

Supporting Information

Table S1. Total energies ($E_h/a.u.$), zero point energies (ZPE/kcal.mol⁻¹) and entropy values (S/cal.mol⁻¹ K⁻¹) of ketones and ketones-I₂/ICl

	$-E_{HF/LANL2DZ^*}$	$-E_{MP2/LANL2DZ^*}$	ZPE	S_{Tot}
1	190.7564526	191.3005	0.066055	64.00
1-I₂	213.1000806	213.8462389	0.067181	104.48
1-ICl	216.6323065	217.4043075	0.067883	96.62
2	229.834567	230.5040534	0.098055	71.91
2-I₂	252.178822	253.0507963	0.099240	112.34
2-ICl	255.7114571	256.6092546	0.099800	103.74
3	268.9074538	269.7055494	0.13076	73.78
3-I₂	291.2521675	292.2532378	0.131859	113.12
3-ICl	294.785162	295.8120431	0.132563	105.25
4	307.9507943	308.8785838	0.162577	78.17
4-I₂	330.2954848	331.4262955	0.163666	117.77
4-ICl	333.8284309	334.984999	0.164375	110.07
5	346.9782902	348.0376855	0.193676	84.49
5-I₂	369.3230397	370.5854891	0.194761	124.16
5-ICl	372.8560365	374.1443261	0.195483	116.37

Table S2. Total energies ($E_h/a.u.$), zero point energies (ZPE/kcal.mol⁻¹) and entropy values (S/cal.mol⁻¹ K⁻¹) of lactones and lactones-I₂/ICl.

	-E _{HF/LANL2DZ*}	-E _{MP2/ANL2DZ*}	ZPE	S _{Tot}
6	226.6119261	227.2059782	0.042328	62.48
6-I₂ (syn)	248.9544869	249.7492536	0.043334	105.33
6-I₂ (anti)	248.9546139	249.7497209	0.043384	104.67
6-ICl (syn)	252.4859158	253.3065907	0.043989	97.26
6-ICl (anti)	252.4859849	253.3070177	0.044043	96.85
7	265.6922893	266.4076226	0.074731	67.35
7-I₂ (syn)	288.0360644	288.9523735	0.075778	108.58
7-I₂ (anti)	288.0360465	288.953065	0.075813	108.22
7-Icl (syn)	291.568414	292.510356	0.076451	100.81
7-Icl (anti)	291.5682676	292.5110474	0.076504	100.41
8	304.7606283	305.6008739	0.106773	72.23
8-I₂ (syn)	327.1055837	328.1474841	0.107825	112.21
8-I₂ (anti)	327.1052496	328.1476512	0.107828	112.37
8-Icl (syn)	330.6387502	331.706140	0.108514	104.59
8-Icl (anti)	330.6381163	331.7062055	0.108532	104.45
9	343.7957029	344.7647989	0.137812	77.92
9-I₂ (syn)	366.1413795	367.3126824	0.138913	117.19
9-I₂ (anti)	366.1406485	367.312166	0.138885	117.92
9-Icl (syn)	369.6750287	370.8717261	0.139612	109.54
9-Icl (anti)	369.6737818	370.8709739	0.139586	110.07
10	382.8316872	383.9324963	0.169084	82.23
10-I₂ (syn)	405.1774421	406.4806208	0.170179	121.38
10-I₂ (anti)	405.176629	406.4799551	0.170153	122.32
10-Icl (syn)	408.7111294	410.0397204	0.170880	113.73
10-Icl (anti)	408.7097123	410.0386612	0.170855	114.46