-325182.53	-518.163503	-325150.67	-14.582	8.680	-24.760	-1.323	-10.178	-10.003
	pNMe2acetophenone_COO	-1	1	-706.851964	-443554.49	-706.792530	-443517.20						
	pNMe2acetophenone_COO_TS	-1	1	-706.814893	-443531.23	-706.755181	-443493.76						
17	Benzoylacetonitrile_anion	-1	1	-476.586084	-299060.44	-476.540736	-299031.99	9.805	16.154	-0.783	5.593	-10.588	-10.561
	Benzoylacetonitrile_COO	-1	1	-665.184916	-417408.02	-665.131554	-417374.54						
	Benzoylacetonitrile_COO_TS	-1	1	-665.174798	-417401.67	-665.121393	-417368.16						
18	Phbenzylketone_anion	-1	1	-615.296022	-386102.26	-615.243510	-386069.31	-1.008	12.717	-11.843	1.831	-10.835	-10.886
	Phbenzylketone_COO	-1	1	-803.912086	-504460.65	-803.851953	-504422.92						
	Phbenzylketone_COO_TS	-1	1	-803.890214	-504446.93	-803.830163	-504409.24						
19	2-Facetophenone_anion	-1	1	-483.560058	-303436.68	-483.517030	-303409.68	-13.566	8.392	-24.236	-1.849	-10.670	-10.241
	2-Facetophenone_COO	-1	1	-672.196134	-421807.63	-672.145223	-421775.68						
	2-Facetophenone_COO_TS	-1	1	-672.161141	-421785.67	-672.109546	-421753.29						
20	phepropanone_anion	-1	1	-423.593386	-265807.02	-423.548703	-265778.98	-10.920	9.366	-22.499	-1.390	-11.579	-10.756
	phepropanone_COO	-1	1	-612.225246	-384175.32	-612.174128	-384143.24						
	phepropanone_COO_TS	-1	1	-612.192917	-384155.03	-612.140488	-384122.13						
21	acetic acid tert-butyl ester_anion	-1	1	-385.722142	-242042.45	-385.678231	-242014.89	-18.469	6.245	-29.475	-2.758	-11.006	-9.003
	acetic acid tert-butyl ester_COO	-1	1	-574.366031	-360418.30	-574.314772	-360386.13						
	acetic acid tert-butyl ester_COO_TS	-1	1	-574.326647	-360393.58	-574.272196	-360359.42						
22	^{t}BuPhenylacetate_anion	-1	1	-616.715646	-386993.09	-616.659625	-386957.93	-7.466	9.346	-18.802	-0.850	-11.336	-10.196
	^{t}BuPhenylacetate_COO	-1	1	-805.342001	-505357.94	-805.279158	-505318.50						
	^{t}BuPhenylacetate_COO_TS	-1	1	-805.315209	-505341.12	-805.250549	-505300.55						
23	Etacetoacetate_anion	-1	1	-459.799940	-288526.98	-459.753001	-288497.52	4.971	13.881	-5.732	3.658	-10.703	-10.223
	Etacetoacetate_COO	-1	1	-648.406475	-406879.39	-648.351706	-406845.02						
	Etacetoacetate_COO_TS	-1	1	-648.392276	-406870.48	-648.336742	-406835.63						
24	diMemalonate_anion	-1	1	-495.740274	-311079.88	-495.693686	-311050.65	4.037	14.900	-6.820	4.390	-10.857	-10.510
	diMemalonate_COO	-1	1	-684.348298	-429433.23	-684.294125	-429399.23						
	diMemalonate_COO_TS	-1	1	-684.330987	-429422.36	-684.276261	-429388.02						
25	diMeacetoacetamid_anion	-1	1	-439.899292	-276039.13	-439.851955	-276009.42	-1.772	12.579	-11.653	1.840	-9.881	-10.739
	diMeacetoacetamid_COO	-1	1	-628.516573	-394398.28	-628.460095	-394362.84						
	diMeacetoacetamid_COO_TS	-1	1	-628.493704	-394383.93	-628.438593	-394349.35						
26	3-oxo-3-pyrrolidin-1-yl-propionitrile_anion	-1	1	-456.921803	-286720.92	-456.875961	-286692.15	0.847	11.711	-10.193	1.411	-11.040	-10.301
	3-oxo-3-pyrrolidin-1-yl-propionitrile_COO	-1	1	-645.534911	-405077.45	-645.481775	-405044.11						
	3-oxo-3-pyrrolidin-1-yl-propionitrile_COO_TS	-1	1	-645.517597	-405066.59	-645.463283	-405032.51						
27	calcone_DA	-2	1	-654.037138	-410412.68	-653.981641	-410377.86	-27.570	6.186	-38.096	-4.168	-10.526	-10.355
	calcone_COO	-2	1	-842.695530	-528797.63	-842.631921	-528757.72						
	calcone_COO_TS	-2	1	-842.641737	-528763.88	-842.577854	-528723.79						
28	flavone_DA	-2	1	-728.077459	-456873.70	-728.023297	-456839.71	-28.338	5.832	-40.483	-4.798	-12.145	-10.630
	flavone_COO	-2	1	-916.737075	-575259.42	-916.677381	-575221.96						
	flavone_COO_TS	-2	1	-916.682622	-575225.25	-916.620513	-575186.27						

Table S6. Gibbs Energies, Enthalpic and Entropic contributions obtained at b2plypd/aug-cc-pvtz//ωb97xd/def2tzvp level, IEFPCM(CH_3CN).

i	b2plypd/aug-cc-pvtz//wb97xd/def2tzvp	species	charge	mult.	wb97xd/def2tzvp Gibbs (hartree)	wb97xd/def2tzvp Enthalpy (hartree)	Electronic Energy wb97xD def2tzvp	Electronic Energy b2plypd aug-cc	CORRECTED: +1,90 kcal/mol Gibbs (kcal/mol)	Enthalpy (hartree)	CORRECTED: +1,90 kcal/mol Enthalpy (kcal/mol)	ΔG^0	ΔG *	ΔH^0	ΔH *	$T\Delta S^0$	$T\Delta S$ *
		CO_2	0	1	-188.617485	-188.592598	-188.607960	-188.348669	-118194.68	-188.333307	-118179.06						
	1	cyclopentadiene_anion	-1	1	-193.560277	-193.529044	-193.613560	-193.236344	-121222.33	-193.151828	-121202.73	2.868	17.552	-7.539	7.115	-10.407	-10.436
		cyclopentadiene_COO	-1	1	-382.170002	-382.130467	-382.233410	-381.597064	-239414.13	-381.494121	-239389.32						
		cyclopentadiene_COO_TS	-1	1	-382.151681	-382.112192	-382.212510	-381.571086	-239399.45	-381.470768	-239374.67						
	2	indene_anion	-1	1	-347.166230	-347.128857	-347.263500	-346.607614	-217436.67	-346.472971	-217413.22	-3.378	15.189	-14.030	5.008	-10.652	-10.181
		indene_COO	-1	1	-535.785294	-535.740009	-535.893630	-534.979229	-335634.72	-534.825608	-335606.30						
		indene_COO_TS	-1	1	-535.760670	-535.714634	-535.865060	-534.945695	-335616.15	-534.795269	-335587.27						
	3	malonitrile_anion	-1	1	-224.514966	-224.481943	-224.519270	-224.152596	-140653.30	-224.115269	-140632.58	10.305	16.550	-0.408	6.491	-10.713	-10.060
		malonitrile_COO	-1	1	-413.115246	-413.074409	-413.129440	-412.501229	-258837.67	-412.446198	-258812.05						
		malonitrile_COO_TS	-1	1	-413.106598	-413.064719	-413.117580	-412.488065	-258831.43	-412.435204	-258805.15						
	4	acetylene_anion	-1	1	-76.825328	-76.802405	-76.821080	-76.681885	-48119.38	-76.663210	-48105.00	-14.023	9.172	-23.756	1.321	-9.733	-7.851
		acetylene_COO	-1	1	-265.464498	-265.432198	-265.468310	-265.067459	-166328.08	-265.031347	-166307.81						
		acetylene_COO_TS	-1	1	-265.427988	-265.392690	-265.426360	-265.025054	-166304.89	-264.991384	-166282.74						
	5	phenylacethylene_anion	-1	1	-307.813196	-307.775762	-307.881470	-307.318054	-192800.29	-307.212346	-192776.80	-15.181	9.909	-24.891	1.479	-9.710	-8.429
		phenylacetylene_COO	-1	1	-496.453310	-496.406463	-496.529930	-495.705759	-311010.14	-495.582292	-310980.75						
		phenylacetylene_COO_TS	-1	1	-496.414670	-496.365782	-496.486840	-495.661326	-310985.05	-495.540268	-310954.38						
	6	diphenylmethane_anion	-1	1	-501.928287	-501.880882	-502.088450	-501.141717	-314368.83	-500.934149	-314339.09	-19.876	9.445	-30.013	0.100	-10.136	-9.345
		diphenylmethane_COO	-1	1	-690.575659	-690.519520	-690.746860	-689.539597	-432583.39	-689.312257	-432548.16						
		diphenylmethane_COO_TS	-1	1	-690.531730	-690.474330	-690.697600	-689.487539	-432554.06	-689.264269	-432518.05						
	7	pCNtoluene_anion	-1	1	-363.208897	-363.168689	-363.290370	-362.634638	-227503.69	-362.512957	-227478.46	-18.052	11.107	-28.467	1.483	-10.415	-9.624
		pCNtoluene_COO	-1	1	-551.851904	-551.803406	-551.944760	-551.029955	-345716.42	-550.888601	-345685.99						
		pCNtoluene_COO_TS	-1	1	-551.809478	-551.759720	-551.896980	-550.978133	-345687.26	-550.840873	-345656.04						
	8	pCOPhtoluene_anion	-1	1	-615.272522	-615.220511	-615.439900	-614.332100	-385392.36	-614.112711	-385359.72	-16.646	11.798	-27.111	2.598	-10.464	-9.200
		pCOPhtoluene_COO	-1	1	-803.913754	-803.853532	-804.092670	-802.725332	-503603.68	-802.486194	-503565.89						
		pCOPhtoluene_COO_TS	-1	1	-803.872256	-803.810019	-804.044770	-802.673601	-503575.24	-802.438850	-503536.18						
	9	pNO2toluene_anion	-1	1	-475.501742	-475.459439	-475.586160	-474.787024	-297878.54	-474.660303	-297852.00	-7.366	16.835	-17.259	6.906	-9.893	-9.929
		pNO2toluene_COO	-1	1	-664.132416	-664.080992	-664.227050	-663.164144	-416080.58	-663.018086	-416048.31						
		pNO2toluene_COO_TS	-1	1	-664.095783	-664.044416	-664.186660	-663.121821	-416056.38	-662.979577	-416024.15						
	10	acetone_anion	-1	1	-192.615488	-192.583402	-192.660010	-192.320622	-120653.20	-192.244014	-120633.06	-11.013	11.381	-21.107	1.859	-10.095	-9.522
		acetone_COO	-1	1	-381.249859	-381.208973	-381.304510	-380.703467	-238858.89	-380.607930	-238833.23						
		acetone_COO_TS	-1	1	-381.216194	-381.174396	-381.266540	-380.663475	-238836.49	-380.571331	-238810.26						
	11	dimethylpentanone_anion	-1	1	-349.762574	-349.716322	-349.911320	-349.236546	-219054.05	-349.041548	-219025.02	-13.927	10.823	-26.925	-0.072	-12.998	-10.894
		dimethylpentanone_COO	-1	1	-538.401217	-538.350792	-538.565400	-537.629344	-337262.65	-537.414736	-337231.01						
		dimethylpentanone_COO_TS	-1	1	-538.364384	-538.310606	-538.521520	-537.582856	-337237.90	-537.371942	-337204.15						
	12	cyclobutanone_anion	-1	1	-230.683917	-230.651406	-230.734980	-230.324058	-144496.61	-230.240484	-144476.21	-13.027	10.165	-23.497	0.073	-10.470	-10.092
		cyclobutanone_COO	-1	1	-419.320992	-419.280279	-419.382350	-418.710279	-262704.32	-418.608208	-262678.77						
		cyclobutanone_COO_TS	-1	1	-419.286123	-419.244807	-419.343950	-418.669789	-262681.12	-418.570646	-262655.20						
	13	cyclohexanone_anion	-1	1	-309.291258	-309.254072	-309.399050	-308.824220	-193720.62	-308.679242	-193697.29	-12.484	11.497	-23.501	1.129	-11.017	-10.368
		cyclohexanone_COO	-1	1	-497.926870	-497.882353	-498.046410	-497.211029	-311927.78	-497.046972	-311899.85						
		cyclohexanone_COO_TS	-1	1	-497.892122	-497.846571	-498.007290	-497.168441	-311903.80	-497.007722	-311875.22						
	14	acetophenone_anion	-1	1	-384.303018	-384.264859	-384.397680	-383.715392	-240723.79	-383.582571	-240699.85	-11.438	10.862	-20.203	2.456	-8.766	-8.405
		acetophenone_COO	-1	1	-572.936777	-572.887700	-573.040440	-572.097786	-358929.90	-571.945046	-358899.11						
		acetophenone_COO_TS	-1	1	-572.904409	-572.854758	-573.004100	-572.058278	-358907.60	-571.908936	-358876.45						
	15	pCNacetophenone_anion	-1	1	-476.558307	-476.513412	-476.647660	-475.830870	-298530.47	-475.696622	-298502.30	-7.020	12.903	-17.269	2.973	-10.248	-9.931
		pCNacetophenone_COO	-1	1	-665.185271	-665.131821	-665.284930	-664.207530	-416732.16	-664.054421	-416698.62						
		pCNacetophenone_COO_TS	-1	1	-665.156741	-665.102785	-665.252580	-664.171959	-416712.24	-664.022164	-416678.38						
	16	pNMe2acetophenone_anion	-1	1	-518.214269	-518.163503	-518.374780	-517.433785	-324592.04	-517.222508	-324560.19	-13.774	11.329	-23.951	1.326	-10.178	-10.003
		pNMe2acetophenone_COO	-1	1	-706.851964	-706.792530	-707.022970	-705.821396	-442800.49	-705.590956	-442763.20						
		pNMe2acetophenone_COO_TS	-1	1	-706.814893	-706.755181	-706.981920	-705.777413	-442775.39	-705.550674	-442737.92						
	17	Benzoylacetonitrile_anion	-1	1	-476.586084	-476.540736	-476.675910	-475.857950	-298547.16	-475.722776	-298518.71	11.317	19.134	0.729	8.573	-10.588	-10.561
		Benzoylacetonitrile_COO	-1	1	-665.184916	-665.131554	-665.284470	-664.204810	-416730.52	-664.051894	-416697.04						
		Benzoylacetonitrile_COO_TS	-1	1	-665.174798	-665.121393	-665.272190	-664.190190	-416722.71	-664.039393	-416689.19						
	18	Phbenzylketone_anion	-1	1	-615.296022	-615.243510	-615.463880	-614.355993	-385407.05	-614.135623	-385374.10	0.257	15.957	-10.578	5.071	-10.835	-10.886
		Phbenzylketone_COO	-1	1	-803.912086	-803.851953	-804.091060	-802.721866	-503601.47	-802.482759	-503563.74						
		Phbenzylketone_COO_TS	-1	1	-803.890214	-803.830163	-804.066460	-802.694119	-503585.77	-802.457822	-503548.09						
	19	2-Facetophenone_anion	-1	1	-483.560058	-483.517030	-483.644000	-482.861432	-302945.61	-482.734462	-302918.61	-13.103	10.963	-23.773	0.722	-10.670	-10.241
		2-Facetophenone_COO	-1	1	-672.196134	-672.145223	-672.291020	-671.248422	-421153.39	-671.102625	-421121.44						
		2-Facetophenone_COO_TS	-1	1	-672.161141	-672.109546	-672.251820	-671.205864	-421129.32	-671.063590	-421096.94						
	20	phepropanone_anion	-1	1	-423.593386	-423.548703	-423.712120	-422.946094	-265326.33	-422.782677	-265298.29	-10.278	12.196	-21.857	1.440	-11.579	-10.756
		phepropanone_COO	-1	1	-612.225246	-612.174128	-612.356580	-611.330239	-383531.28	-611.147787	-383499.20						
		phepropanone_COO_TS	-1	1	-612.192917	-612.140488	-612.319670	-611.289844	-383508.81	-611.110662	-383475.91						
	21	acetic acid tert-butyl ester_anion	-1	1	-385.722142	-385.678231	-385.848670	-385.161580	-241611.29	-384.991141	-241583.74	-17.883	8.809	-28.889	-0.194	-11.006	-9.003
		acetic acid tert-butyl ester_COO	-1	1	-574.366031	-574.314772	-574.504990	-573.557676	-359823.85	-573.367458	-359791.68						
		acetic acid tert-butyl ester_COO_TS	-1	1	-574.326647	-574.272196	-574.457830	-573.507363	-359797.16	-573.321729	-359762.99						
	22	^{t}BuPhenylacetate_anion	-1	1	-616.715646	-616.659625	-616.916700	-615.803868	-386294.78	-615.546793	-386259.62	-6.485	12.281	-17.821	2.085	-11.336	-10.196
		^{t}BuPhenylacetate_COO	-1	1	-805.342001	-805.279158	-805.555710	-804.182024	-504495.94	-803.905472	-504456.50						
		^{t}BuPhenylacetate_COO_TS	-1	1	-805.315209	-805.250549	-805.523420	-804.146621	-504477.17	-803.873750	-504436.60						
	23	Etacetoacetate_anion	-1	1	-459.799940	-459.753001	-459.907660	-459.142227	-288046.66	-458.987568	-288017.21	6.828	17.124	-3.875	6.900	-10.703	-10.223
		Etacetoacetate_COO	-1	1	-648.406475	-648.351706	-648.524550	-647.496867	-406234.51	-647.324023	-406200.14						
		Etacetoacetate_COO_TS	-1	1	-648.392276	-648.336742	-648.507110	-647.477219	-406224.21	-647.306851	-406189.36						
24	c2	diMemalonate_anion	-1	1	-495.738251	-495.691933	-495.823280	-495.043361	-310589.21	-494.912014	-310560.14	4.500	16.602	-6.187	6.261	-10.688	-10.341
		diMemalonate_COO	-1	1	-684.348298	-684.294125	-684.443920	-683.401949	-428779.38	-683.252154	-428745.39						
		diMemalonate_COO_TS	-1	1	-684.330987	-684.276261	-684.423240	-683.379296	-428767.28	-683.232317	-428732.94						
	25	diMeacetoacetamid_anion	-1	1	-439.899292	-439.851955	-440.019140	-439.257739	-275561.34	-439.090554	-275531.64	0.124	16.041	-9.757	5.302	-9.881	-10.739
		diMeacetoacetamid_COO	-1	1	-628.516573	-628.460095	-628.645490	-627.621777	-393755.89	-627.436382	-393720.45						
		diMeacetoacetamid_COO_TS	-1	1	-628.493704	-628.438593	-628.621590	-627.595381	-393739.98	-627.412384	-393705.39						
	26	3-oxo-3-pyrrolidin-1-yl-propionitrile_anion	-1	1	-456.921803	-456.875961	-457.040510	-456.237321	-286216.91	-456.072772	-286188.14	3.068	14.516	-7.972	4.216	-11.040	-10.301
		3-oxo-3-pyrrolidin-1-yl-propionitrile_COO	-1	1	-645.534911	-645.481775	-645.664760	-644.598741	-404408.52	-644.415756	-404375.17						
		3-oxo-3-pyrrolidin-1-yl-propionitrile_COO_TS	-1	1	-645.517597	-645.463283	-645.643650	-644.576700	-404397.07	-644.396333	-404362.99						
	27	calcone_DA	-2	1	-654.037138	-653.981641	-654.216510	-653.025980	-409665.61	-652.791111	-409630.79	-26.088	8.810	-36.615	-1.544	-10.526	-10.355
		calcone_COO	-2	1	-842.695530	-842.631921	-842.887170	-841.434989	-527886.38	-841.179740	-527846.46						
		calcone_COO_TS	-2	1	-842.641737	-842.577854	-842.828460	-841.374457	-527851.48	-841.123851	-527811.39						
	28	flavone_DA	-2	1	-728.077459	-728.023297	-728.240500	-726.964502	-456072.99	-726.747299	-456039.01	-27.080	8.186	-39.226	-2.444	-12.145	-10.630
		flavone_COO	-2	1	-916.737075	-916.677381	-916.914670	-915.377378	-574294.75	-915.140089	-574257.29						
		flavone_COO_TS	-2	1	-916.682622	-916.620513	-916.853400	-915.314360	-574259.48	-915.081473	-574220.51						

Table S7. Gibbs Energies, Enthalpic and Entropic contributions obtained by b3lyp/g-311g(d,p)//b3lyp/g-311g(d,p) , IEFPCM(CH_3CN).

	b3lyp/6-311g(d,p)				CORRECTED + 1,90 (kcal/mol)		CORRECTED + 1,90 (kcal/mol)	(kcal/mol)					
i	species	charge	mult.	Gibbs (hartree)	Gibbs (kcal/mol)	Enthalpy (hartree)	Enthalpy (kcal/mol)	ΔG^0	ΔG	ΔH^0	ΔH	$T\Delta S^0$	$T\Delta S$
	CO_2	0	1	-188.653398	-118379.92	-188.628475	-118364.28						
1	cyclopentadiene_anion	-1	1	-193.606336	-121487.93	-193.574996	-121468.27	8.265	13.341	-2.378	3.037	-10.643	-10.304
	cyclopentadiene_COO	-1	1	-382.243535	-239859.59	-382.204232	-239834.92						
	cyclopentadiene_COO_TS	-1	1	-382.235446	-239854.51	-382.195603	-239829.51						
2	indene_anion	-1	1	-347.253266	-217902.86	-347.215757	-217879.32	5.136	12.819	-5.722	2.612	-10.858	-10.208
	indene_COO	-1	1	-535.895452	-336277.64	-535.850323	-336249.32						
	indene_COO_TS	-1	1	-535.883207	-336269.96	-535.837042	-336240.99						
3	malonitrile_anion	-1	1	-224.573688	-140920.25	-224.540724	-140899.56	13.384	14.196	2.826	4.082	-10.557	-10.114
	malonitrile_COO	-1	1	-413.202730	-259286.78	-413.161667	-259261.01						
	malonitrile_COO_TS	-1	1	-413.201435	-259285.97	-413.159666	-259259.76						
4	acetylene_anion	-1	1	-76.842109	-48217.26	-76.819149	-48202.85	-14.428	4.592	-24.153	-3.014	-9.725	-7.606
	acetylene_COO	-1	1	-265.515472	-166611.61	-265.483087	-166591.29						
	acetylene_COO_TS	-1	1	-265.485162	-166592.59	-265.449400	-166570.15						
5	phenylacethylene_anion	-1	1	-307.891845	-193203.19	-307.854285	-193179.62	-12.000	5.951	-23.697	-2.482	-11.697	-8.432
	phenylacetylene_COO	-1	1	-496.561339	-311595.11	-496.517496	-311567.60						
	phenylacetylene_COO_TS	-1	1	-496.532732	-311577.16	-496.483687	-311546.38						
6	diphenylmethane_anion	-1	1	-502.058930	-315044.90	-502.011478	-315015.12	-8.309	8.901	-18.821	-0.568	-10.513	-9.470
	diphenylmethane_COO	-1	1	-690.722541	-433433.13	-690.666919	-433398.22						
	diphenylmethane_COO_TS	-1	1	-690.695115	-433415.92	-690.637831	-433379.97						
7	pCNtoluene_anion	-1	1	-363.305237	-227975.62	-363.264917	-227950.32	-8.230	8.212	-18.789	-0.990	-10.558	-9.202
	pCNtoluene_COO	-1	1	-551.968723	-346363.77	-551.920306	-346333.39						
	pCNtoluene_COO_TS	-1	1	-551.942521	-346347.33	-551.891942	-346315.59						
8	pCOPhtoluene_anion	-1	1	-615.423300	-386182.13	-615.371160	-386149.41	-6.427	9.585	-16.999	0.103	-10.572	-9.482
	pCOPhtoluene_COO	-1	1	-804.083912	-504568.47	-804.023696	-504530.69						
	pCOPhtoluene_COO_TS	-1	1	-804.058396	-504552.46	-803.996443	-504513.59						
9	pNO2toluene_anion	-1	1	-475.609539	-298447.65	-475.567107	-298421.03	0.444	12.201	-9.579	2.670	-10.024	-9.532
	pNO2toluene_COO	-1	1	-664.259201	-416827.13	-664.207820	-416794.88						
	pNO2toluene_COO_TS	-1	1	-664.240465	-416815.37	-664.188300	-416782.63						
10	acetone_anion	-1	1	-192.653207	-120889.84	-192.620954	-120869.60	-8.707	6.648	-18.611	-2.329	-9.905	-8.977
	acetone_COO	-1	1	-381.317452	-239278.46	-381.276060	-239252.49						
	acetone_COO_TS	-1	1	-381.292983	-239263.11	-381.250113	-239236.21						
11	dimethylpentanone_anion	-1	1	-349.835181	-219523.03	-349.789306	-219494.25	-8.341	8.512	-20.290	-1.913	-11.950	-10.424
	dimethylpentanone_COO	-1	1	-538.498843	-337911.29	-538.447088	-337878.82						
	dimethylpentanone_COO_TS	-1	1	-538.471987	-337894.44	-538.417801	-337860.44						
12	cyclobutanone_anion	-1	1	-230.728407	-144782.39	-230.695796	-144761.93	-8.745	6.381	-19.452	-3.005	-10.707	-9.386
	cyclobutanone_COO	-1	1	-419.392713	-263171.05	-419.352242	-263145.66						
	cyclobutanone_COO_TS	-1	1	-419.368609	-263155.93	-419.326032	-263129.21						
13	cyclohexanone_anion	-1	1	-309.351492	-194119.13	-309.314139	-194095.69	-6.333	7.594	-17.319	-2.371	-10.986	-9.965
	cyclohexanone_COO	-1	1	-498.011955	-312505.38	-497.967186	-312477.29						
	cyclohexanone_COO_TS	-1	1	-497.989760	-312491.46	-497.943365	-312462.34						
14	acetophenone_anion	-1	1	-384.391843	-241207.67	-384.353454	-241183.58	-5.722	7.265	-15.092	-0.996	-9.369	-8.262
	acetophenone_COO	-1	1	-573.051332	-359593.31	-573.002951	-359562.95						
	acetophenone_COO_TS	-1	1	-573.030635	-359580.32	-572.980489	-359548.86						
15	pCNacetophenone_anion	-1	1	-476.670138	-299113.19	-476.627307	-299086.31	1.767	8.187	-7.228	0.017	-8.994	-8.170
	pCNacetophenone_COO	-1	1	-665.317693	-417491.34	-665.264272	-417457.82						
	pCNacetophenone_COO_TS	-1	1	-665.307461	-417484.92	-665.252727	-417450.57						
16	pNMe2acetophenone_anion	-1	1	-518.327480	-325253.57	-518.276970	-325221.87	-6.281	6.340	-15.803	-2.197	-9.522	-8.537
	pNMe2acetophenone_COO	-1	1	-706.987859	-443639.77	-706.927601	-443601.96						
	pNMe2acetophenone_COO_TS	-1	1	-706.967747	-443627.15	-706.905918	-443588.35						
17	Benzoylacetonitrile_anion	-1	1	-476.699234	-299131.45	-476.654275	-299103.23	15.459	16.551	5.020	5.951	-10.439	-10.600
	Benzoylacetonitrile_COO	-1	1	-665.324968	-417495.90	-665.271722	-417462.49						
	Benzoylacetonitrile_COO_TS	-1	1	-665.323229	-417494.81	-665.270239	-417461.56						
18	Phbenzylketone_anion	-1	1	-615.445817	-386196.26	-615.393651	-386163.52	8.106	13.569	-2.763	3.160	-10.870	-10.410
	Phbenzylketone_COO	-1	1	-804.083269	-504568.07	-804.023502	-504530.57						
	Phbenzylketone_COO_TS	-1	1	-804.074563	-504562.61	-804.014063	-504524.64						
19	2-Facetophenone_anion	-1	1	-483.660057	-303499.43	-483.616510	-303472.10	-2.421	7.444	-13.847	-2.130	-11.426	-9.574
	2-Facetophenone_COO	-1	1	-672.314286	-421881.77	-672.264024	-421850.23						
	2-Facetophenone_COO_TS	-1	1	-672.298565	-421871.90	-672.245352	-421838.51						
20	phepropanone_anion	-1	1	-423.692435	-265869.17	-423.647797	-265841.16	-4.226	8.404	-15.939	-1.670	-11.713	-10.074
	phepropanone_COO	-1	1	-612.349539	-384253.31	-612.298644	-384221.38						
	phepropanone_COO_TS	-1	1	-612.329412	-384240.68	-612.275905	-384207.11						
21	acetic acid tert-butyl ester_anion	-1	1	-385.798139	-242090.14	-385.755989	-242063.69	-12.581	5.603	-22.301	-2.204	-9.719	-7.807
	acetic acid tert-butyl ester_COO	-1	1	-574.468559	-360482.64	-574.416975	-360450.27						
	acetic acid tert-butyl ester_COO_TS	-1	1	-574.439580	-360464.45	-574.384948	-360430.17						
22	^{t}BuPhenylacetate_anion	-1	1	-616.854400	-387080.16	-616.798590	-387045.14	3.010	11.548	-7.861	0.843	-10.870	-10.705
	^{t}BuPhenylacetate_COO	-1	1	-805.499974	-505457.07	-805.436564	-505417.28						
	^{t}BuPhenylacetate_COO_TS	-1	1	-805.486367	-505448.53	-805.422694	-505408.57						
23	Etacetoacetate_anion	-1	1	-459.892036	-288584.77	-459.844203	-288554.75	10.347	13.001	-0.271	3.055	-10.618	-9.947
	Etacetoacetate_COO	-1	1	-648.525917	-406954.34	-648.470082	-406919.30						
	Etacetoacetate_COO_TS	-1	1	-648.521687	-406951.68	-648.464782	-406915.98						
24 c2	diMemalonate_anion	-1	1	-495.833848	-311138.60	-495.786940	-311109.16	9.356	13.853	-1.460	3.495	-10.816	-10.358
	diMemalonate_COO	-1	1	-684.469308	-429509.16	-684.414714	-429474.90						
	diMemalonate_COO_TS	-1	1	-684.462142	-429504.66	-684.406818	-429469.95						
25	diMeacetoacetamid_anion	-1	1	-439.990113	-276096.12	-439.941627	-276065.69	6.708	12.631	-4.360	2.173	-11.068	-10.458
	diMeacetoacetamid_COO	-1	1	-628.629793	-394469.33	-628.574022	-394434.33						
	diMeacetoacetamid_COO_TS	-1	1	-628.620354	-394463.41	-628.563611	-394427.80						
26	3-oxo-3-pyrrolidin-1-yl-propionitrile_anion	-1	1	-457.016137	-286780.11	-456.969833	-286751.06	6.628	11.773	-4.910	1.433	-11.538	-10.340
	3-oxo-3-pyrrolidin-1-yl-propionitrile_COO	-1	1	-645.655945	-405153.40	-645.603105	-405120.25						
	3-oxo-3-pyrrolidin-1-yl-propionitrile_COO_TS	-1	1	-645.647746	-405148.26	-645.592997	-405113.90						
27	calcone_DA	-2	1	-654.198454	-410513.91	-654.142435	-410478.76	-14.222	7.531	-25.142	-2.351	-10.919	-9.882
	calcone_COO	-2	1	-842.871489	-528908.05	-842.807948	-528868.18						
	calcone_COO_TS	-2	1	-842.836823	-528886.30	-842.771629	-528845.39						
28	flavone_DA	-2	1	-728.246328	-456979.66	-728.191484	-456945.25	-14.667	8.012	-26.931	-2.356	-12.263	-10.367
	flavone_COO	-2	1	-916.920072	-575374.25	-916.859848	-575336.46						
	flavone_COO_TS	-2	1	-916.883931	-575351.57	-916.820685	-575311.88						

F. MARCUS FITTING

ΔG^0 and $\Delta G^{\ddagger}$ data for the carbanion series were evaluated by the Marcus model for group transfer in bimolecular reactions.

$$\Delta G^{\ddagger} = \Delta G_0^{\ddagger} + 0.5 \cdot \Delta G^0 + \{(\Delta G^0)^2/(16 \cdot \Delta G_0^{\ddagger})\} \qquad \text{(eq. 3 in the main manuscript)}$$

The data fitting gives values of $\Delta G_0^{\ddagger}$ of 14.2±0.4 kcalmol^{-1} which are similar to the ones obtained with the linear fitting showed in Figure 2A in the main text: $\Delta G_0^{\ddagger}$= 12.7±0.3 kcalmol^{-1}; obtained with the same by ωb97XD/aug-cc-pvtz//ωb97XD/def2tzvp level of theory.

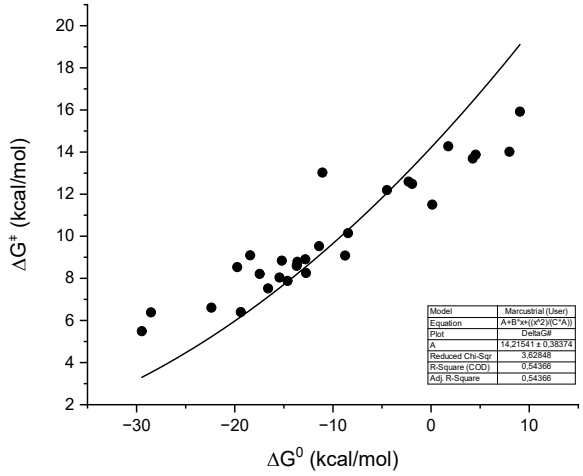


Figure S6. Quadratic fitting of calculated $\Delta G^{\ddagger}$ vs ΔG^0, according to the Marcus model for group transfer reactions (eq. 3 in the manuscript) for ωb97XD/aug-cc-pvtz//ωb97XD/def2tzvp level of theory.

G. ELECTROPHILICITY VALUES OF CO_2

Electrophilicity values of CO_2 were estimated from the Mayr-Patz equation (eq. 6 in the main text) for the carbanions with reported values of N and S_N.

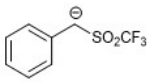
$\log k(20°C) = S_N(N + E)$ (eq. 6 in the main text)

log k(20°C) was determined from the calculated $\Delta G^{\ddagger}$ according to the Eyring equation, assuming a unitary transmission coefficient:

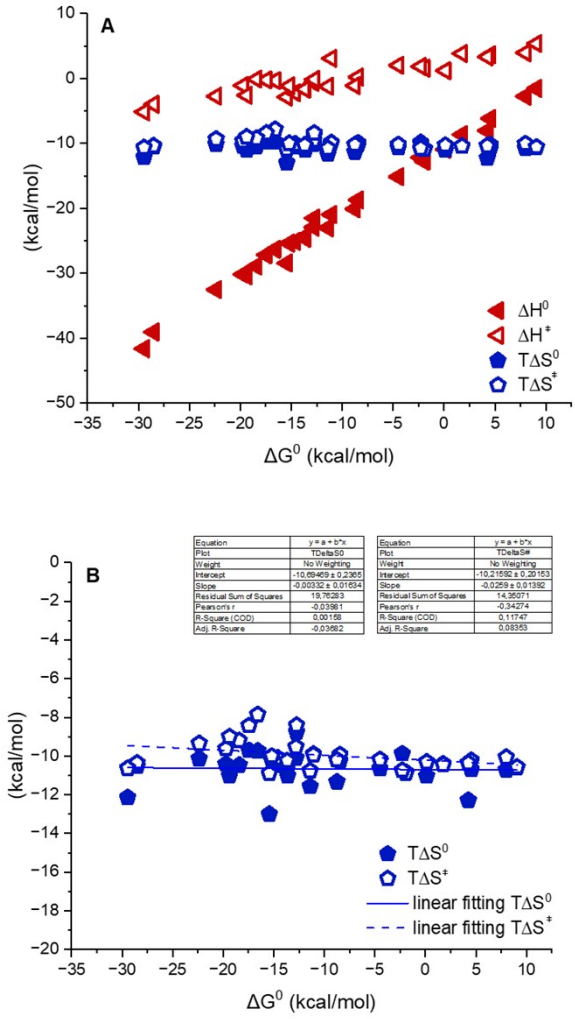
$k = (k_B T/\hbar) \times \exp(-\Delta G^{\ddagger}/RT)$, and rearranging:

$\log k(20°C) = 12.78 - \Delta G^{\ddagger}/(2.303 \times 0.582)$

Table S8. $\Delta G^{\ddagger}$, log k(20°C) and electrophilicity of CO_2.

Carbanion	N	S_N	$\Delta G^{\ddagger}$ (kcalmol^{-1})	log k(20°C)	E(CO_2)	Ref
R_2^-	24.16	0.68	12.2	3.67	-18.8	this work
R_2^-	24.16	0.68	/	5.32	-16.33	Experimental From ref. [1]
R_2^-	24.16	0.68	7.93	6.86	-14.07	b3lyp-D3/6-311+G(d,p) From ref. [1]
R_3^-	19.36	0.67	14.0	2.33	-15.9	this work
R_3^-	19.36	0.67	11.18	4.44	-12.73	b3lyp-D3/6-311+G(d,p) From ref. [1]
R_{17}^-	16.55	0.78	15.9	0.91	-15.4	this work
R_{23}^-	18.82	0.69	13.9	2.41	-15.3	this work
R_{24}^-	20.22	0.65	13.7	2.56	-16.3	this work
	18.67	0.68	8.38	6.53	-9.1	b3lyp-D3/6-311+G(d,p) From ref. [1]

H. ENTHALPIC AND ENTROPIC CONTRIBUTIONS



Equation	y = a + b*x
Plot	TDeltaS0
Weight	No Weighting
Intercept	-10,69469 ± 0,2365
Slope	-0,00332 ± 0,01634
Residual Sum of Squares	19,76283
Pearson's r	-0,03981
R-Square (COD)	0,00158
Adj. R-Square	-0,03682

Equation	y = a + b*x
Plot	TDeltaS‡
Weight	No Weighting
Intercept	-10,21592 ± 0,20153
Slope	-0,0259 ± 0,01392
Residual Sum of Squares	14,35071
Pearson's r	-0,34274
R-Square (COD)	0,11747
Adj. R-Square	0,08353

Figure S7. A) Dependence of enthalpic (ΔH^0 and $\Delta H^{\ddagger}$, red symbols) and entropic ($T\Delta S^0$ and $T\Delta S^{\ddagger}$, blue symbols) respect to ΔG^0 of the carboxylation step. B) Linear fitting of the data for $T\Delta S^0$ and $T\Delta S^{\ddagger}$ give slope of 0.00±0.01 and and intercept of -0.03±0.01 $kcalmol^{-1}$ respectively.

I. $\Delta E^{\ddagger}$ DISTORTION: DIFFERENCE BETWEEN CARBANION AND CO_2 DISTORTION AT THE TRANSITION STATE

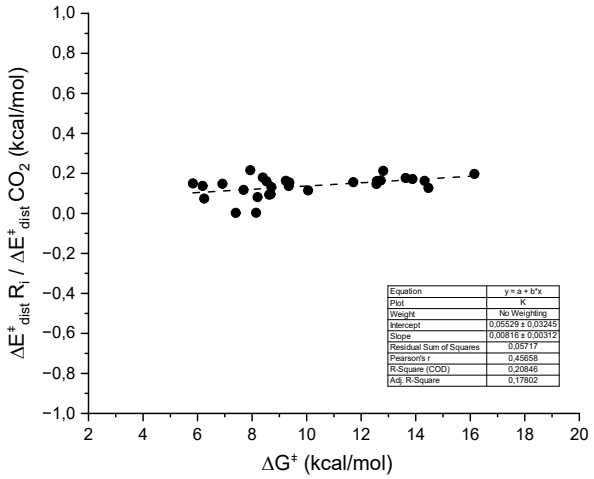


Figure S8. $\Delta E_{distortion}^{\ddagger}$ ratio between carbanion and CO_2 (SPE calculated at transition state geometries) respect to $\Delta G^{\ddagger}$ of the carboxylation step.

L. $\Delta E^{\ddagger}$ DISTORTION: ENERGY TABLES

Table S9. Potential energy of activation ($\Delta E^{\ddagger}$) values calculated considering the electronic energies of CO_2, R_i^- and R_i-TSs, obtained at ωb97XD/ def2tzvp//ωb97XD/def2tzvp level of theory.

	wb97xd/def2tzvp				(kcal/mol)			
i	species	charge	mult.	E (hartree)	E	ΔE distortion total	ΔE distortion anion	ΔE distortion CO_2
	CO_2	0	1	-188.608	-118353			
1	cyclopentadiene_anion	-1	1	-193.614	-121494	23.0163	2.599333	20.417
	cyclopentadiene_distorted	-1	1	-193.609	-121492			
	distorted CO_2	0	1	-188.575	-118333			
2	indene_anion	-1	1	-347.264	-217911	17.81098	2.280872	15.530
	indene_distorted	-1	1	-347.26	-217909			
	distorted CO_2	0	1	-188.583	-118338			
3	malonitrile_anion	-1	1	-224.519	-140888	17.68184	2.472388	15.209
	malonitrile_distorted	-1	1	-224.515	-140886			
	distorted CO_2	0	1	-188.584	-118338			
4	acetylene_anion	-1	1	-76.8211	-48206	7.940193	0.021273	7.919
	acetylene_distorted	-1	1	-76.821	-48205.9			
	distorted CO_2	0	1	-188.595	-118345			
5	phenylacethylene_anion	-1	1	-307.881	-193199	8.100145	0.023406	8.077
	phenylacetylene_distorted	-1	1	-307.881	-193199			
	distorted CO_2	0	1	-188.595	-118345			
6	diphenylmethane_anion	-1	1	-502.088	-315065	8.74786	1.126191	7.622
	diphenylmethane_distorted	-1	1	-502.087	-315064			
	distorted CO_2	0	1	-188.596	-118346			
7	pCNtoluene_anion	-1	1	-363.29	-227968	9.63974	1.121109	8.519
	pCNtoluene_distorted	-1	1	-363.289	-227967			
	distorted CO_2	0	1	-188.594	-118345			
8	pCOPhtoluene_anion	-1	1	-615.44	-386194	11.20757	1.570343	9.637
	pCOPhtoluene_distorted	-1	1	-615.437	-386193			
	distorted CO_2	0	1	-188.593	-118344			
9	pNO2toluene_anion	-1	1	-475.586	-298435	14.83157	2.598894	12.233
	pNO2toluene_distorted	-1	1	-475.582	-298432			
	distorted CO_2	0	1	-188.588	-118341			
10	acetone_anion	-1	1	-192.66	-120896	10.03639	0.857743	9.179
	acetone_distorted	-1	1	-192.659	-120895			
	distorted CO_2	0	1	-188.593	-118344			
11	dimethylpentanone_anion	-1	1	-349.911	-219573	8.423187	1.495606	6.928
	dimethylpentanone_distorted	-1	1	-349.909	-219571			
	distorted CO_2	0	1	-188.597	-118346			
12	cyclobutanone_anion	-1	1	-230.735	-144788	8.582951	0.900476	7.682
	cyclobutanone_distorted	-1	1	-230.734	-144788			
	distorted CO_2	0	1	-188.596	-118346			
13	cyclohexanone_anion	-1	1	-309.399	-194151	9.784004	1.351844	8.432
	cyclohexanone_distorted	-1	1	-309.397	-194150			
	distorted CO_2	0	1	-188.595	-118345			
14	acetophenone_anion	-1	1	-384.398	-241213	10.49184	0.787274	9.705
	acetophenone_distorted	-1	1	-384.396	-241212			
	distorted CO_2	0	1	-188.592	-118344			
15	pCNacetophenone_anion	-1	1	-476.648	-299101	12.11614	1.244916	10.871
	pCNacetophenone_distorted	-1	1	-476.646	-299100			
	distorted CO_2	0	1	-188.591	-118342			
16	pNMe2acetophenone_anion	-1	1	-518.375	-325285	9.573663	0.838165	8.735
	pNMe2acetophenone_distorted	-1	1	-518.373	-325284			
	distorted CO_2	0	1	-188.594	-118345			
17	Benzoylacetonitrile_anion	-1	1	-476.676	-299119	20.95926	3.456135	17.503
	Benzoylacetonitrile_distorted	-1	1	-476.67	-299115			
	distorted CO_2	0	1	-188.58	-118336			
18	Phbenzylketone_anion	-1	1	-615.464	-386209	16.84311	2.380018	14.463
	Phbenzylketone_distorted	-1	1	-615.46	-386207			
	distorted CO_2	0	1	-188.585	-118339			
19	2-Facetophenone_anion	-1	1	-483.644	-303491	8.708578	1.324422	7.384
	2-Facetophenone_distorted	-1	1	-483.642	-303490			
	distorted CO_2	0	1	-188.596	-118346			
20	phepropanone_anion	-1	1	-423.712	-265883	10.82661	1.451743	9.375
	phepropanone_distorted	-1	1	-423.71	-265882			
	distorted CO_2	0	1	-188.593	-118344			
21	acetic acid tert-butyl ester_anion	-1	1	-385.849	-242124	7.187432	0.492972	6.694
	acetic acid tert-butyl ester_distorted	-1	1	-385.848	-242123			
	distorted CO_2	0	1	-188.597	-118347			
22	^{t}BuPhenylacetate_anion	-1	1	-616.917	-387121	12.2055	1.465486	10.740
	^{t}BuPhenylacetate_distorted	-1	1	-616.914	-387120			
	distorted CO_2	0	1	-188.591	-118343			
23	Etacetoacetate_anion	-1	1	-459.908	-288596	18.89193	2.773404	16.119
	Etacetoacetate_distorted	-1	1	-459.903	-288594			
	distorted CO_2	0	1	-188.582	-118341			
24	diMemalonate_anion	-1	1	-495.825	-311145	17.87589	2.685515	15.190
	diMemalonate_distorted	-1	1	-495.821	-311142			
	diMemalonate_COO_TS	0	1	-188.583	-118338			
25	diMeacetoacetamid_anion	-1	1	-440.019	-276116	16.42488	2.281939	14.143
	diMeacetoacetamid_distorted	-1	1	-440.016	-276114			
	distorted CO_2	0	1	-188.585	-118339			
26	3-oxo-3-pyrrolidin-1-yl-propionitrile_anion	-1	1	-457.041	-286797	14.60987	1.972388	12.637
	3-oxo-3-pyrrolidin-1-yl-propionitrile_dist	-1	1	-457.037	-286795			
	distorted CO_2	0	1	-188.588	-118341			
27	calcone_DA	-2	1	-654.217	-410527	5.284133	0.637487	4.647
	calcone_distorted	-2	1	-654.216	-410527			
	distorted CO_2	0	1	-188.601	-118349			
28	flavone_DA	-2	1	-728.24	-456978	4.536141	0.591051	3.945
	flavone_distorted	-2	1	-728.24	-456977			
	distorted CO_2	0	1	-188.602	-118349			

M. O-C-O ANGLE DISTORTION AND C-C DISTANCE IN THE TRANSITION STATE

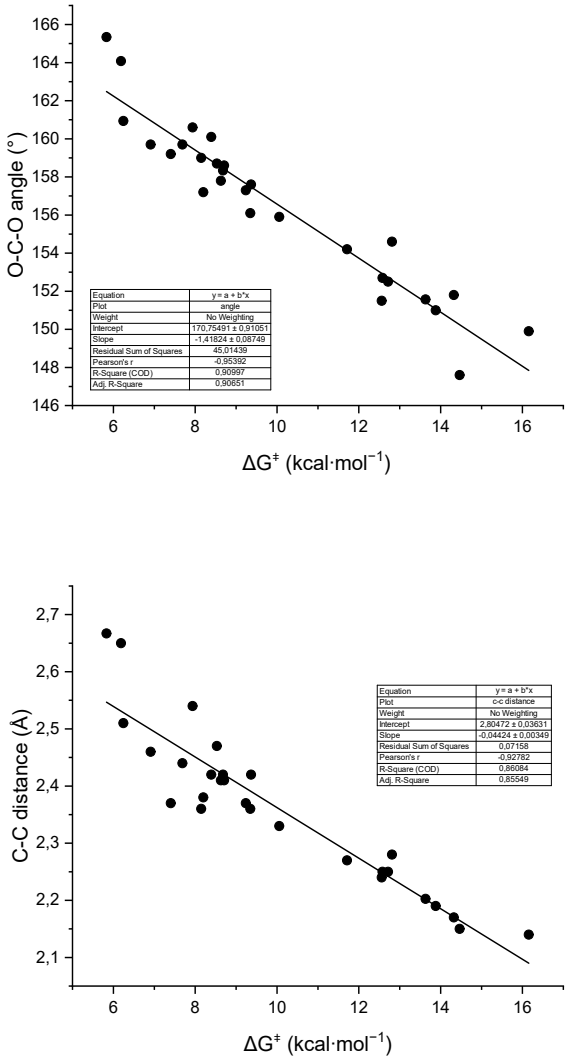


Figure S9. Dependence of O-C-O angle (bending of CO_2, panel A) and of C-C distance (formation of the new C-C bond between $\mathbf{R_i}^-$ and CO_2, panel B) in the transition state with respect to $\Delta G^{\ddagger}$ of the carboxylation reaction. Linear fittings of the data give slope values of -1.41±0.09° for the O-C-O angle and to a concomitant reduction of the C-C distance with a slope value of -0.044±0.003.

N. OPTIMIZED GEOMETRIES

28 organic molecules (R_i-H) were considered for the linear correlations. The carbon atom which is considered to attack the CO_2 from the anion $\mathbf{R_i^-}$ is evidenced.

$$R_i^- + CO_2 \rightleftharpoons R_i\text{-}COO^- \qquad \Delta G^0, \Delta G^{\ddagger}$$

N.1 B3LYP/6-311G(D,P)

CO_2			
	0 1 C 0.00000000 0.00000000 0.00003100 O 0.00000000 0.00000000 1.16031300 O 0.00000000 0.00000000 -1.16033700		
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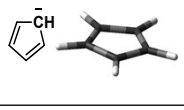
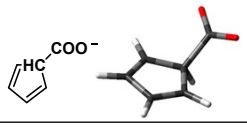
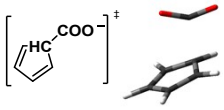
1			
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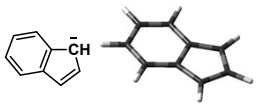
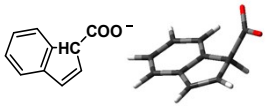
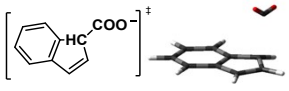
2			
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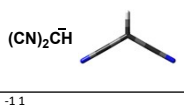
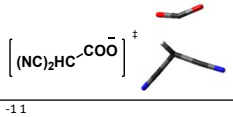
3			
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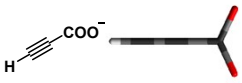
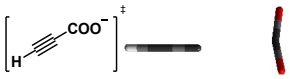
4			
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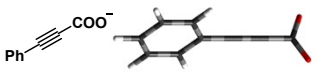
5			
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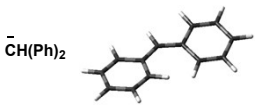
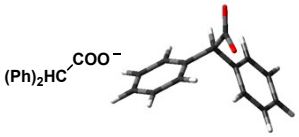
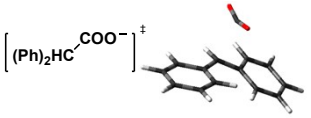
6			
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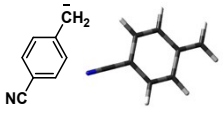
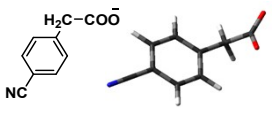
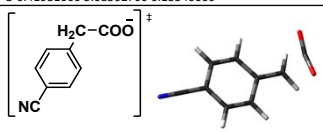
7			
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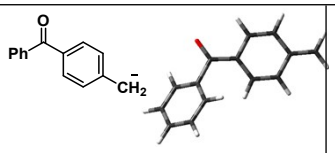
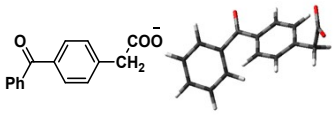
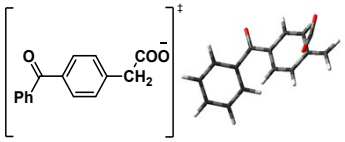
8			
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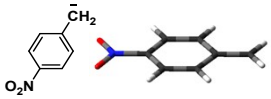
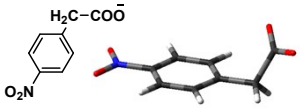
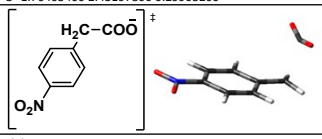
9			
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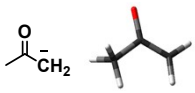
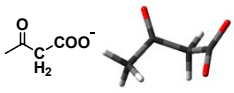
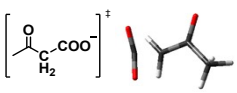
10			
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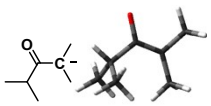
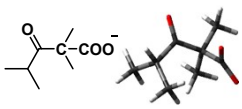
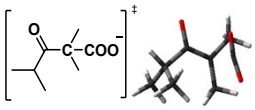
11			
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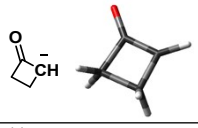
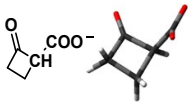
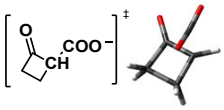
12			
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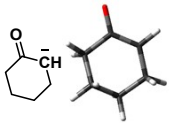
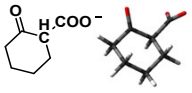
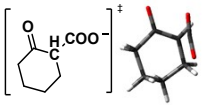
13			
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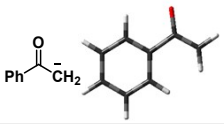
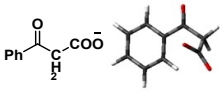
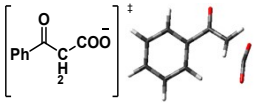
14			
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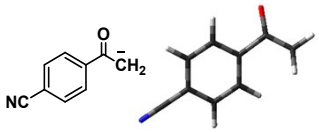
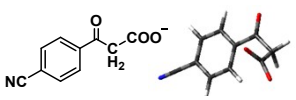
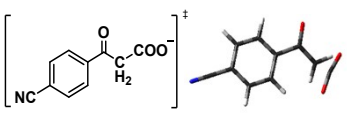
15			

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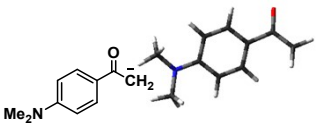
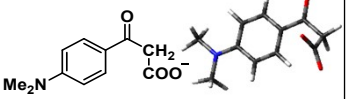
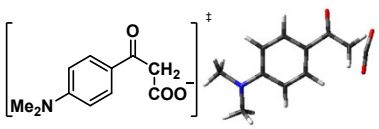
16			
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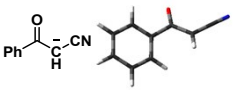
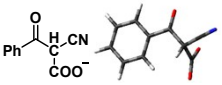
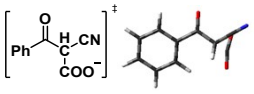
17			
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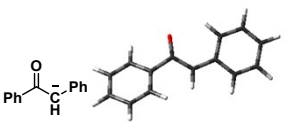
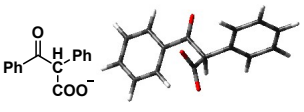
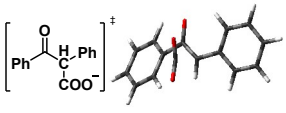
18			

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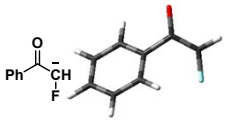
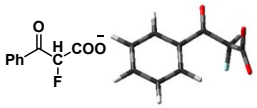
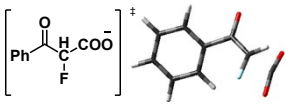
19			
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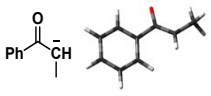
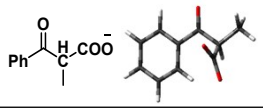
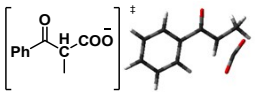
20			
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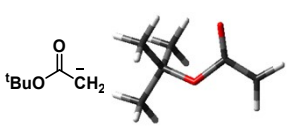
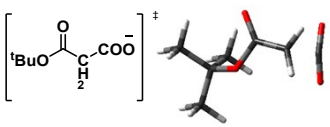
21			
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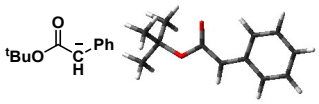
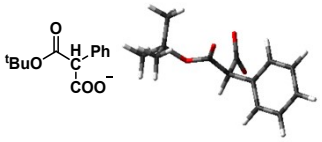
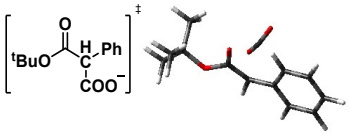
22			
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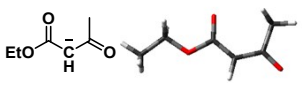
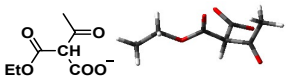
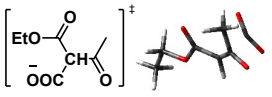
23 c_1			
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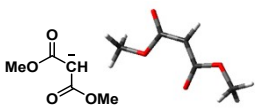
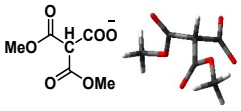
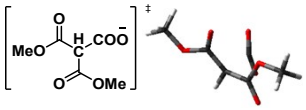
24 c_2			
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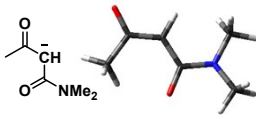
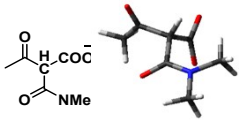
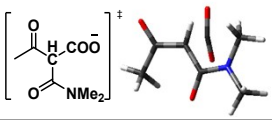
25 c_1			
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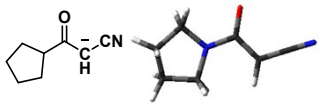
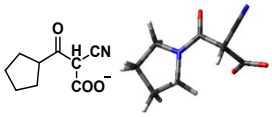
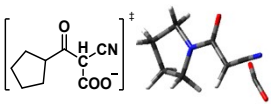
26			
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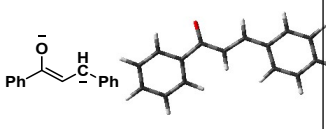
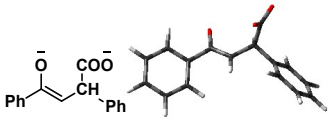
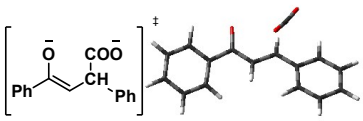
27			

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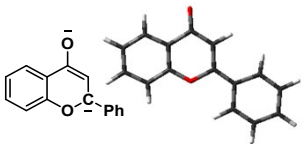
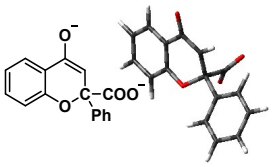
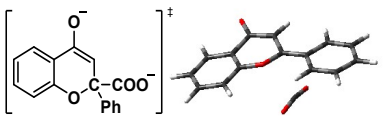
28			
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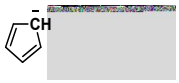
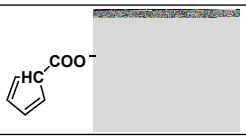
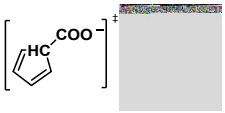
1			
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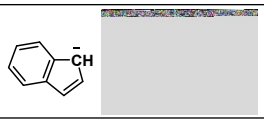
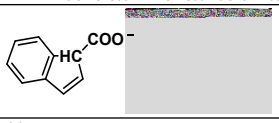
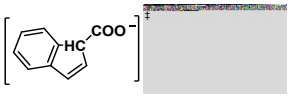
2			
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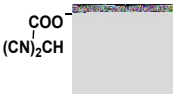
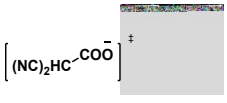
3			
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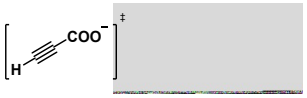
4			
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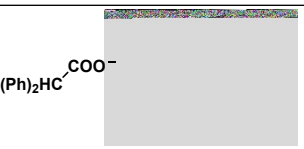
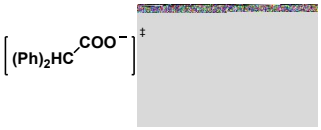
6			
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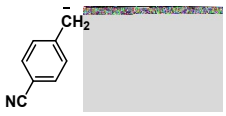
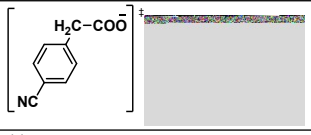
7			
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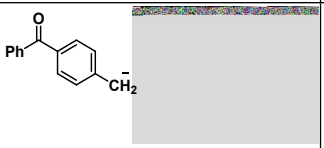
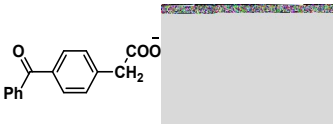
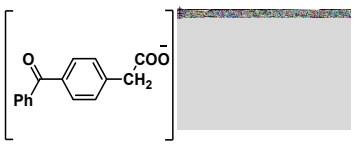
8			
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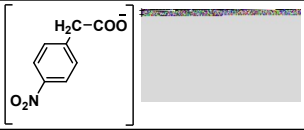
9			
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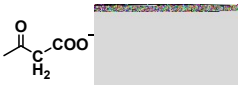
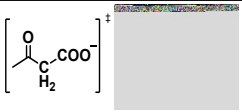
10			
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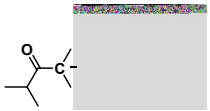
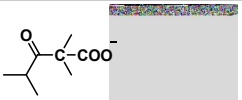
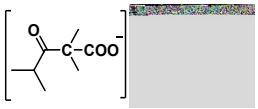
11			
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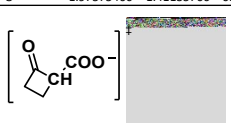
12			

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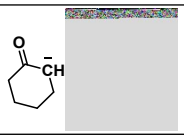
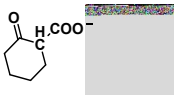
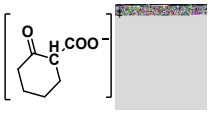
13			
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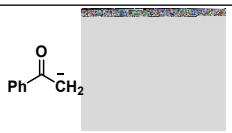
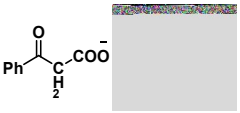
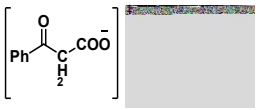
14			
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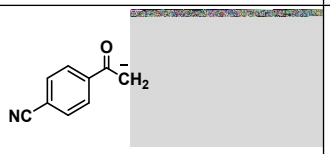
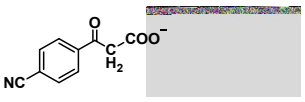
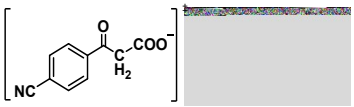
15			
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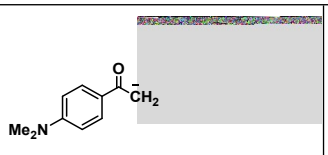

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C	3.41334300	1.24363400	0.02882500
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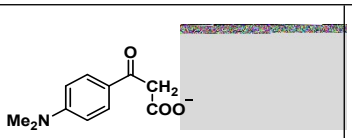

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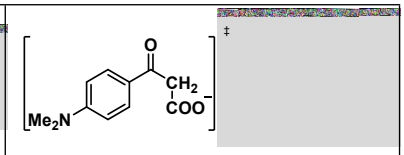
C	0.59729100	0.71151900	-0.27086200
C	-0.38082000	1.65378500	0.05398300
C	0.17822700	-0.60410200	-0.47788900
C	-1.70920200	1.31436600	0.16642000
H	-0.07714900	2.67965600	0.22031300
C	-1.14633100	-0.96865200	-0.36515200
H	0.90036200	-1.37375000	-0.72102800
C	-2.13555900	-0.01671600	-0.04016700
H	-2.42453600	2.08345500	0.41787100
H	-1.41517500	-2.00150100	-0.52954000
O	2.34906100	2.27762300	-0.13844300
C	3.03429800	0.09560900	-0.78156200
H	2.72322600	-0.42056900	-1.68956300
H	3.96957100	0.61928200	-0.98516000
C	3.31580800	-0.95081500	0.33580000
O	3.34066500	-0.51541800	1.50525400
O	3.51663800	-2.12325800	-0.04125900
C	-3.85337900	-1.73961100	-0.12755000
H	-3.61001100	-2.09185800	-1.13441800
H	-3.37682600	-2.41111200	0.59333700
H	-4.92916700	-1.81533400	0.00299600
C	-4.43893000	0.62896500	0.41587200
H	-4.24104700	1.07682700	1.39459600
H	-4.48063700	1.43266600	-0.32531900
H	-5.41700400	0.15778600	0.45396500
N	-3.44635100	-0.36543000	0.07032800



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C	-0.07112400	0.59461900	0.69583600
C	1.26652900	0.91991800	0.55587300
C	2.20149000	-0.02570300	0.09893500
H	2.36751500	-2.05959900	-0.61965600
H	0.00108100	-2.57851500	-0.37197700
H	-0.74860900	1.36565100	1.03930800
H	1.58073700	1.92396400	0.80240800
C	-2.01470800	-1.08046400	0.51433200
C	-2.88201200	-0.25213800	1.22173100
H	-3.88368400	-0.61479300	1.42395500
H	-2.51086300	0.54215500	1.85331100
O	-2.35783600	-2.15479700	-0.05480300
C	-3.55071000	1.15353900	-0.62869800
O	-4.22503100	0.41363200	-1.23782400
O	-3.01746900	2.15857200	-0.34207100
N	3.54422200	0.27697600	-0.00387300
C	3.96239500	1.65668200	0.10710000
H	3.69647700	2.07109700	1.08153600
H	5.04481400	1.70848900	0.01538100
H	3.51971000	2.29712000	-0.66724400
C	4.41213500	-0.62745000	-0.72486800
H	4.11291300	-0.75467100	-1.77363500
H	5.42735200	-0.23824700	-0.70408600
H	4.43001600	-1.61355900	-0.25649600

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-1 1

C	-2.73442200	0.96306600	0.26805000
C	-1.36566300	1.16828500	0.19250700
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C	-1.03200200	-1.16400700	-0.23278600
C	-2.40253500	-1.37155400	-0.17011100
C	-3.25841700	-0.30968900	0.08564200
H	-3.39512900	1.79798300	0.46701800
H	-0.95030800	2.15946500	0.32016000
H	-0.37930800	-2.00033200	-0.44884900
H	-2.80317800	-2.36549900	-0.32674000
H	-4.32783500	-0.47205600	0.13702200
C	0.98852200	0.39724600	-0.12747200
C	1.86291400	-0.63823100	0.22857500
H	1.50686000	-1.59307400	0.58381900
O	1.33897200	1.54281600	-0.48668700
C	3.24603700	-0.44925400	0.17554700
N	4.39709000	-0.29929500	0.13391400

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C	-3.34652100	-0.85438100	0.34662500
C	-2.02434700	-1.25756200	0.37622200
C	-1.01740400	-0.41446300	-0.09368400
C	-1.35707500	0.84224200	-0.59219200
C	-2.68312500	1.24540700	-0.61902600
C	-3.67781400	0.39919800	-0.15268500
H	-4.12141600	-1.51534400	0.71275900
H	-1.75319400	-2.23040000	0.76381000
H	-0.59456500	1.52343500	-0.94566200
H	-2.93869100	2.22356300	-1.00503200
H	-4.71278300	0.71612500	-0.17660900
C	0.39014800	-0.90706500	-0.03925200
C	1.48054200	0.02670500	-0.54032100
H	1.20626000	0.46944300	-1.49621700
O	0.66005800	-1.99791100	0.40931500
C	1.69697800	1.22037900	0.52461500
O	1.65380100	2.35715100	0.04391300
O	1.87748100	0.83689500	1.68532900
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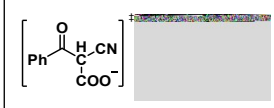

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C	-1.39798300	0.83960900	-0.59914500
C	-2.72390800	1.24360500	-0.64288500
C	-3.72371200	0.41041400	-0.16226500
H	-4.16644300	-1.48264400	0.74760100
H	-1.79419000	-2.18531000	0.84221300
H	-0.63192800	1.51051900	-0.96399400
H	-2.97596400	2.21354300	-1.05258500
H	-4.75889800	0.72555800	-0.20121000
C	0.36652700	-0.89542600	0.02082300
C	1.37691700	-0.18338700	-0.72256000
H	1.07098700	0.40298600	-1.57728100
O	0.62445500	-1.85437700	0.74695200
C	1.88234900	1.39019000	0.63273500
O	1.63702700	2.38201800	0.02842900
O	2.28112400	0.86060900	1.61462300
C	2.62069900	-0.83632400	-0.89034000
N	3.65341800	-1.33978900	-1.01508000

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-1 1

C	-4.22550600	-0.74277100	0.46481700
C	-2.88191200	-1.07685600	0.38641700
C	-1.93133600	-0.15556500	-0.05168500
C	-2.37754500	1.10894400	-0.43685400
C	-3.72238800	1.44501200	-0.37158200
C	-4.65326300	0.52256800	0.08584100
H	-4.94281700	-1.47293900	0.82038400
H	-2.54697400	-2.06806500	0.66427100
H	-1.66889600	1.83645900	-0.81227100
H	-4.04523000	2.43017100	-0.68639700
H	-5.70270900	0.78482900	0.13876900
C	-0.47638000	-0.58652000	-0.11582600
C	0.48045100	0.40207800	0.06905000
H	0.13048800	1.40697300	0.27091400
O	-0.26720600	-1.82128400	-0.30816500
C	1.91536500	0.24294200	0.05235000
C	2.73827200	1.36562900	0.28784900
C	2.58030000	-0.97715500	-0.19022300
C	4.11797500	1.28031500	0.28231300
H	2.26721900	2.32469600	0.47829800
C	3.96538300	-1.05514800	-0.19475700
H	1.97998200	-1.85642000	-0.37354300
C	4.75181400	0.06492400	0.04021900
H	4.70806700	2.17081900	0.46842500
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H	5.83243200	-0.00439800	0.03512300

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C	4.20213000	-1.36449600	0.19367600
C	2.84307800	-1.46558200	0.43369700
C	1.96836700	-0.47111600	-0.00077900
C	2.48330600	0.63134300	-0.68064500
C	3.84546400	0.73579600	-0.91704300
C	4.70633300	-0.26145600	-0.48314600
H	4.87069100	-2.14491800	0.53413500
H	2.44009700	-2.31952000	0.96180400
H	1.83093000	1.42449400	-1.02115000
H	4.23460000	1.59882300	-1.44180800
H	5.76946700	-0.17957200	-0.67134900
C	0.50306000	-0.63780500	0.28462200
O	0.11881400	-1.58517700	0.93597300
C	-1.88977800	-0.02897700	-0.26565100
C	-2.54420900	-0.28410100	-1.46676100
C	-2.60462000	-0.17049500	0.92231000
C	-3.87769700	-0.67124400	-1.48703500
H	-2.00426300	-0.17693500	-2.40068400
C	-3.93544600	-0.55680500	0.90609200
H	-2.10859500	0.03209500	1.86238300
C	-4.57842200	-0.80975400	-0.29902000
H	-4.36769100	-0.86264300	-2.43378000
H	-4.47523500	-0.66017800	1.83951500
H	-5.61867100	-1.11032800	-0.31012900
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H	-0.15885500	0.60448700	-1.30658200
C	-0.27957200	1.75784400	0.51494800
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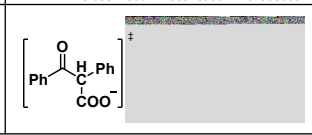
O	-0.45040700	2.79414700	-0.15252100



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C	2.48808800	0.78894100	-0.56289400
C	3.83323400	0.98043500	-0.84291300
C	4.74152800	-0.05229600	-0.65696200
H	4.99501900	-2.08853100	-0.02834400
H	2.59790000	-2.40541900	0.50257700
H	1.79945000	1.61148000	-0.70360200
H	4.17341300	1.94263000	-1.20575900
H	5.79054800	0.09694000	-0.88061900
C	0.57459600	-0.71392300	0.26057900
C	-0.40571600	0.10604300	-0.34687400
H	-0.05947700	0.72161700	-1.16603700
O	0.34927200	-1.63637700	1.06733100
C	-0.43167600	1.75723500	1.17508900
O	-0.22551900	2.71287600	0.50844300
O	-0.67507700	1.23150800	2.20239600
C	-1.83553800	-0.18257200	-0.39592100
C	-2.62566600	0.48445900	-1.34877700
C	-2.49698000	-1.06940100	0.46908300
C	-3.99130000	0.28062700	-1.43673100
H	-2.14645000	1.17747100	-2.03216500
C	-3.86644000	-1.27313700	0.37519500
H	-1.91590900	-1.59610800	1.21077500
C	-4.62736000	-0.60387500	-0.57304900
H	-4.56439500	0.81395600	-2.18634100
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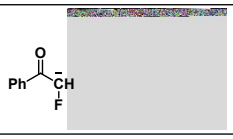

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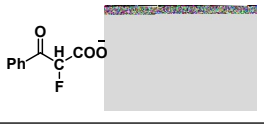
C	0.51122800	-0.99587500	-0.50030400
C	2.26723600	0.91716500	0.46159100
H	0.52956500	2.16052400	0.67705200
C	1.87078300	-1.27001400	-0.43442600
H	-0.16643600	-1.74648500	-0.88493000
C	2.75458500	-0.31765400	0.05285400
H	2.94826900	1.66966400	0.84113500
H	2.24146400	-2.23127000	-0.76999200
H	3.81469300	-0.53270500	0.10748800
O	-1.72174100	1.81699700	-0.54977900
C	-2.40438000	-0.30200800	0.13426500
H	-3.46954400	-0.11813300	0.11613500
F	-2.10343300	-1.57664800	0.59769200



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C	-0.45721300	1.15270000	0.17914500
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C	2.00653800	1.13438100	-0.08395600
C	0.88424600	-0.98876900	0.08825400
C	3.22115900	0.48586400	-0.21394500
H	1.95458200	2.21504800	-0.09932800
C	2.10149800	-1.63673800	-0.05340100
H	-0.01987500	-1.57130200	0.20518600
C	3.26928000	-0.90264500	-0.20065500
H	4.13178500	1.05993500	-0.32703400
H	2.13798400	-2.71843600	-0.04643700
H	4.21908400	-1.41194600	-0.30497800
O	-0.52293200	2.33387900	-0.08397900
C	-1.71339700	0.41381700	0.61894900
H	-2.46128300	1.16623300	0.87346600
C	-2.28938600	-0.47418200	-0.52757600
O	-2.43441200	0.14032500	-1.60029100
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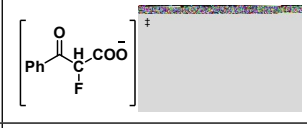

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C	-0.98598900	-0.99746100	0.00110800
C	-2.21853500	-1.58888800	-0.23821600
C	-3.35685200	-0.80658500	-0.37288700
H	-4.13420600	1.19427800	-0.38451000
H	-1.92514000	2.24108600	-0.00084100
H	-0.10531600	-1.61676500	0.10171000
H	-2.28909700	-2.66658500	-0.32281200
H	-4.31888100	-1.26974500	-0.55431000
C	0.44365500	1.10032100	0.31355700
C	1.43615500	0.50070800	1.07197600
H	2.29683700	1.05522800	1.42372600
O	0.60837000	2.21758400	-0.25322200
C	2.65394300	-0.54633000	-0.74180100
O	3.01510700	0.37787900	-1.36228400
O	2.51899100	-1.65900900	-0.39945200
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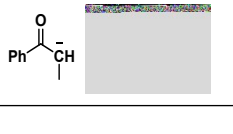

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C	3.00936000	-0.25403800	0.08461900
C	2.17948700	-1.33964800	-0.16371600
C	0.80419400	-1.16991600	-0.23229100
H	0.62453900	2.14699300	0.29126500
H	3.08069800	1.86023500	0.44330200
H	4.08314400	-0.38584400	0.13696400
H	2.60664800	-2.32423500	-0.31399000
H	0.17646500	-2.02603300	-0.44631600
C	-1.27506200	0.33433700	-0.11543100
C	-2.11746200	-0.68979300	0.22404000
H	-1.71118000	-1.64036500	0.54540100
C	-3.60987700	-0.52474700	0.21809100
H	-3.97395100	-0.10340100	-0.72596400
H	-4.11649200	-1.48162200	0.36561000
H	-3.97050800	0.15213700	1.00515600
O	-1.64348400	1.51614100	-0.45524700

-1 1

C	0.87957000	-0.39684400	-0.11461700
C	1.95360600	-1.18581200	0.29419300
C	3.23705600	-0.66957900	0.32553500
C	3.46327800	0.64829100	-0.05096700
C	2.40145000	1.44316200	-0.45663600
C	1.11580800	0.92427900	-0.49118300
H	1.76534300	-2.21048800	0.58615000
H	4.06326300	-1.29278300	0.64340300
H	4.46664500	1.05468000	-0.02719100
H	2.57353600	2.47151300	-0.74764600
H	0.29763600	1.56164800	-0.79996000
C	-0.49211700	-1.00868300	-0.13678000
C	-2.90413700	-0.99132200	-0.85692000
H	-3.23444200	-1.47149700	0.06377600
H	-3.70696200	-0.34857400	-1.22136900
H	-2.72505400	-1.77024600	-1.59959500
O	-0.64504500	-2.15862200	0.22320100
C	-1.64879500	-0.16255800	-0.61351900
H	-1.35519000	0.33025500	-1.54145400
C	-1.95642500	0.95923200	0.43395900
O	-1.98779700	0.59722700	1.62773400
O	-2.17222500	2.10070600	-0.02024800

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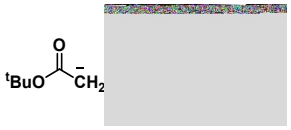
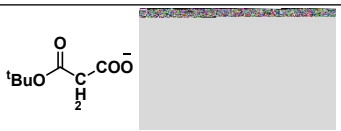
C	-0.86721700	-0.42147300	0.13456300
C	-1.83792900	-1.11002900	-0.59091700
C	-3.14865200	-0.65979000	-0.65584100
C	-3.51969200	0.50094300	0.00680300
C	-2.56432100	1.20244100	0.73072500
C	-1.25647700	0.74621900	0.79381900
H	-1.53844500	-2.01278700	-1.10647300
H	-3.88259100	-1.21743800	-1.22553800
H	-4.54132400	0.85745500	-0.04024000
H	-2.83905000	2.11339100	1.24896400
H	-0.53169200	1.32070800	1.35329800
C	0.54114000	-0.99262200	0.16751400
C	1.50751100	-0.38127900	0.95763400
H	1.20751700	0.36355200	1.68104100
C	2.84061300	-1.03945700	1.16363300
H	3.30685200	-1.28969100	0.20746700
H	3.52634700	-0.38524900	1.70725800
H	2.76653300	-1.97777400	1.72924700
C	2.05490100	1.30165700	-0.68514900
O	0.75955100	-2.01031100	-0.55142500
O	2.76408500	0.69292300	-1.39393300
O	1.47968800	2.23590900	-0.26610700

21



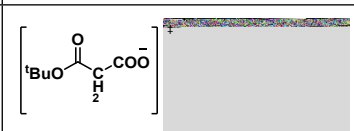
-1 1

C	1.51021100	-0.03250000	-0.12602100
O	1.54512100	-1.27621100	0.01548900
O	0.28853100	0.57686900	-0.47156700
C	-0.95853500	0.05871200	0.00663100
C	-1.36878400	-1.20748600	-0.74569600
H	-0.67415100	-2.01623500	-0.53342100
H	-2.37804200	-1.50702500	-0.45248900
H	-1.36852400	-1.01798700	-1.82149000
C	-1.95716700	1.17265900	-0.29602000
H	-1.97260500	1.38732900	-1.36626800
H	-2.96257000	0.87860800	0.01118300
H	-1.68432400	2.08586000	0.23591800
C	-0.90796300	-0.18820100	1.51278400
H	-0.20514300	-0.98563900	1.74756400
H	-0.59726300	0.72031700	2.03317300
H	-1.89725500	-0.47048600	1.87855400
C	2.54075100	0.87486800	-0.02767200
H	2.36931700	1.93457100	-0.15558100
H	3.55026300	0.51711100	0.12744000



-1 1

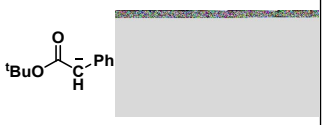
C	-0.33255300	0.81955300	-0.08577300
O	-0.05555100	1.63735200	0.76145100
C	-1.68470700	0.69577900	-0.72125500
H	-1.59326200	0.37275600	-1.75801400
H	-2.17009300	1.67111800	-0.70440700
O	0.51345700	-0.08739500	-0.57173500
C	1.87592700	-0.24876300	-0.07280500
C	-2.60729300	-0.31695900	0.02020700
O	-2.13439000	-0.90387200	1.01368100
O	-3.74938000	-0.43715300	-0.46453100
C	2.68963000	1.01219600	-0.33551400
H	2.34837900	1.84125700	0.27969200
H	3.73791600	0.81415000	-0.10625000
H	2.61873800	1.29568400	-1.38699500
C	2.40882000	-1.40502300	-0.90702000
H	2.39677800	-1.15044400	-1.96770000
H	3.43551200	-1.62931600	-0.61589700
H	1.80155300	-2.29821400	-0.75470300
C	1.85733600	-0.62507900	1.40285800
H	1.48414200	0.19186900	2.01588200
H	1.23155000	-1.50432900	1.56186700
H	2.87272100	-0.86619900	1.72139600



-1 1

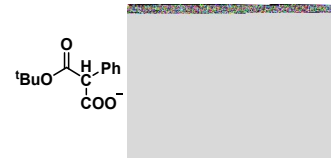
C	-0.26474600	1.13562400	-0.44557200
O	-0.04897600	1.86698700	0.53666600
C	-1.40638400	1.08858700	-1.23961100
H	-1.41331100	0.49349200	-2.14156400
H	-2.12213200	1.89548600	-1.14863900
O	0.69869600	0.21320200	-0.85186700
C	1.68183600	-0.30568200	0.05695500
C	-2.53931900	-0.62825300	0.20077200
O	-2.86598700	0.04175300	1.10084400
O	-2.39786000	-1.56373200	-0.48684800
C	2.72903300	0.74734600	0.41601300
H	2.28357700	1.54774900	1.00070900
H	3.53666000	0.28633900	0.98947000
H	3.15755900	1.17303200	-0.49395300
C	2.34304000	-1.42992500	-0.73479300
H	2.79198700	-1.03790900	-1.64926800
H	3.12672900	-1.90309800	-0.14052000
H	1.60763800	-2.18873000	-1.00755300
C	1.01841100	-0.88102500	1.30610700
H	0.53300600	-0.09625200	1.88283600
H	0.27264300	-1.62781700	1.02522400
H	1.76743800	-1.36800400	1.93367900

22



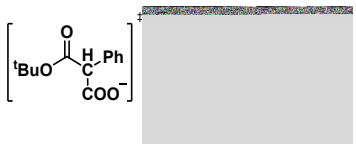
-1 1

C	-3.10209500	-0.07977900	0.00003000
C	-4.04619900	-1.27908200	0.00007100
H	-3.88095200	-1.89493200	0.88587300
H	-5.08468400	-0.94370500	0.00018800
H	-3.88112600	-1.89486400	-0.88580900
C	-3.33326400	0.74809900	-1.26286200
H	-4.37590900	1.07028800	-1.30669200
H	-2.68974500	1.62398100	-1.27628500
H	-3.12629300	0.14393000	-2.14880300
C	-3.33312200	0.74806800	1.26295000
H	-3.12619300	0.14386400	2.14887600
H	-2.68954000	1.62390300	1.27636800
H	-4.37573600	1.07036300	1.30683400
O	-1.80010100	-0.68410600	-0.00006700
C	-0.62418900	0.05923400	-0.00008000
O	-0.66828400	1.29929900	-0.00015100
C	0.49439600	-0.78010300	-0.00003100
H	0.30174500	-1.84588300	-0.00001500
C	1.86666800	-0.36861900	-0.00000200
C	2.88788600	-1.35042500	-0.00002100
C	2.31046700	0.97522400	0.00005300
C	4.22981100	-1.02184100	-0.00001200
H	2.59951900	-2.39700800	-0.00004500
C	3.65934100	1.29423200	0.00006500
H	1.56804000	1.76036200	0.00007900
C	4.63972500	0.30924900	0.00002300
H	4.96979800	-1.81510600	-0.00003000
H	3.95054400	2.33962600	0.00010300
H	5.69106200	0.56810000	0.00000600



-1 1

C	3.11974600	-0.53082800	0.08153200
C	4.10205500	0.08805700	1.06566800
H	3.85870100	-0.20684100	2.08727000
H	5.11410900	-0.24892300	0.83916000
H	4.07550500	1.17648700	0.99983800
C	3.43351100	-0.07543700	-1.33734400
H	4.45245400	-0.37329500	-1.58934800
H	2.75175300	-0.52076700	-2.05793900
H	3.36716800	1.01108200	-1.40952800
C	3.12070200	-2.04830300	0.21487800
H	2.82404600	-2.33906500	1.22404400
H	2.44553100	-2.51104200	-0.50099600
H	4.13020400	-2.42149600	0.03565500
O	1.83628100	0.01318200	0.51652000
C	0.68878900	-0.25731800	-0.10407900
O	0.57097100	-1.01156800	-1.03821700
C	-0.43279000	0.52501400	0.54614900
H	-0.25508800	0.51868400	1.62091400
C	-0.37132500	2.02693300	0.08809600
O	-0.88768200	2.84183700	0.87431200
O	0.15623100	2.25601200	-1.01806300
C	-1.79599900	-0.05709500	0.27020700
C	-2.52369900	-0.65250600	1.29500700
C	-2.36143200	-0.00306100	-1.00237200
C	-3.78498900	-1.18433200	1.05973700
H	-2.09928500	-0.70042300	2.29133100
C	-3.61903700	-0.53328400	-1.24138600
H	-1.80726800	0.46419600	-1.80629700
C	-4.33649500	-1.12769700	-0.21074700
H	-4.33546900	-1.64257100	1.87214800
H	-4.04333900	-0.48154600	-2.23663900
H	-5.31963300	-1.54104900	-0.39810100



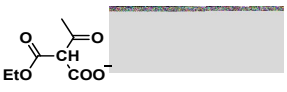
-1 1

C	3.12664900	-0.43933200	0.18775700
C	4.06398400	0.17023200	1.22471000
H	3.95147700	-0.33662500	2.18458500
H	5.10097100	0.07065400	0.90039600
H	3.84313000	1.22976900	1.36342500
C	3.26478500	0.30991200	-1.13464400
H	4.29774900	0.25263700	-1.48291500
H	2.61449800	-0.11444200	-1.89630800
H	3.00963000	1.36274600	-0.99720000
C	3.43372900	-1.92652100	0.03079000
H	3.27114800	-2.44371800	0.97864800
H	2.80003900	-2.37723900	-0.72838000
H	4.48035600	-2.05602500	-0.25279000
O	1.82015200	-0.22808600	0.75865900
C	0.66199200	-0.52654500	0.07546000
O	0.67980700	-1.25055000	-0.92111900
C	-0.45154200	0.11716900	0.66940600
H	-0.25348500	0.59571500	1.61925500
C	-0.15601900	2.09635300	-0.57427400
O	-0.59397500	1.81434400	-1.62727500
O	0.33179700	2.79731800	0.23551100
C	-1.83646000	-0.21677800	0.41211400
C	-2.82477600	0.22364800	1.31514400
C	-2.28912200	-0.92756300	-0.71466100
C	-4.16910000	-0.02907900	1.11181900
H	-2.51596800	0.77737300	2.19581800
C	-3.63861500	-1.18120400	-0.91170100
H	-1.56136000	-1.27450700	-1.43325200
C	-4.59423100	-0.73809100	-0.00712400
H	-4.89397500	0.32836100	1.83456000
H	-3.94810800	-1.73347500	-1.79234800
H	-5.64600400	-0.93863400	-0.16848000

23 c_1

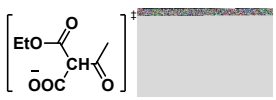
-1 1

C	0.19403000	0.21135000	0.00130000
O	0.17802500	1.44148700	0.00356600
O	1.40498300	-0.44497500	-0.00079900
C	2.57238900	0.36438200	0.00275700
H	2.57508300	1.01650200	-0.87426900
H	2.57654900	1.00629700	0.88735400
C	-2.25576300	-0.38795400	-0.00069900
O	-3.14710100	-1.26758300	0.00222200
C	-2.70423200	1.06446500	-0.00508000
H	-2.29292400	1.60138000	-0.86043800
H	-3.79289300	1.09676600	-0.03562000
H	-2.34617600	1.58613100	0.88371500
C	3.77390800	-0.55271100	-0.00360300
H	3.77722900	-1.18436800	-0.89329800
H	4.69062100	0.03903500	-0.00014200
H	3.77796500	-1.19590500	0.87777400
C	-0.88425700	-0.70595900	0.00075200
H	-0.62915900	-1.75870200	0.00244100



-1 1

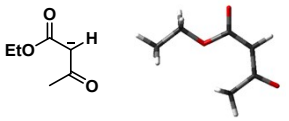
C	-0.57313900	-0.40540000	0.26809400
O	-0.57557600	-0.97485300	1.33285700
C	0.64538200	0.05626200	-0.48219200
H	0.39009900	0.17037500	-1.53510500
O	-1.68514800	-0.09172800	-0.39436300
C	-2.93193800	-0.38955600	0.25324100
H	-2.98285400	-1.46252600	0.44378800
H	-2.95851500	0.12769500	1.21353500
C	1.09407800	1.49002900	0.02414800
O	0.29697000	2.09849000	0.75418000
O	2.20787000	1.84919500	-0.39228900
C	1.83168900	-0.88676800	-0.40651400
O	2.31500800	-1.33321700	-1.42346100
C	2.39680800	-1.22920600	0.94368300
H	1.78013000	-2.01373300	1.38575500
H	3.41721000	-1.59035900	0.83291200
H	2.36234200	-0.37654200	1.62039200
C	-4.04434600	0.06796400	-0.65651200
H	-4.00680600	-0.45557300	-1.61240500
H	-5.00566700	-0.14313000	-0.18689800
H	-3.98012800	1.14075000	-0.84107200



-1 1

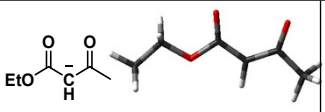
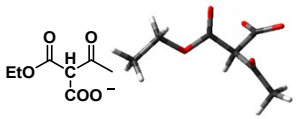
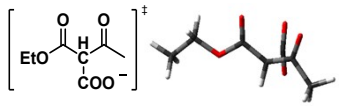
C	-0.56174000	-0.61757500	0.06384700
O	-0.62105400	-1.35306400	1.03434800
C	0.60468600	-0.15715300	-0.64600200
H	0.39785000	0.31662700	-1.59645200
O	-1.69198500	-0.07794500	-0.46835300
C	-2.92483900	-0.40753400	0.16818100
H	-3.06839100	-1.49005200	0.14604000
H	-2.88752000	-0.09901200	1.21513000
C	1.06751500	1.68293900	0.44618900
O	0.84469500	1.45785700	1.58669800
O	1.41522500	2.41603100	-0.41551900
C	1.90055500	-0.77098400	-0.55810100
O	2.75628400	-0.58611300	-1.43261900
C	2.25764800	-1.62002400	0.64169300
H	1.72154200	-2.56963600	0.59632500
H	3.33020800	-1.80842300	0.63638300
H	1.95808900	-1.13707600	1.57073600
C	-4.03182900	0.30475100	-0.57223400
H	-4.06828600	-0.01066100	-1.61592500
H	-4.99192200	0.07185100	-0.10972500
H	-3.88886600	1.38573300	-0.54039800

23 c_2



-1 1

C	-0.16473200	1.07302800	-0.00002200
O	-0.74452200	2.16232200	-0.00007800
O	-0.90187100	-0.07522800	0.00003900
C	-2.31663600	0.06241100	-0.00015000
H	-2.63419000	0.62504000	0.88094000
H	-2.63392700	0.62536100	-0.88112400
C	2.03538400	-0.26006400	0.00024500
O	3.28747600	-0.20132200	0.00009100
C	1.41259400	-1.64876400	0.00035800
H	0.77786600	-1.79796600	-0.87360000
H	2.21276600	-2.38772000	0.00049300
H	0.77773300	-1.79778500	0.87424600
C	-2.91252000	-1.32653500	-0.00048300
H	-2.60197600	-1.88349900	0.88489900
H	-4.00166600	-1.26133100	-0.00059600
H	-2.60176900	-1.88315700	-0.88600800

	C 1.24340000 0.90558900 0.00010300 H 1.79155400 1.84088800 0.00002500		
23 c_3			
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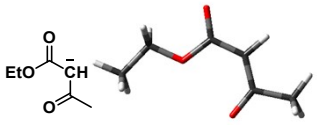
23 c_4			
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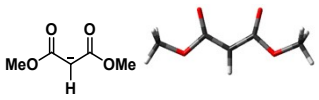
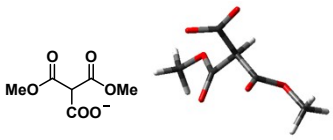
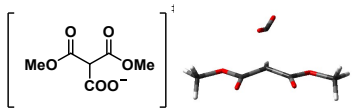
24 c_1			
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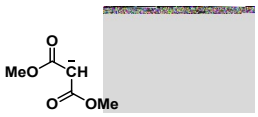
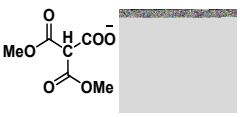
24 c_2



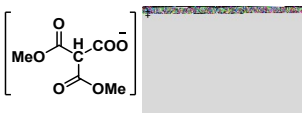
-1 1

C	1.12876200	-0.04467700	0.00012900
O	1.12277100	-1.27310900	0.00045200
O	2.34347500	0.61691300	-0.00028100
C	3.49740600	-0.19969700	-0.00018400
H	4.34783000	0.48011300	-0.00106000
H	3.54016400	-0.83542800	0.88649100
H	3.53937000	-0.83680400	-0.88587800
C	-1.32337200	0.61327300	0.00015000
O	-2.20994500	1.47303700	0.00013900
O	-1.67285300	-0.70573400	0.00001100
C	-3.06107900	-0.98431900	-0.00030700
H	-3.14696900	-2.06950900	-0.00001200
H	-3.55208200	-0.57797500	0.88571200
H	-3.55150800	-0.57861500	-0.88698900
C	0.06336400	0.88195400	0.00008400
H	0.32511700	1.93015600	-0.00005800



-1 1

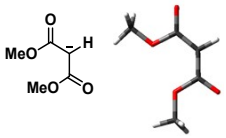
C	1.16799600	-0.52530700	-0.00821400
O	1.04945900	-1.34575600	-0.88346000
C	0.05776100	0.28899900	0.60309300
H	0.29123600	0.46142500	1.65194700
O	2.33551700	-0.21478400	0.55274000
C	3.48987500	-0.85543500	0.00964900
H	4.33326100	-0.47744700	0.58002800
H	3.41462200	-1.93686500	0.11866800
H	3.60346700	-0.60371100	-1.04434400
C	-0.05791300	1.70900600	-0.08232600
O	0.72806400	1.94780800	-1.01176600
O	-0.93701500	2.43431800	0.41146000
C	-1.27277300	-0.42338200	0.56103600
O	-1.80932500	-0.90887600	1.52696000
O	-1.79906400	-0.44580000	-0.65736700
C	-3.06201800	-1.09665900	-0.79643400
H	-3.31996100	-1.01793400	-1.84835100
H	-2.98646200	-2.14313600	-0.50290200
H	-3.81481600	-0.60093800	-0.18440700



-1 1

C	-1.13227600	-0.64517100	-0.12362300
O	-1.12942900	-1.43439500	0.80311900
C	-0.03717800	0.07235700	-0.71925700
H	-0.26771000	0.54319900	-1.66401800
O	-2.30660800	-0.28644900	-0.72034000
C	-3.48533100	-0.85831000	-0.17668800
H	-4.30945900	-0.46008000	-0.76434000
H	-3.46901500	-1.94635800	-0.25374000
H	-3.61085600	-0.58072500	0.87092600
C	-0.02230700	1.94969900	0.45235900
O	-0.51849900	1.68254100	1.49146500
O	0.47690200	2.71529900	-0.29733000
C	1.34972600	-0.29130500	-0.60325400
O	2.21860700	0.06796200	-1.38787500
O	1.66632800	-1.03042200	0.48290200
C	3.03632100	-1.37193900	0.63312900
H	3.09466100	-1.96915000	1.54021500
H	3.39388000	-1.95461600	-0.21680200
H	3.65636600	-0.48055100	0.73622700

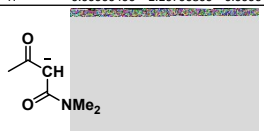
24 c_3



-1 1

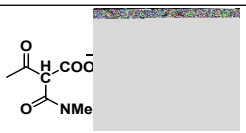
C	1.29128400	-0.60969200	-0.00257400
O	2.34351100	-1.25658200	-0.02936000
O	1.35245800	0.75327700	0.03379100
C	2.64940900	1.32024600	0.00952900
H	2.50357600	2.39850900	0.04341100
H	3.24286700	1.00332100	0.86871800
H	3.18658100	1.05236900	-0.90199900
C	-1.29128200	-0.60968600	0.00261900
O	-2.34351800	-1.25657000	0.02920500
O	-1.35245000	0.75328200	-0.03364800
C	-2.64941100	1.32023800	-0.00961700
H	-2.50355800	2.39852600	-0.04263600
H	-3.24242200	1.00395800	-0.86935800
H	-3.18705200	1.05167700	0.90142500
C	0.00000000	-1.18587200	0.00012400
H	-0.00000400	-2.26700800	0.00004800

25 c_1



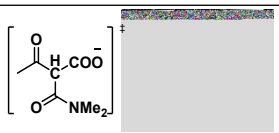
-1 1

C	0.44166300	-0.36633400	-0.00494200
O	0.30360500	-1.60705800	0.03751200
C	-2.00632000	0.31940900	0.03070200
O	-2.86409100	1.22853000	0.16346500
C	-2.53619100	-1.09008800	-0.17151800
H	-2.55614200	-1.61691400	0.78609600
H	-3.55702200	-1.02604000	-0.54949300
H	-1.91024800	-1.67806700	-0.83852900
C	2.02211200	1.55650800	-0.14895900
H	1.89623300	2.03431900	0.83127400
H	3.05913700	1.69412300	-0.45627100
H	1.39225300	2.07859100	-0.86865900
N	1.73215300	0.14160400	-0.12695700
C	2.86182600	-0.71391200	0.15355300
H	3.29354900	-0.50156700	1.14052100
H	2.53765400	-1.74933300	0.12938100
H	3.64605800	-0.56871100	-0.59413500
C	-0.62640300	0.58436200	0.06150400
H	-0.38277400	1.63092600	0.17865600



-1 1

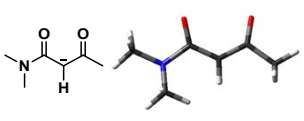
C	0.70802900	-0.67853000	-0.04913100
O	0.55177000	-1.70880900	-0.70168600
C	-0.48776500	0.08645500	0.49111000
H	-0.34813500	0.29380400	1.55135700
C	-0.73220200	1.44687200	-0.25046200
O	-0.18404000	1.59379000	-1.35730800
O	-1.48403400	2.23684900	0.35113200
C	-1.73384100	-0.78648100	0.40043700
O	-2.15218300	-1.35381300	1.38525600
C	-2.44010900	-0.87529500	-0.92154200
H	-1.72184500	-1.02430900	-1.72567200
H	-3.17282000	-1.67905000	-0.90236000
H	-2.95057900	0.07381000	-1.10474700
C	2.20319000	1.08890600	0.84568400
H	3.01084300	0.98977200	1.57257100
H	2.50648600	1.81119300	0.08292900
H	1.33291100	1.48227900	1.36000700
N	1.93782600	-0.20392100	0.24897900
C	3.10194200	-0.87190000	-0.29792500
H	3.90804200	-0.84748600	0.43622300
H	2.85563300	-1.90265000	-0.53182600
H	3.44711400	-0.37420800	-1.20951700



-1 1

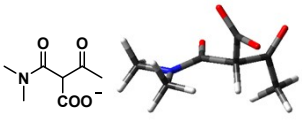
C	-0.78274700	-0.67541400	0.02468500
O	-0.76414500	-1.63890400	0.80462300
C	0.39786400	-0.12710200	-0.62203300
H	0.23678300	0.48868300	-1.49555400
C	0.94242600	1.55749700	0.76892200
O	1.32864900	2.38416700	0.01892300
O	0.68542900	1.15933200	1.84994200
C	1.68661100	-0.74862900	-0.62344700
O	2.54247000	-0.44837800	-1.47320800
C	2.06696900	-1.75262000	0.44383100
H	1.57977700	-2.70736100	0.23953800
H	3.14830300	-1.88704000	0.43039700
H	1.72872000	-1.43863600	1.42960000
C	-2.10670300	1.09154000	-1.12771300
H	-2.04915500	0.81057800	-2.18524200
H	-3.07826200	1.55393300	-0.95639000
H	-1.34467200	1.84368000	-0.92780400
N	-1.97831500	-0.04645500	-0.24295700
C	-3.21877800	-0.62305100	0.22345400
H	-3.84609600	-0.93379000	-0.61878600
H	-2.99745700	-1.48923300	0.83857200
H	-3.78281200	0.10131000	0.81793300

25 c_2



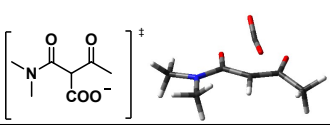
-1 1

C	0.52038100	-0.44268200	0.00320000
O	0.52727500	-1.68653000	-0.03738300
C	-1.99160500	-0.05649200	0.01156800
O	-2.42309000	-1.21938900	0.17933500
C	-3.05408700	1.03432100	-0.13429300
H	-2.64057700	2.03426300	-0.26854600
H	-3.68921800	0.79870500	-0.99178600
H	-3.69429000	1.03296700	0.75111100
C	1.86654800	1.65596300	0.13180500



-1 1

C	0.65471400	-0.63018100	0.18793100
O	0.49135100	-1.52754000	1.01168300
C	-1.79321600	-0.71591600	-0.09530100
O	-2.58216200	-0.40201700	0.76363000
C	-2.01314500	-1.91694900	-0.97360400
H	-1.08846900	-2.47971900	-1.10143300
H	-2.79153800	-2.55503900	-0.56089600
H	-2.32187100	-1.56549000	-1.96206200
C	2.16685300	0.89829500	-1.04984900



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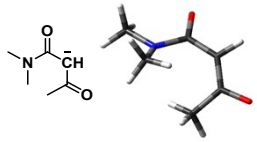
C	-0.85936800	-0.66917400	-0.12995100
O	-0.95631000	-1.55480800	-0.98662300
C	1.64175400	-0.93730000	0.34505300
O	1.94355000	-1.79377100	-0.49328700
C	2.70264400	-0.54582600	1.36849500
H	2.68225800	-1.27098200	2.18658300
H	3.68963700	-0.58950200	0.90786100
H	2.53785500	0.44506500	1.79078100
C	-2.00014700	1.00726500	1.32277400

	H 2.88255000 1.91100200 0.43403000 H 1.68140000 2.11900600 -0.84578500 H 1.18560600 2.10094800 0.85702800 N 1.74134900 0.21709400 0.10506100 C 2.96736600 -0.50695300 -0.13631500 H 3.70068300 -0.29473100 0.64687300 H 2.75370400 -1.57105600 -0.14200000 H 3.41358300 -0.23045300 -1.09995500 C -0.65747100 0.37975800 -0.05031500 H -0.52314900 1.44355700 -0.16590700	H 1.27700700 1.27542400 -1.54235200 H 2.57839000 1.69863100 -0.42837300 H 2.89991900 0.64329300 -1.81686600 N 1.88316500 -0.27386300 -0.24741100 C 3.04773800 -0.90360200 0.34283500 H 3.44677100 -0.30006100 1.16396700 H 2.78059800 -1.88372200 0.72503100 H 3.82164600 -1.00828400 -0.41812000 C -0.54298200 0.10572200 -0.39210600 H -0.45598600 0.16367000 -1.47879000 C -0.67728100 1.55553800 0.17178300 O -1.30775200 2.34909300 -0.55273400 O -0.14952700 1.77682600 1.27762600	H -1.22893100 1.75774700 1.15480500 H -2.96327000 1.51592000 1.30204100 H -1.86514300 0.58474600 2.32491200 N -1.99522400 -0.00558900 0.28793300 C -3.29528700 -0.47973000 -0.13051400 H -3.90051900 0.34944700 -0.50559600 H -3.16825900 -1.21288500 -0.92043100 H -3.83457600 -0.94575800 0.70198500 C 0.39862700 -0.23683000 0.46749700 H 0.32092300 0.33990700 1.37569400 C 0.96294400 1.51638300 -0.79447700 O 1.26035500 2.33259900 0.00886700 O 0.80110500 1.15806700 -1.90738700
25 c_3			
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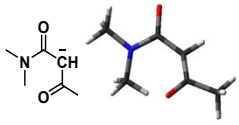
25 c_4			
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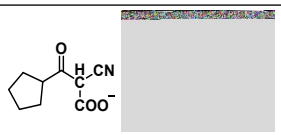
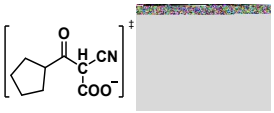
26			
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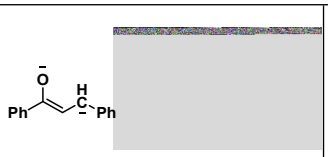
27



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C	3.96729700	1.69394500	-0.08322800
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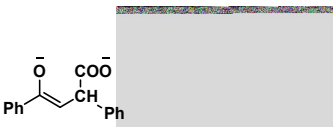
C	2.56060600	-0.33872500	0.00587900
C	3.80846700	-1.06286800	0.01379700
C	5.03340900	-0.44179200	-0.02383000
C	5.15455900	0.95677500	-0.07309400
H	4.01671000	2.77927900	-0.12082700
H	1.84528300	1.72815100	-0.05619500
H	3.76649000	-2.14833300	0.05194900
H	5.93032100	-1.05535800	-0.01462700
H	6.12247000	1.44048900	-0.10180200
C	0.03625100	-0.37521300	0.04746500
H	0.01008100	0.70667700	-0.00533700
C	-1.17541000	-1.03635700	0.08250400
O	-1.30785000	-2.33229900	0.11500300
C	-2.43464000	-0.23148300	0.03905100
C	-3.65276900	-0.90236200	-0.15815000
C	-2.51548200	1.16594700	0.19571000
C	-4.86467400	-0.22811500	-0.21869400
H	-3.61652300	-1.97845600	-0.26384900
C	-3.72210100	1.83895500	0.13712600
H	-1.61721500	1.74061200	0.38294400
C	-4.91563100	1.15069600	-0.07499000
H	-5.77987800	-0.78818600	-0.37887100
H	-3.73615800	2.91562200	0.26640300
H	-5.85953300	1.68012600	-0.11686000
C	1.33251000	-0.99703800	0.04783800
H	1.35769200	-2.08289900	0.09277200



-2 1

C	3.58918000	-1.80841800	1.00510300
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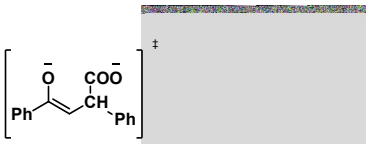
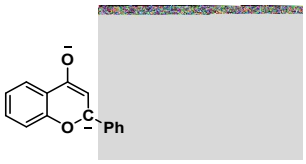
C	2.27542700	-0.16727700	-0.20058000
C	3.08270400	-0.39272100	-1.31330100
C	4.12546000	-1.31026900	-1.27519600
C	4.38375300	-2.02376000	-0.11446600
H	3.78257000	-2.35787100	1.91894600
H	1.94103600	-0.72174500	1.83965400
H	2.88883000	0.15847600	-2.22669700
H	4.73617800	-1.46723100	-2.15642900
H	5.19532000	-2.74011300	-0.08024500
C	-0.19219000	0.18915000	-0.00489900
H	-0.23895400	-0.62279200	0.70933500
C	-1.33801000	0.64517800	-0.59768100
O	-1.42702700	1.65022900	-1.39394000
C	-2.63643000	-0.06291400	-0.26317300
C	-3.83100700	0.65328400	-0.34175800
C	-2.71286800	-1.40637200	0.11179000
C	-5.04938000	0.06615800	-0.03140400
H	-3.78333200	1.68893800	-0.65346100
C	-3.92844700	-2.00125600	0.41691200
H	-1.80820000	-2.00060200	0.14982100
C	-5.10552400	-1.26668500	0.35239200
H	-5.95998800	0.65114300	-0.09011100
H	-3.95809900	-3.04742000	0.69844300
H	-6.05509600	-1.73052600	0.58993100
C	1.14186000	0.83405400	-0.24928200
H	1.13115400	1.26728600	-1.25048300
C	1.49993300	2.02144900	0.70584700
O	1.15317300	1.94548900	1.90526600
O	2.14940100	2.96188400	0.18709100



-2 1

C	3.53528600	-2.15220800	0.63773000
C	2.33205500	-1.53260400	0.35933700
C	2.24806000	-0.36005100	-0.46700800
C	3.51333600	0.08547500	-0.98260300
C	4.69977400	-0.54513200	-0.69020400
C	4.74730300	-1.68144400	0.13099000
H	3.53081300	-3.03335900	1.27367600
H	1.42661300	-1.93971100	0.79427000
H	3.52133500	0.96108800	-1.62461300
H	5.62014400	-0.15161500	-1.11254800
H	5.68333500	-2.17760100	0.35350500
C	-0.27067900	-0.14706500	-0.44940300
H	-0.36547400	-1.11311300	0.03271200
C	-1.42678400	0.56386000	-0.69157900
O	-1.46242600	1.76134800	-1.19619300
C	-2.73959900	-0.04606200	-0.30713600
C	-3.87087700	0.78009300	-0.23964700
C	-2.94157400	-1.40699300	-0.01747900
C	-5.11820900	0.28981700	0.12075500
H	-3.73864300	1.82726800	-0.47749100
C	-4.18427000	-1.89860700	0.34223100
H	-2.11378100	-2.10079400	-0.09395900
C	-5.28929900	-1.05448700	0.41916900
H	-5.96559800	0.96524500	0.16764400
H	-4.29706400	-2.95600900	0.55441300
H	-6.26230600	-1.44238300	0.69460700
C	1.05567300	0.31877700	-0.75743300
H	1.12709800	1.17345800	-1.42190300
C	1.60372700	2.12739100	1.10068800
O	1.03031000	1.64322100	1.99266100
O	2.24086700	2.83830100	0.42968800

28



-2 1

C	3.58026700	0.48491300	0.09211000
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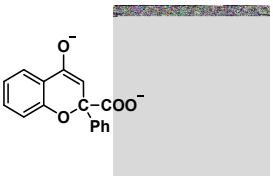
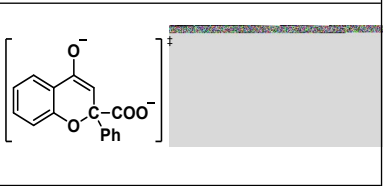
C	1.53193300	-0.74918500	-0.05739700
C	2.25496700	-1.93779200	-0.02198700
C	3.64466400	-1.91133100	0.06942800
C	4.31309700	-0.70124000	0.12897100
H	4.07666300	1.44669900	0.13107400
H	1.71776900	-2.87746300	-0.06944400
H	4.19477200	-2.84461200	0.09556200
H	5.39361300	-0.67407100	0.20103000
C	1.40817500	1.75510200	-0.04747600
O	2.04195400	2.87793000	-0.05355500
O	0.19712700	-0.85287000	-0.16591600
C	-1.97213200	0.04599700	-0.01594500
C	-2.53501100	-1.29901900	-0.05245300
C	-2.97541600	1.10145400	0.07647200
C	-3.88971000	-1.52245300	-0.01080100
H	-1.86194100	-2.14480200	-0.11482000
C	-4.31911000	0.82777200	0.11484500
H	-2.65468300	2.13579500	0.12126500
C	-4.83217200	-0.48243700	0.07202200
H	-4.23971200	-2.55192600	-0.04255100
H	-5.00980900	1.66506600	0.18430800
H	-5.89594300	-0.67841000	0.10524700
C	0.04733500	1.57596900	-0.07373100
H	-0.57585800	2.46333400	-0.09077000
C	-0.62800200	0.30046300	-0.06836800



-2 1

C	3.60507100	0.54267100	-0.48046900
C	2.21807300	0.46617200	-0.44080100
C	1.63077500	-0.77562200	-0.17683700
C	2.41639900	-1.90728600	0.01189300
C	3.79861000	-1.80484400	-0.03309300
C	4.40019800	-0.57520600	-0.27062400
H	4.04677300	1.50726500	-0.69925600
H	1.93093000	-2.85680000	0.20072300
H	4.40540600	-2.68847800	0.12437000
H	5.47961600	-0.49237600	-0.30134000
C	1.34442100	1.64288300	-0.75855500
O	1.88914700	2.68534800	-1.26454700
O	0.29154400	-0.93188700	-0.16057300
C	-1.92336800	-0.09745700	-0.16468400
C	-2.29025300	-1.33037100	-0.69425400
C	-2.91895500	0.86103200	0.02761700
C	-3.61186900	-1.59526400	-1.03331500
H	-1.53494900	-2.08748400	-0.84818000
C	-4.23680900	0.59708600	-0.30764900
H	-2.65320800	1.81554700	0.46145000
C	-4.59203400	-0.63456500	-0.84345900
H	-3.87269400	-2.56146500	-1.44860800
H	-4.99190200	1.35769600	-0.14908300
H	-5.62174200	-0.84084300	-1.10790000
C	0.01746600	1.44533200	-0.49554200
H	-0.69052100	2.24342200	-0.68120500
C	-0.48390500	0.21615900	0.21754500
C	-0.45594800	0.34291900	1.80112600
O	-0.13078900	-0.67277300	2.44753500
O	-0.80052000	1.44952200	2.26453900



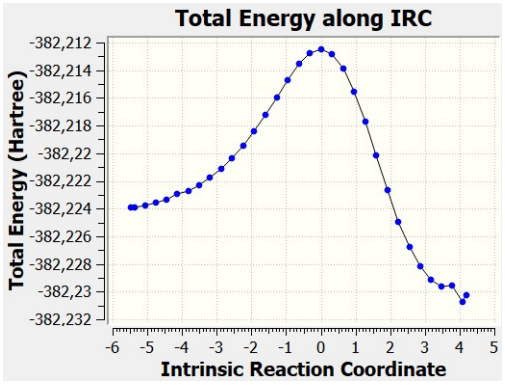
-2 1

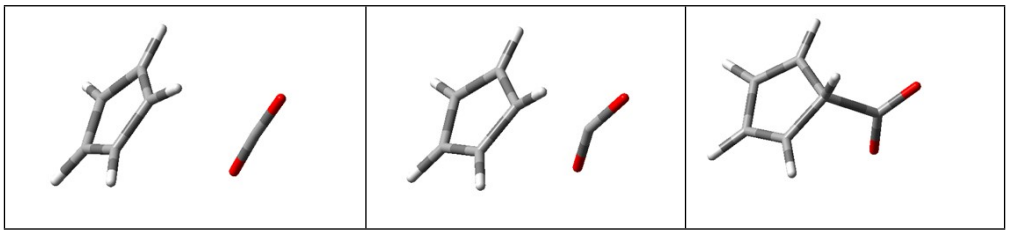
C	3.69888000	0.50395800	-0.13667000
C	2.32551300	0.49268000	-0.34421500
C	1.67855200	-0.75087700	-0.42203200
C	2.40149500	-1.93230500	-0.29328000
C	3.77656600	-1.89164200	-0.08565600
C	4.43081200	-0.67344700	-0.00296500
H	4.18627100	1.47025600	-0.09274400
H	1.87514000	-2.87688800	-0.35950500
H	4.32861500	-2.81866200	0.01463000
H	5.50117800	-0.63625300	0.15930000
C	1.53933800	1.75138900	-0.51277900
O	2.17084300	2.87246400	-0.56652000
O	0.35992000	-0.85985000	-0.66203900
C	-1.82556700	0.00326400	-0.51778400
C	-2.36023500	-1.33982000	-0.62213100
C	-2.83318500	1.04461100	-0.47841000
C	-3.71351400	-1.58565900	-0.60924900
H	-1.67157500	-2.17154900	-0.69342500
C	-4.17625100	0.75541000	-0.46874300
H	-2.52336100	2.08128200	-0.42795700
C	-4.66576600	-0.55953600	-0.52028100
H	-4.04968300	-2.61733600	-0.67812000
H	-4.88004500	1.58281100	-0.42502700
H	-5.72753800	-0.76934100	-0.51856600
C	0.18199500	1.56189600	-0.58117500
H	-0.45015600	2.43940300	-0.65981500
C	-0.47223500	0.27444300	-0.48230000
C	-0.76509100	0.11104600	2.16378400
O	-0.31878100	-0.96392600	2.23160300
O	-1.20156800	1.16678900	2.39252400

O. INTRINSIC REACTION COORDINATE (IRC) ANALYSIS

R_1^-

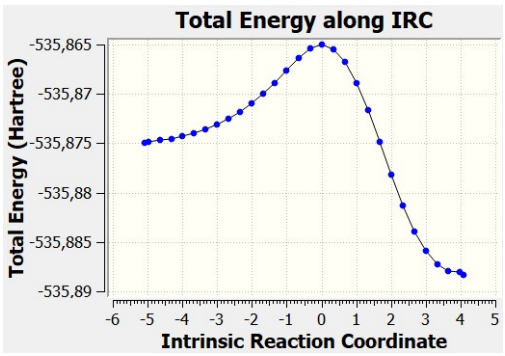
TS imaginary frequency = 410.22 cm^{-1}

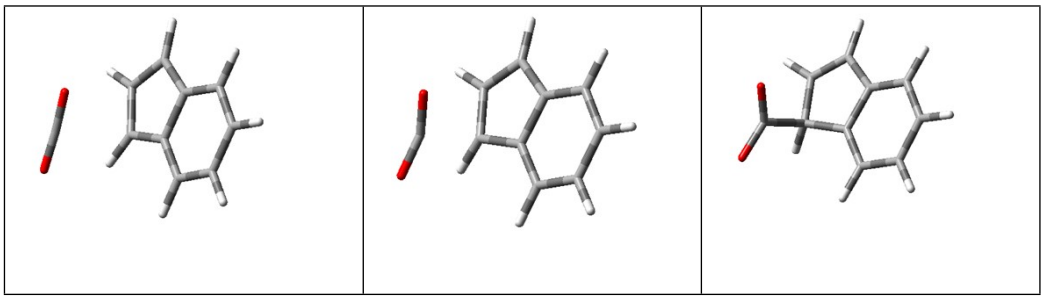




R_2^-

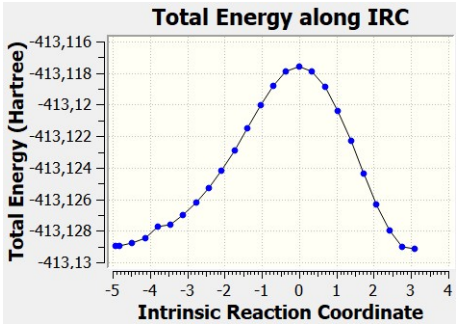
TS imaginary frequency = 438.50 cm^{-1}

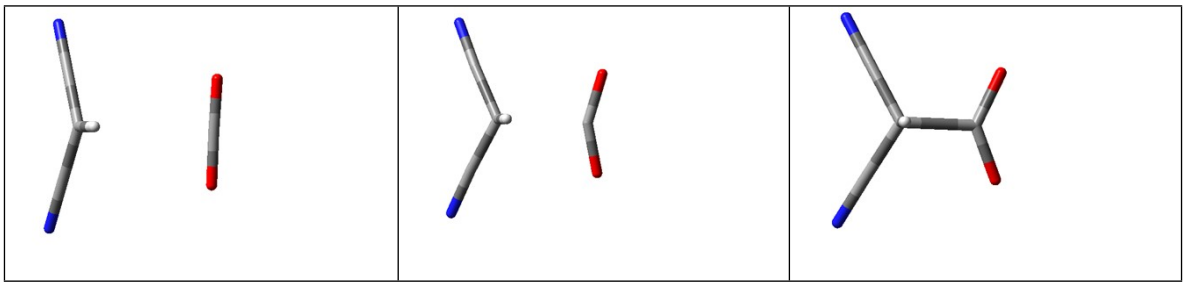




R_3^-

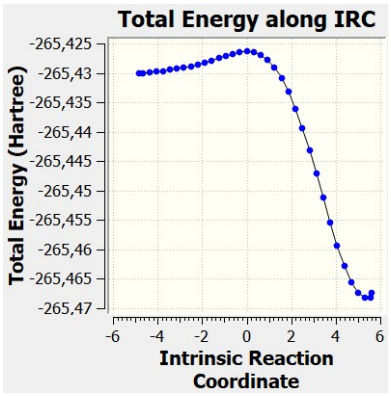
TS imaginary frequency = 384.07 cm^{-1}

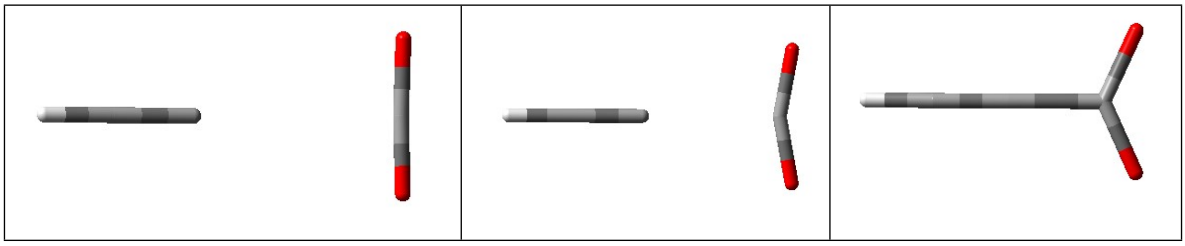




R_4^-

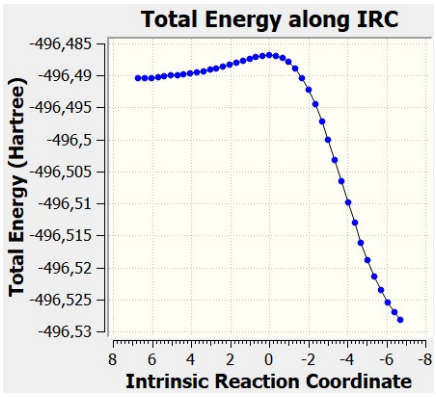
TS imaginary frequency = 247.35 cm^{-1}

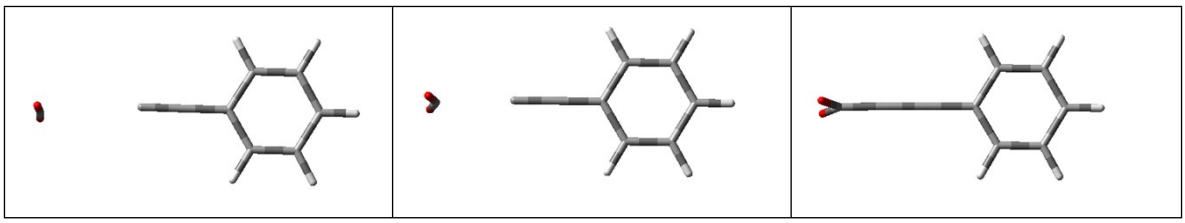




R_5^-

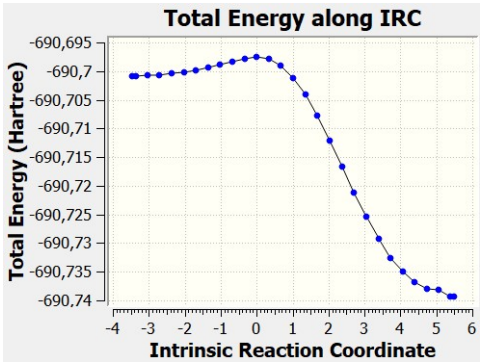
TS imaginary frequency = 197.77 cm^{-1}

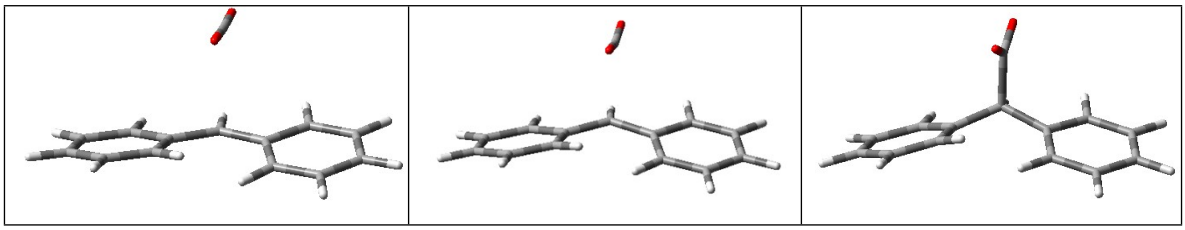




R_6^-

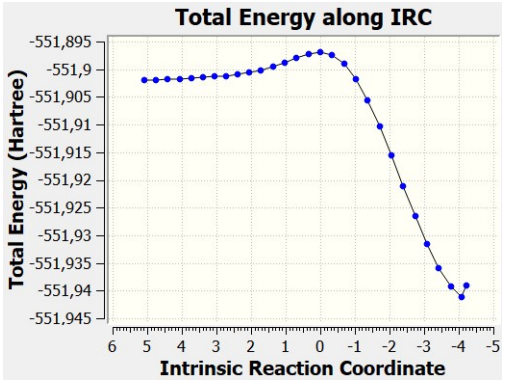
TS imaginary frequency = 362.00 cm^{-1}

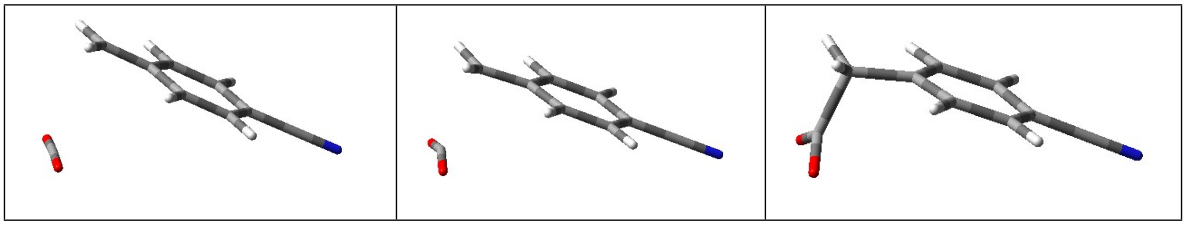




R_7^-

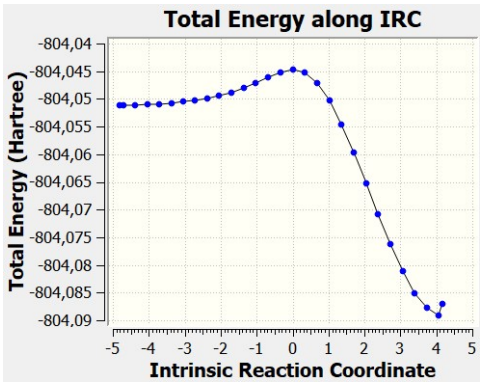
TS imaginary frequency = 426.14 cm^{-1}

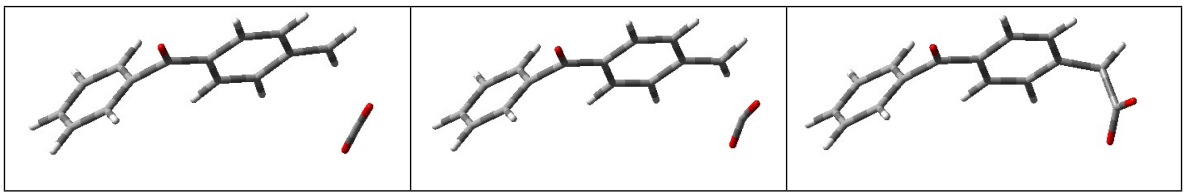




R_8^-

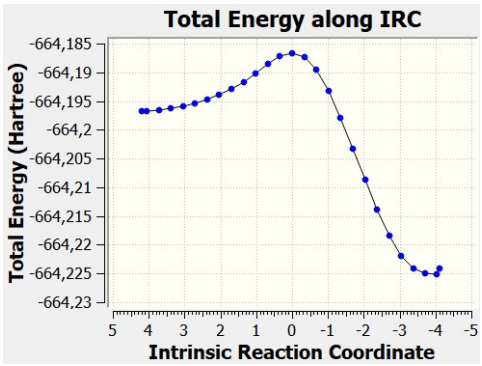
TS imaginary frequency = 477.30 cm^{-1}

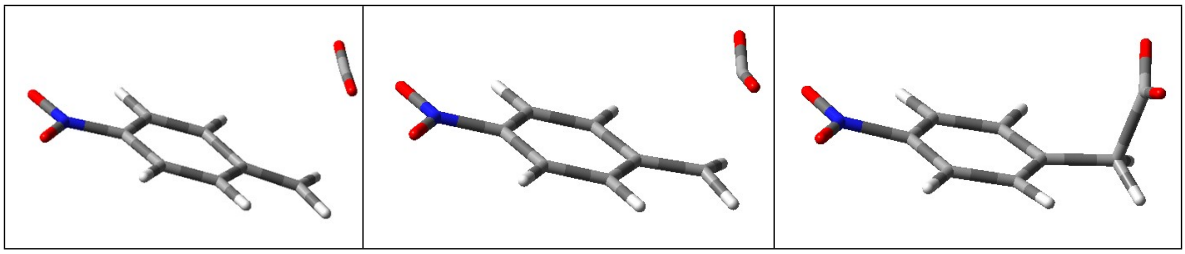




R_9^-

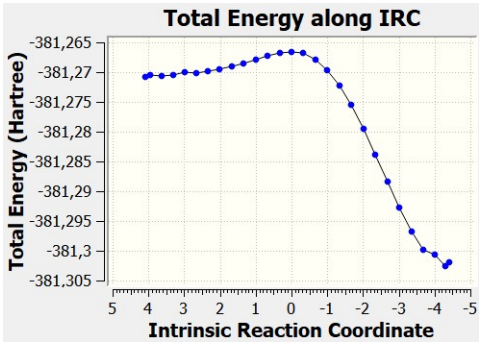
TS imaginary frequency = 552.72 cm^{-1}

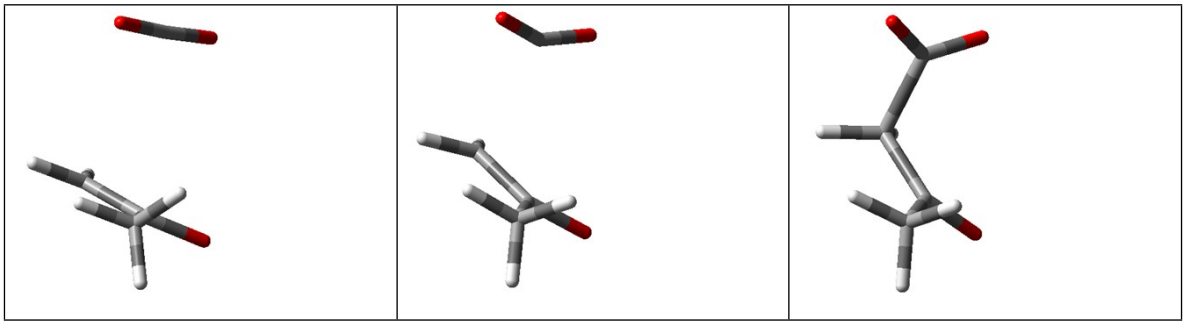




R_{10}^-

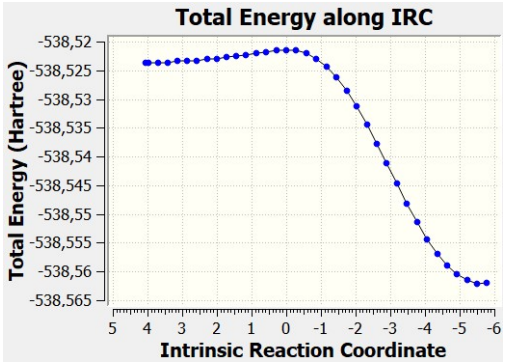
TS imaginary frequency = 351.56 cm^{-1}

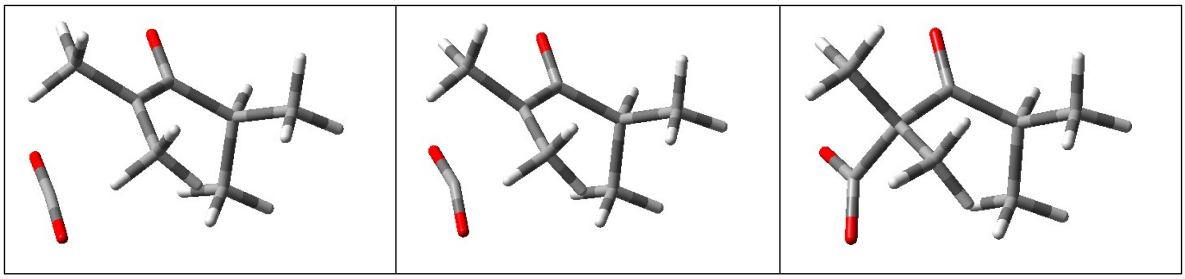




R_{11}^-

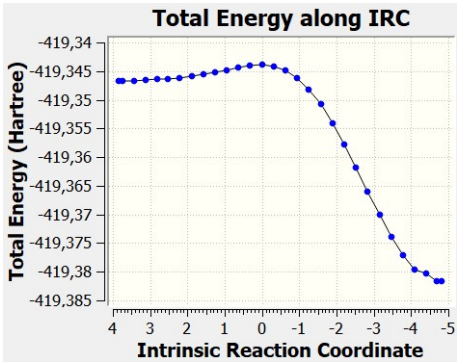
TS imaginary frequency = 277.11 cm^{-1}

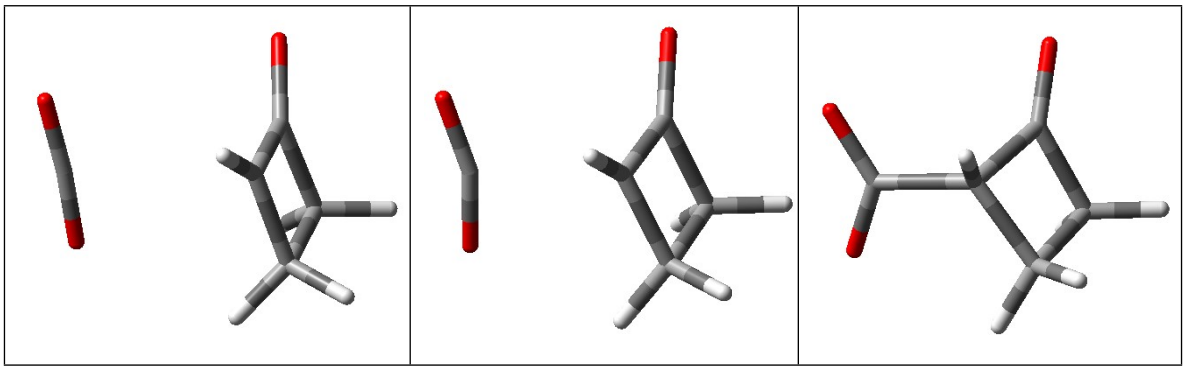




R_{12}^-

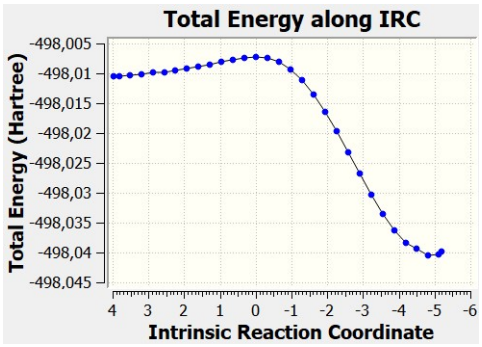
TS imaginary frequency = 301.67 cm^{-1}

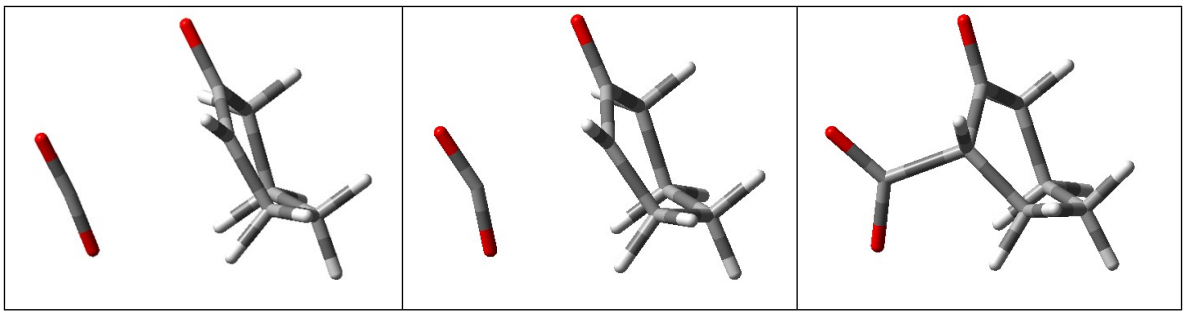




R_{13}^-

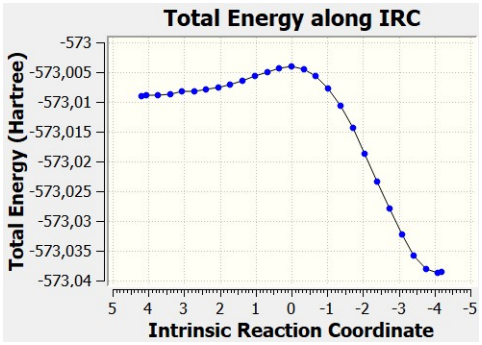
TS imaginary frequency = 292.94 cm^{-1}

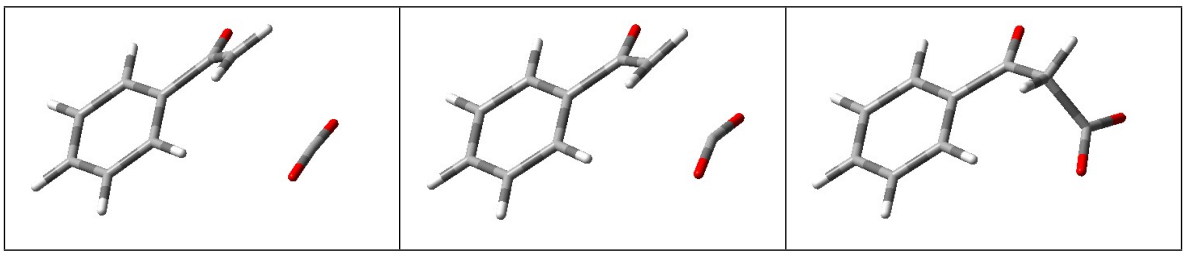




R_{14}^-

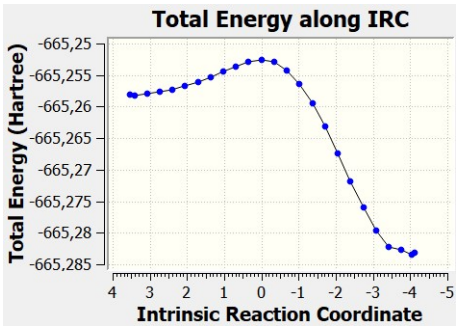
TS imaginary frequency = 376.05 cm^{-1}

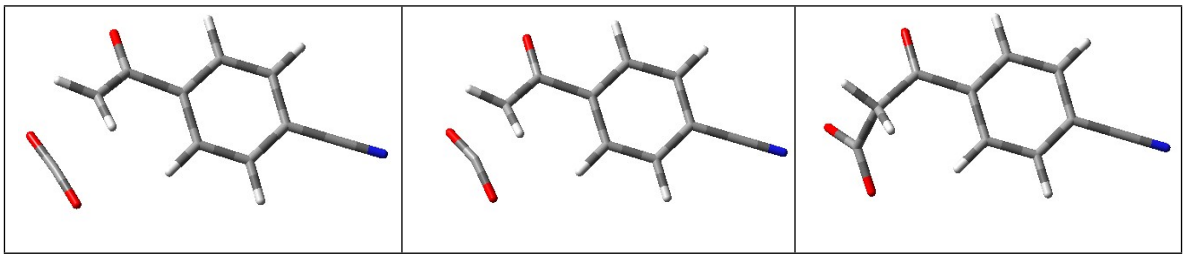




R_{15}^-

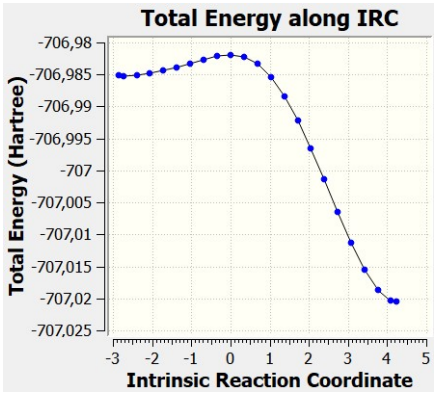
TS imaginary frequency = 391.92 cm^{-1}

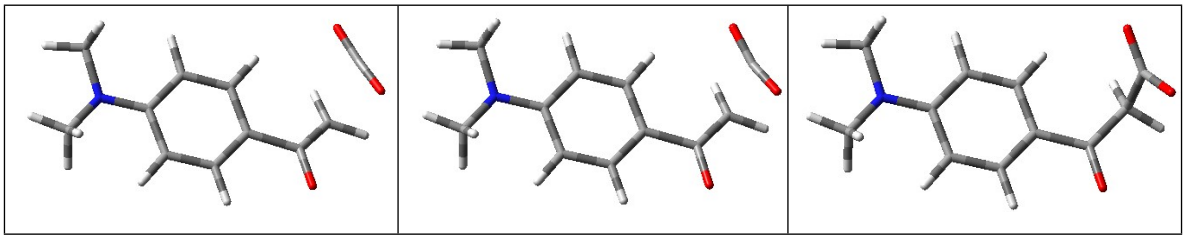




R_{16}^-

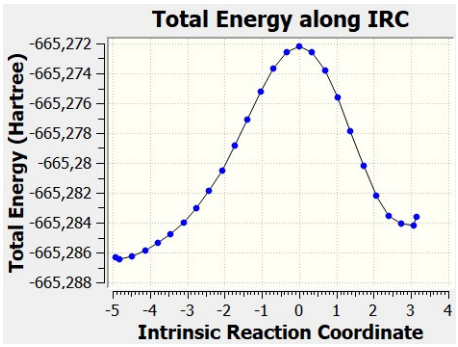
TS imaginary frequency = 357.14 cm^{-1}

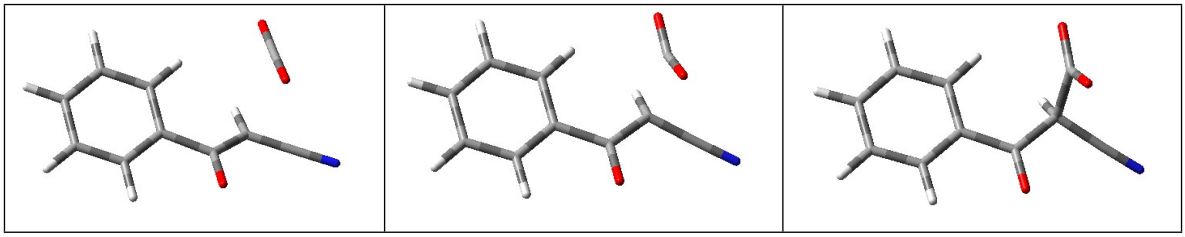




R_{17}^-

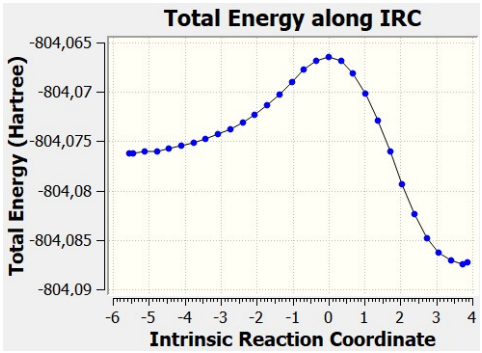
TS imaginary frequency = 424.47 cm^{-1}

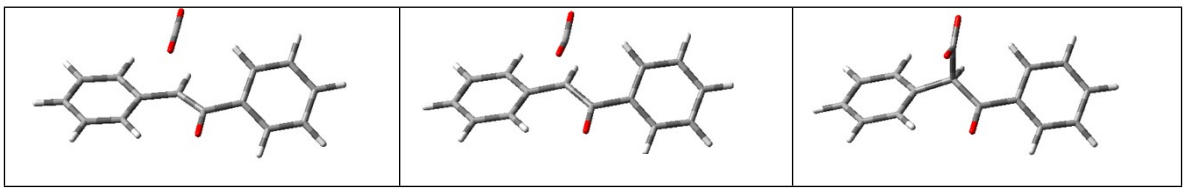




R_{18}^-

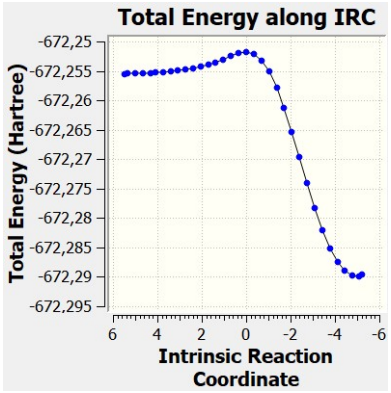
imaginary frequency = 421.27 cm^{-1}

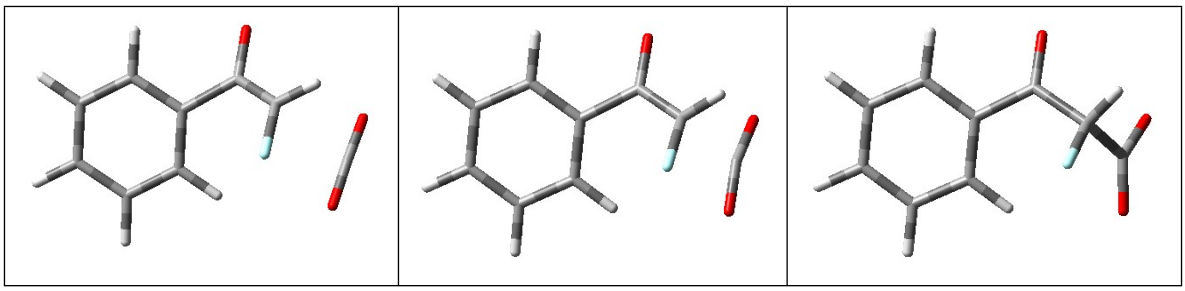




R_{19}^-

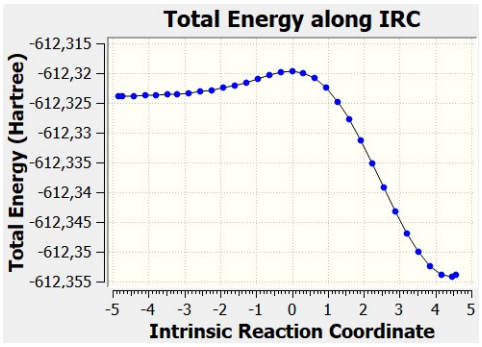
TS imaginary frequency = 342.63 cm^{-1}

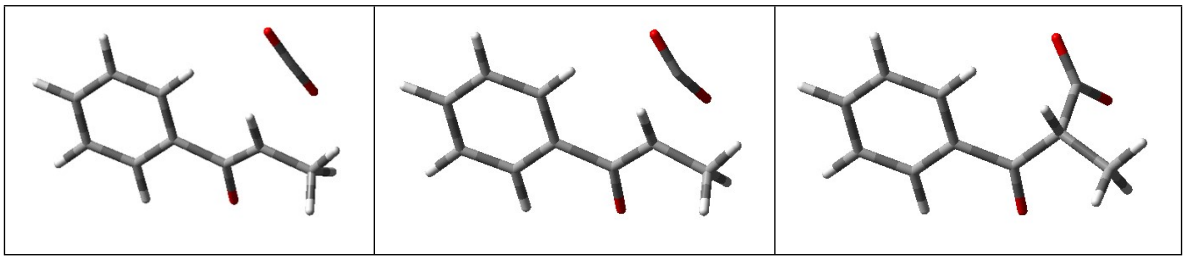




R_{20}^-

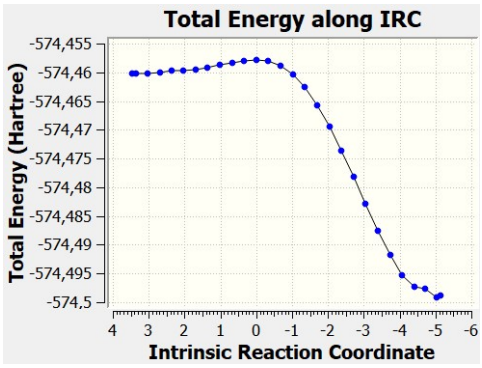
TS imaginary frequency = 348.58 cm^{-1}

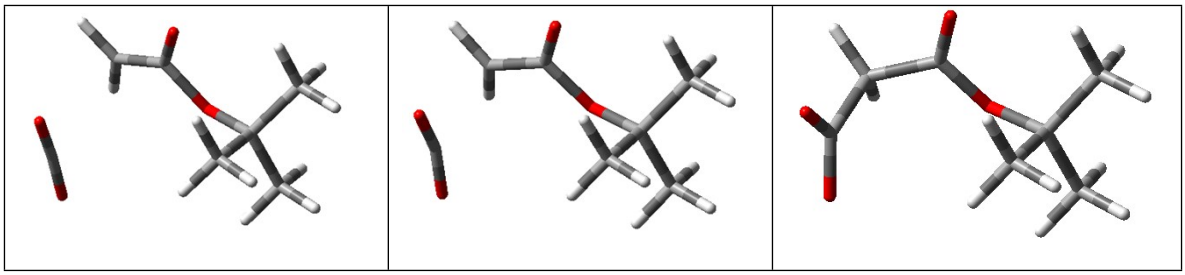




R_{21}^-

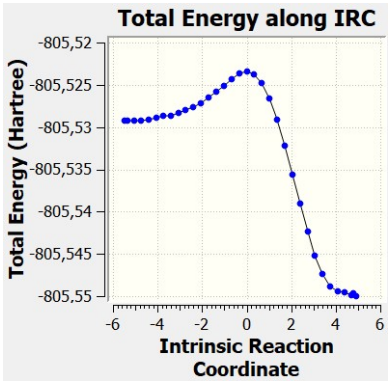
TS imaginary frequency = 296.69 cm^{-1}

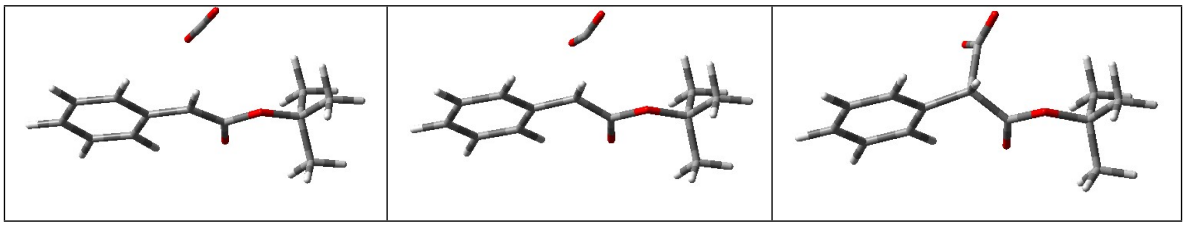




R_{22}^-

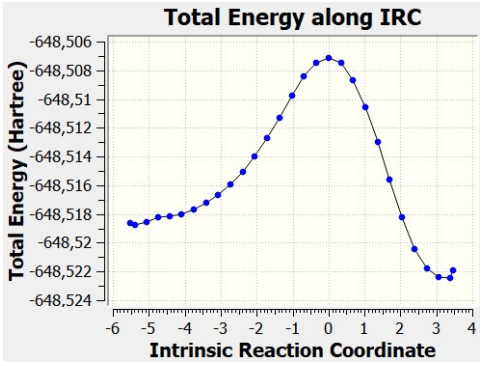
TS imaginary frequency = 369.81 cm^{-1}

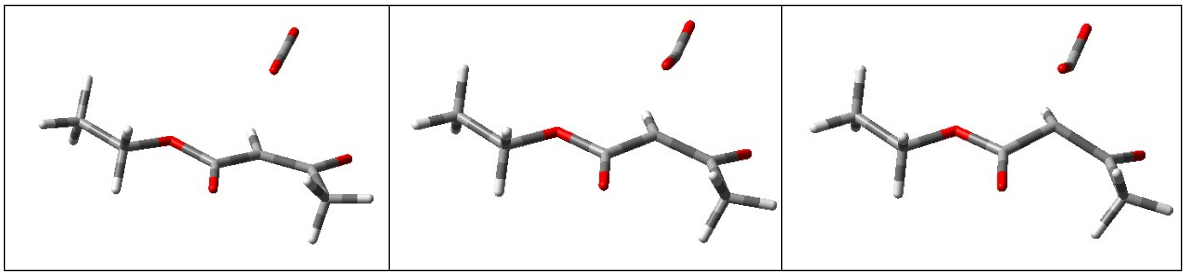




R_{23}^- c_1 (reported in the main text)

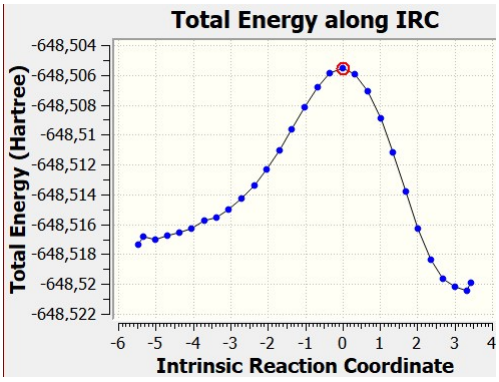
TS imaginary frequency = 412.06 cm^{-1}

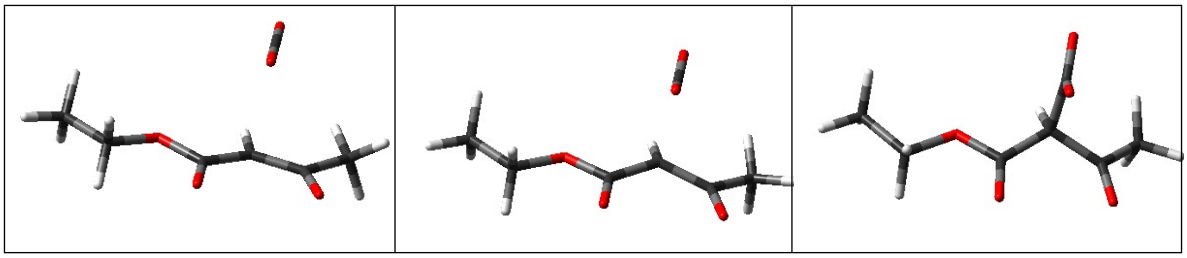




R_{23}^- c_3

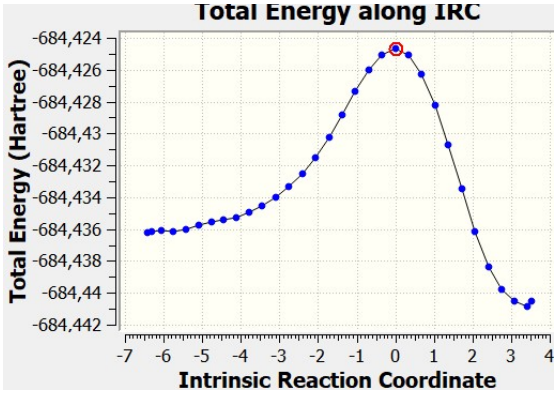
TS imaginary frequency = -409.92 cm^{-1}





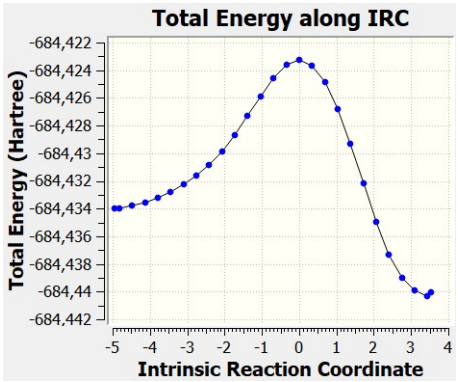
R_{24}^- c_1 (reported in the main text)

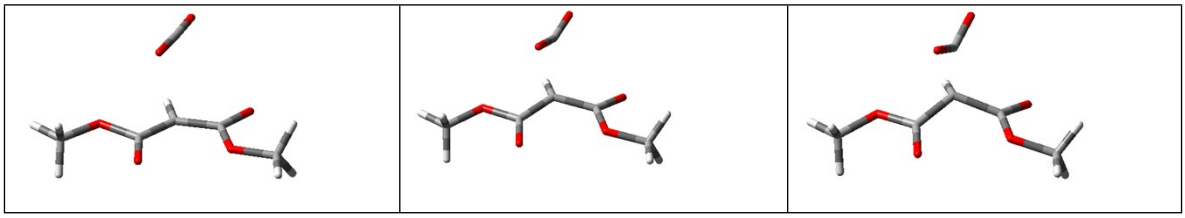
TS imaginary frequency = 418.06 cm^{-1}



R_{24}^- c_2

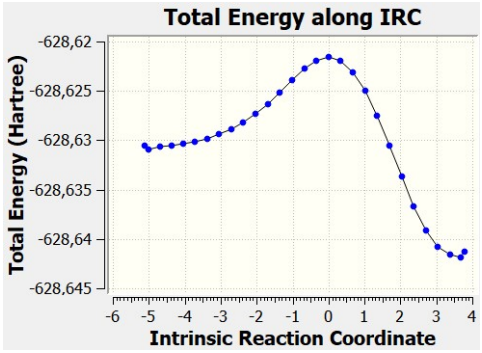
TS imaginary frequency = 416.64 cm^{-1}

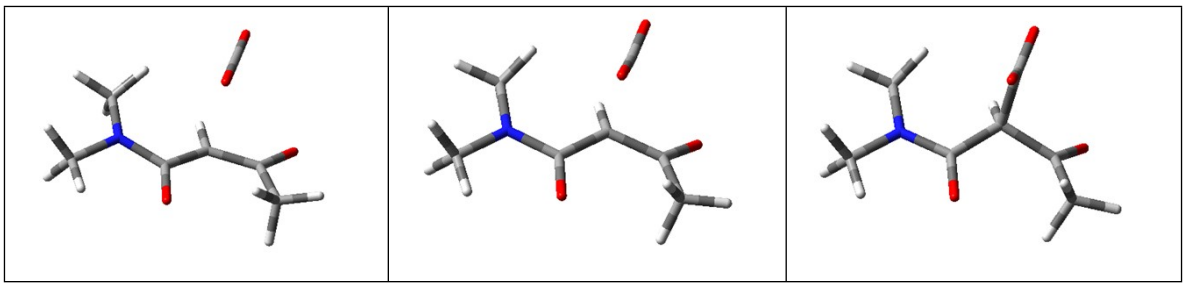




R_{25}^- c_1 (reported in the main text)

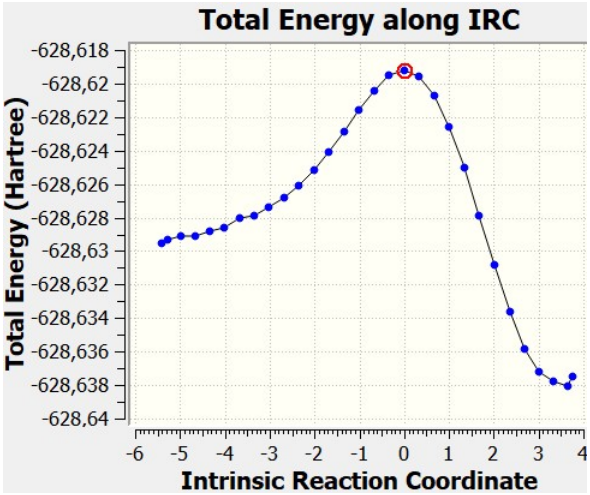
TS imaginary frequency = 403.79 cm^{-1}





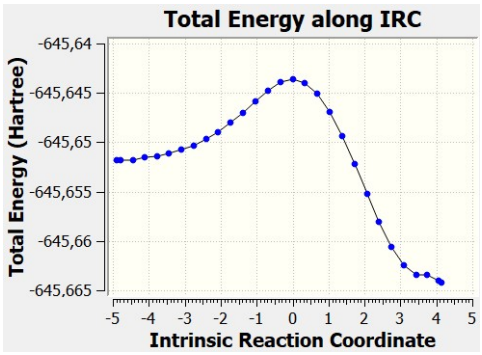
R_{25}^- c_2

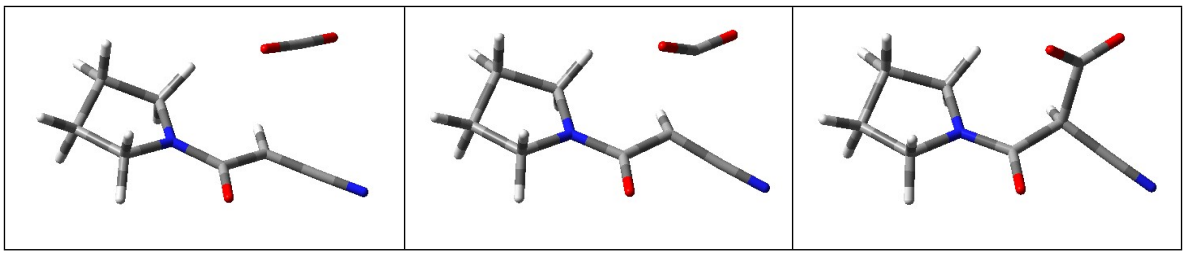
TS imaginary frequency = 408.70 cm^{-1}



R_{26}^-

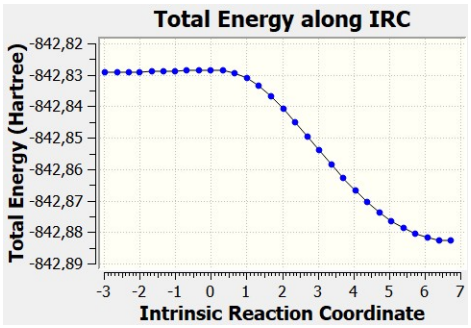
TS imaginary frequency = 385.63 cm^{-1}

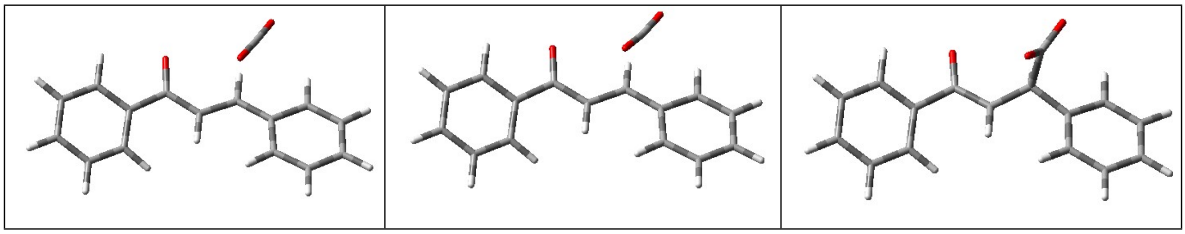




R_{27}^-

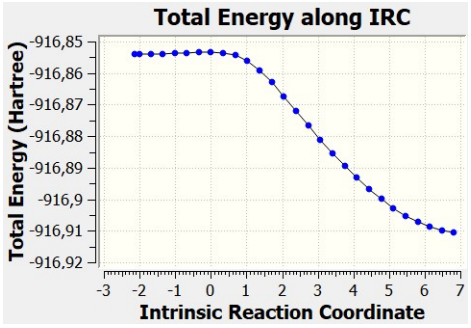
TS imaginary frequency = 243.80 cm^{-1}

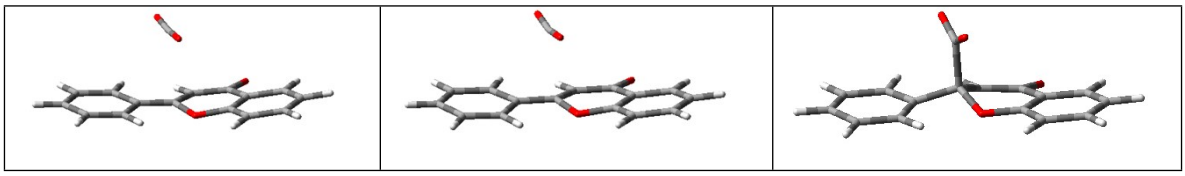




R_{28}^-

TS imaginary frequency = 259.54 cm^{-1}





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