Supporting info:

A Substrate Descriptor Based Approach for the prediction of the Regioselectivity of hydroformylation

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All DFT calculations were performed with the Amsterdam Density Functional[1,2] (ADF) program. The BL3YP-D3(BJ)[3,4] density functional was used together with a small core TZ2P basis set. Relativistic effects were accounted for by running calculations with zeroth-order regular approximation (ZORA).[5–7] All local minima were characterized by having zero imaginary frequencies after running a frequency calculation. Also, these XYZ coordinates were used to calculate the Sterimol parameters.[8] To determine the computer-aided drug design (CADD) descriptors, RDKit: Open-source cheminformatics; http://www.rdkit.org was used. [9]

Substrate details

CAS	*st_L*	*st_B1*	*st_B5*	*int_{IR}(C=C)*	*$\Delta^{13}C$ shift*	*ΔΔE **CAT1***	*ΔΔE **CAT2***	*ΔΔE cage_effect*
2114-42-3	4.75	1.81	6.33	13.13	22. 5	-0.78	0.55	1.33
3724-55-8	4.75	1.85	4.52	13.36	11.6	-0.92	0.14	1.07
818-57-5	4.75	1.81	3.72	15.65	21.2	-0.45	0.45	0.90
109-49-9	4.75	1.82	4.63	20.21	21.9	-0.41	0.54	0.96
591-87-7	4.74	1.85	4.66	4.310	14.4	-0.67	-0.31	0.36
1746-13-0	4.76	1.88	5.34	5.660	18.7	-0.35	-0.12	0.24
300-57-2	4.75	1.84	6.02	16.75	21.7	-0.61	0.52	1.13
4696-30-4	4.75	1.8	4.36	14.61	18.9	-0.64	0.57	1.21
1736-60-3	4.75	1.81	6.66	13.59	15.8	-0.51	0.05	0.56
768-56-9	4.75	1.82	3.61	19.88	23.1	-0.39	0.57	0.96
111-66-0	4.75	1.83	5.92	20.13	25.1	-0.34	0.63	0.97
1587-04-8	4.75	1.8	4.36	18.8	21.0	-0.67	0.53	1.21
3333-20-8	4.75	1.84	6.3	16.07	22.0	-0.41	0.59	1.00
3333-13-9	4.75	1.84	7.06	18.97	21.4	-0.78	0.61	1.38
3698-28-0	4.75	1.84	6.03	19.79	26.7	-0.38	0.59	0.97
61142-41-4	4.75	2.48	4.00	19.48	34.8	0.45	1.04	0.59
140-67-0	4.75	1.84	7.84	21.85	22.6	-0.73	0.64	1.38
77446-17-4	4.76	1.84	6.73	16.18	22.2	-0.2	0.57	0.77
4810-05-3	4.76	1.87	7.17	21.55	21.9	-1.26	0.58	1.83
2489-86-3	4.75	1.89	7.26	14.12	20.8	-0.38	0.44	0.82
3524-73-0	4.75	1.82	4.62	20.75	25.2	-0.36	0.68	1.05
2489-87-4	4.75	1.84	8.28	17.04	21.3	-0.73	0.49	1.23
557-31-3	4.75	1.89	4.54	4.370	18.6	-0.38	0.14	0.52
3739-64-8	4.75	1.89	6.18	4.410	18.7	-0.33	0.17	0.50
3840-33-3	4.75	1.86	7.15	19.33	20.7	-0.69	0.57	1.26
1587-05-9	4.76	1.87	6.06	19.13	20.5	-1.02	0.47	1.48
1813-97-4	4.75	1.83	7.63	13.59	19.7	-1.12	0.33	1.46
93-15-2	4.75	1.84	8.25	17.30	18.7	-0.39	0.57	0.96
30984-53-3	4.75	1.84	6.22	13.65	21.4	-0.66	0.41	1.07
487-11-6	4.75	1.84	8.25	14.31	21.2	-0.38	0.53	0.91
3840-17-3	4.75	1.84	7.04	14.34	19.1	-0.59	0.36	0.95
3769-23-1	4.75	1.79	4.44	16.94	22.3	-0.51	0.54	1.06
42918-20-7	4.75	1.83	6.09	14.31	19.0	-0.69	0.38	1.07
24743-14-4	4.75	1.84	7.00	12.10	21.3	-0.42	0.52	0.94
1737-16-2	4.75	1.84	7.00	18.36	21.4	-0.82	0.50	1.32
3404-61-3	4.76	2.43	4.70	16.88	32.9	0.12	1.05	0.93
691-37-2	4.76	1.84	4.43	16.23	22.4	-0.43	0.54	0.97

762-62-9	4.75	1.8	4.42	14.20	19.6	-0.49	0.25	0.73
3742-34-5	4.76	2.43	3.29	23.36	31.6	-0.47	0.91	1.38
695-12-5	4.76	2.45	3.50	20.24	33.3	-0.11	1.02	1.13
3524-75-2	4.75	1.79	5.71	11.60	23.9	-0.56	0.62	1.18

Computer-aided drug design descriptors of substrates

CAS	K_1	K_2	K_3	*L-SASA*	*Eccentricity*	*Alpha*
3524-73-0	0.57	3.91	5.74	65.91	0.98	-0.26
3769-23-1	0.57	3.91	3.57	65.91	0.97	-0.26
3404-61-3	0.57	3.91	3.57	65.91	0.97	-0.26
111-66-0	0.68	6.74	5.74	75.08	0.99	-0.26
691-37-2	0.46	2.95	3.74	56.73	0.97	-0.26
762-62-9	0.57	2.15	5.74	65.91	0.91	-0.26
3742-34-5	0.63	2.15	1.05	62.09	0.97	-0.26
695-12-5	0.74	2.91	1.36	71.27	0.95	-0.26
61142-41-4	0.97	4.54	2.55	89.62	0.91	-0.26
3524-75-2	0.74	2.91	1.36	71.27	0.95	-0.26
2114-42-3	0.86	3.71	2.21	80.44	0.96	-0.26
3724-55-8	0.97	3.40	3.03	54.02	0.95	-0.79
818-57-5	1.06	4.37	3.40	63.20	0.97	-0.79
300-57-2	1.20	3.08	1.73	69.89	0.96	-1.04
1736-60-3	5.48	3.77	1.49	83.69	0.90	-1.39
768-56-9	1.29	3.89	2.06	79.06	0.99	-1.04
591-87-7	0.97	3.40	5.21	54.02	0.98	-0.79
1746-13-0	1.50	3.72	1.94	75.00	0.99	-1.24
109-49-9	0.79	3.59	5.41	58.09	0.99	-0.59
4810-05-3	1.50	3.57	1.76	97.41	0.92	-1.04
2489-86-3	2.09	3.44	1.48	95.38	0.92	-1.56
2489-87-4	2.09	3.44	1.62	95.38	0.98	-1.56
4696-30-4	0.58	4.70	3.70	52.67	0.97	-0.30
1587-04-8	1.29	3.21	1.47	79.06	0.92	-1.04
3333-20-8	1.29	3.21	1.73	79.06	0.95	-1.04
3333-13-9	1.29	3.21	1.73	79.06	0.98	-1.04
140-67-0	1.58	3.81	2.11	84.17	0.98	-1.24
3698-28-0	1.58	3.81	1.84	84.17	0.86	-1.24
77446-17-4	1.39	3.38	2.23	88.24	0.92	-1.04
24743-14-4	1.58	3.81	2.11	84.17	0.95	-1.24
1737-16-2	1.73	3.16	1.69	72.65	0.98	-1.11
1587-05-9	1.39	3.38	1.70	88.24	0.92	-1.04
3840-33-3	1.39	3.38	1.94	88.24	0.97	-1.04
1813-97-4	3.15	3.64	2.61	87.34	0.98	-1.25
93-15-2	1.97	4.55	2.25	98.46	0.94	-1.44
557-31-3	0.58	4.70	3.70	52.67	0.99	-0.30
3739-64-8	0.81	6.70	5.70	71.02	0.99	-0.30
30984-53-3	1.73	3.16	1.69	72.65	0.96	-1.11
487-11-6	2.37	5.29	2.43	112.75	0.89	-1.64
3840-17-3	1.89	3.43	1.89	78.78	0.96	-0.75
42918-20-7	1.98	3.57	1.71	82.35	0.88	-0.56
	R^2					
Free Catalyst	0.094	0.005	0.052	0.035	0.008	0.068
Cage Catlyst	0.058	0.070	0.043	0.005	0.005	0.102
Cage Effect	0.001	0.095	0.153	0.052	0.000	0.007

CAS	*PBF*	*PMI1*	*PMI2*	*PMI3*	Φ	*RadGyr*
3524-73-0	0.55	92.03	425.43	486.57	0.32	2.25
3769-23-1	0.78	102.34	323.02	413.28	0.32	2.09
3404-61-3	0.63	130.56	306.80	363.31	0.32	2.09
111-66-0	0.82	111.21	778.28	600.56	0.57	2.55
691-37-2	0.75	76.12	247.73	274.01	0.23	1.89
762-62-9	0.84	126.83	300.12	308.51	0.18	1.94
3742-34-5	0.74	100.53	296.51	346.82	0.19	1.95
695-12-5	0.74	134.99	350.71	451.74	0.27	2.03
61142-41-4	0.75	241.97	568.85	717.83	0.44	2.30
3524-75-2	0.75	112.00	418.46	486.73	0.27	2.15
2114-42-3	0.81	150.42	547.78	560.43	0.35	2.30
3724-55-8	0.69	100.03	325.47	345.56	0.47	1.94
818-57-5	0.61	87.17	563.03	473.73	0.58	2.37
300-57-2	0.66	145.99	459.50	518.98	0.41	2.18
1736-60-3	0.68	579.76	862.45	1315.66	1.48	2.57
768-56-9	0.47	189.99	591.94	886.93	0.50	2.62
591-87-7	0.52	99.81	322.83	431.27	0.47	2.11
1746-13-0	0.42	120.86	782.01	876.11	0.56	2.57
109-49-9	0.62	75.53	401.17	446.17	0.41	2.19
4810-05-3	0.54	329.30	806.50	1062.58	0.45	2.62
2489-86-3	0.47	407.82	846.26	1109.86	0.55	2.62
2489-87-4	0.61	263.17	1039.72	1203.78	0.55	2.85
4696-30-4	0.51	68.41	337.77	342.44	0.46	1.87
1587-04-8	0.67	246.66	527.48	675.82	0.41	2.31
3333-20-8	0.66	221.45	558.47	691.69	0.41	2.36
3333-13-9	0.71	157.73	688.11	729.18	0.41	2.43
140-67-0	0.70	171.72	927.73	995.31	0.55	2.67
3698-28-0	0.67	395.80	479.17	766.33	0.55	2.35
77446-17-4	0.65	344.54	624.72	865.47	0.43	2.51
24743-14-4	0.65	225.60	708.33	899.69	0.55	2.58
1737-16-2	0.67	154.13	695.86	749.59	0.55	2.42
1587-05-9	0.57	321.34	562.01	720.09	0.43	2.42
3840-33-3	0.66	260.71	685.14	942.26	0.43	2.47
1813-97-4	0.70	221.36	1361.26	1414.43	0.88	2.86
93-15-2	0.68	454.00	987.10	1328.15	0.69	2.78
557-31-3	0.48	66.14	271.36	341.13	0.46	2.06
3739-64-8	0.65	79.35	684.38	820.34	0.68	2.52
30984-53-3	0.66	219.21	571.48	704.20	0.55	2.34
487-11-6	0.64	774.39	1058.18	1704.39	0.84	2.91
3840-17-3	0.66	265.46	775.24	909.48	0.65	2.52
42918-20-7	0.67	459.18	599.09	959.90	0.71	2.26
	R^2					
Free Catalyst	0.130	0.000	0.014	0.014	0.168	0.009
Cage Catlyst	0.004	0.001	0.076	0.035	0.018	0.029
Cage Effect	0.059	0.000	0.027	0.006	0.049	0.006

CAS	*Sphericity*	*Asphericity*	χ_{0n}	X_{1n}	X_{2n}	χ_{3n}
3524-73-0	0.36	0.39	17.50	8.50	0.75	0.25
3769-23-1	0.44	0.30	17.50	8.50	0.75	0.31
3404-61-3	0.44	0.33	17.50	8.50	0.75	0.31
111-66-0	0.27	0.64	20.00	9.75	0.75	0.31
691-37-2	0.44	0.41	15.00	7.25	0.63	0.19
762-62-9	0.61	0.23	17.50	8.50	1.00	0.25
3742-34-5	0.30	0.44	15.50	7.75	1.00	0.56
695-12-5	0.33	0.37	18.00	9.00	1.13	0.63
61142-41-4	0.79	0.14	23.00	11.50	1.38	0.75
3524-75-2	0.38	0.46	18.00	9.00	1.13	0.63
2114-42-3	0.31	0.43	20.50	10.25	1.25	0.69
3724-55-8	0.25	0.33	11.32	5.36	0.64	0.26
818-57-5	0.32	0.58	13.82	6.61	0.76	0.32
300-57-2	0.31	0.38	14.50	7.25	1.25	0.69
1736-60-3	0.31	0.22	11.39	5.69	2.19	1.40
768-56-9	0.13	0.63	17.00	8.50	1.38	0.75
591-87-7	0.34	0.41	11.32	5.36	0.62	0.19
1746-13-0	0.10	0.64	14.91	7.41	1.28	0.68
109-49-9	0.41	0.56	13.41	6.45	0.70	0.24
4810-05-3	0.18	0.34	22.00	11.00	2.00	1.19
2489-86-3	0.13	0.24	18.50	9.50	2.25	1.50
2489-87-4	0.18	0.50	18.50	9.50	2.25	1.44
4696-30-4	0.38	0.41	12.91	6.16	0.45	0.16
1587-04-8	0.28	0.34	17.00	8.50	1.50	0.88
3333-20-8	0.25	0.32	17.00	8.50	1.50	0.81
3333-13-9	0.26	0.49	17.00	8.50	1.50	0.81
140-67-0	0.21	0.56	17.41	8.66	1.56	0.89
3698-28-0	0.25	0.18	17.41	8.66	1.56	0.94
77446-17-4	0.23	0.24	19.50	9.75	1.75	0.94
24743-14-4	0.23	0.29	17.41	8.66	1.56	0.89
1737-16-2	0.31	0.51	13.88	6.94	1.44	0.78
1587-05-9	0.20	0.26	19.50	9.75	1.75	1.06
3840-33-3	0.28	0.34	19.50	9.75	1.75	1.00
1813-97-4	0.27	0.56	15.13	7.57	2.00	1.10
93-15-2	0.20	0.30	20.32	10.07	1.86	1.14
557-31-3	0.31	0.63	12.91	6.16	0.43	0.15
3739-64-8	0.21	0.64	17.91	8.66	0.68	0.27
30984-53-3	0.31	0.34	13.88	6.94	1.44	0.78
487-11-6	0.17	0.21	23.22	11.47	2.17	1.38
3840-17-3	0.31	0.40	13.88	6.94	1.44	0.78
42918-20-7	0.31	0.20	13.88	6.94	1.44	0.83
	R^2					
Free Catalyst	0.086	0.044	0.290	0.292	0.002	0.004
Cage Catlyst	0.189	0.025	0.051	0.042	0.060	0.052
Cage Effect	0.027	0.001	0.058	0.070	0.075	0.074

CAS	χ_{0v}	χ_{1v}	χ_{2v}	χ_{3v}
3524-73-0	3.50	1.50	0.75	0.25
3769-23-1	3.50	1.50	0.75	0.31
3404-61-3	3.50	1.50	0.75	0.31
111-66-0	4.00	1.75	0.75	0.31
691-37-2	3.00	1.25	0.63	0.19
762-62-9	3.50	1.50	1.00	0.25
3742-34-5	3.50	1.75	1.00	0.56
695-12-5	4.00	2.00	1.13	0.63
61142-41-4	5.00	2.50	1.38	0.75
3524-75-2	4.00	2.00	1.13	0.63
2114-42-3	4.50	2.25	1.25	0.69
3724-55-8	3.32	1.36	0.64	0.26
818-57-5	3.82	1.61	0.76	0.32
300-57-2	4.50	2.25	1.25	0.69
1736-60-3	6.39	3.19	2.19	1.40
768-56-9	5.00	2.50	1.38	0.75
591-87-7	3.32	1.36	0.62	0.19
1746-13-0	4.91	2.41	1.28	0.68
109-49-9	3.41	1.45	0.70	0.24
4810-05-3	6.00	3.00	2.00	1.19
2489-86-3	6.50	3.50	2.25	1.50
2489-87-4	6.50	3.50	2.25	1.44
4696-30-4	2.91	1.16	0.45	0.16
1587-04-8	5.00	2.50	1.50	0.88
3333-20-8	5.00	2.50	1.50	0.81
3333-13-9	5.00	2.50	1.50	0.81
140-67-0	5.41	2.66	1.56	0.89
3698-28-0	5.41	2.66	1.56	0.94
77446-17-4	5.50	2.75	1.75	0.94
24743-14-4	5.41	2.66	1.56	0.89
1737-16-2	4.88	2.44	1.44	0.78
1587-05-9	5.50	2.75	1.75	1.06
3840-33-3	5.50	2.75	1.75	1.00
1813-97-4	6.13	3.07	2.00	1.10
93-15-2	6.32	3.07	1.86	1.14
557-31-3	2.91	1.16	0.43	0.15
3739-64-8	3.91	1.66	0.68	0.27
30984-53-3	4.88	2.44	1.44	0.78
487-11-6	7.22	3.47	2.17	1.38
3840-17-3	5.63	2.82	1.82	0.97
42918-20-7	6.46	3.23	2.23	1.42
	R^2			
Free Catalyst	0.000	0.001	0.001	0.002
Cage Catlyst	0.042	0.043	0.067	0.059
Cage Effect	0.035	0.052	0.071	0.071

CAS	*NPR1*	*NPR2*	*#Rotatable Bonds*
3524-73-0	0.31	0.91	5
3769-23-1	0.25	0.90	5
3404-61-3	0.39	0.82	5
111-66-0	0.24	0.90	6
691-37-2	0.31	0.85	4
762-62-9	0.41	0.97	1
3742-34-5	0.24	0.85	1
695-12-5	0.38	0.83	1
61142-41-4	0.35	0.78	1
3524-75-2	0.23	0.89	2
2114-42-3	0.23	0.88	2
3724-55-8	0.29	0.83	3
818-57-5	0.38	0.92	4
300-57-2	0.28	0.89	2
1736-60-3	0.44	0.66	2
768-56-9	0.14	0.91	3
591-87-7	0.18	0.88	3
1746-13-0	0.19	0.89	3
109-49-9	0.17	0.86	4
4810-05-3	0.31	0.76	5
2489-86-3	0.30	0.70	2
2489-87-4	0.21	0.87	2
4696-30-4	0.12	0.96	4
1587-04-8	0.40	0.75	3
3333-20-8	0.32	0.84	3
3333-13-9	0.22	0.93	3
140-67-0	0.17	0.93	4
3698-28-0	0.51	0.61	4
77446-17-4	0.40	0.72	4
24743-14-4	0.26	0.84	4
1737-16-2	0.21	0.93	2
1587-05-9	0.39	0.68	4
3840-33-3	0.31	0.84	4
1813-97-4	0.18	0.97	2
93-15-2	0.34	0.75	6
557-31-3	0.20	0.98	4
3739-64-8	0.14	1.00	6
30984-53-3	0.31	0.81	2
487-11-6	0.47	0.61	8
3840-17-3	0.27	0.84	2
42918-20-7	0.48	0.61	2
	Rsq		
Free Catalyst	0.041	0.011	0.000
Cage Catlyst	0.048	0.006	0.004
Cage Effect	0.001	0.000	0.003

CAS	*ISF*	*SpherocityIndex*	*TPSA*
3524-73-0	0.01	0.46	0.00
3769-23-1	0.01	0.43	0.00
3404-61-3	0.01	0.30	0.00
111-66-0	0.01	0.28	0.00
691-37-2	0.01	0.44	0.00
762-62-9	0.01	0.61	0.00
3742-34-5	0.01	0.38	0.00
695-12-5	0.01	0.51	0.00
61142-41-4	0.00	0.38	0.00
3524-75-2	0.01	0.28	0.00
2114-42-3	0.01	0.32	0.00
3724-55-8	0.01	0.36	26.30
818-57-5	0.00	0.32	26.30
300-57-2	0.01	0.31	0.00
1736-60-3	0.00	0.31	0.00
768-56-9	0.01	0.13	0.00
591-87-7	0.01	0.20	26.30
1746-13-0	0.01	0.30	9.23
109-49-9	0.01	0.41	17.07
4810-05-3	0.00	0.18	0.00
2489-86-3	0.00	0.15	0.00
2489-87-4	0.00	0.19	0.00
4696-30-4	0.02	0.29	9.23
1587-04-8	0.00	0.28	0.00
3333-20-8	0.00	0.27	0.00
3333-13-9	0.01	0.26	0.00
140-67-0	0.01	0.23	9.23
3698-28-0	0.00	0.26	9.23
77446-17-4	0.00	0.24	0.00
24743-14-4	0.00	0.21	9.23
1737-16-2	0.01	0.31	0.00
1587-05-9	0.00	0.20	0.00
3840-33-3	0.00	0.24	0.00
1813-97-4	0.00	0.27	0.00
93-15-2	0.00	0.20	18.46
557-31-3	0.01	0.32	9.23
3739-64-8	0.02	0.20	9.23
30984-53-3	0.00	0.31	0.00
487-11-6	0.00	0.17	27.69
3840-17-3	0.00	0.31	0.00
42918-20-7	0.00	0.31	0.00
Free Catalyst	0.028		
Cage Catlyst	0.005		
Cage Effect	0.045		

DFT-optimized molecular geometries and related output.:

Program: ADF
Functional B3LYP-TZ2P
1-octene 111-66-0
Alkene carbon atoms
Outermost : 15
Innermost: 14
C next to C=C: 1
IR C=C stretch 1698 cm^{-1}
Intensity: 20.13

C	1.15156726	0.31519828	0.15887983
H	0.12737013	-0.06723023	0.08917287
H	1.78276221	-0.52703243	0.47267020
C	1.22543337	1.40927726	1.23973664
H	2.24875285	1.80116858	1.28835573
H	0.58916249	2.24999979	0.94038917
C	0.80441663	0.91180845	2.62638992
H	-0.22045136	0.52291085	2.57636640
H	1.43851666	0.06367632	2.91458370
C	0.88369172	1.99369484	3.70867766
H	0.24947046	2.84184847	3.42073997
C	0.46525331	1.49878478	5.09818833
H	1.90858730	2.38333502	3.75710433
C	1.60518843	0.79766451	-1.19113024
C	0.85462760	0.82754722	-2.29138242
H	2.63144372	1.16131183	-1.24368359
H	-0.17446465	0.47840208	-2.28481719
H	1.24074630	1.19861119	-3.23478658
C	0.54827370	2.58761042	6.17391522
H	-0.10416926	3.43163064	5.92958458
H	1.56843870	2.97369310	6.26365525
H	0.24824473	2.20608215	7.15388155
H	1.09982834	0.65154136	5.38423735
H	-0.55844752	1.10916456	5.04825786

5-methylhexene
Cas: 3524-73-0
IR stretch: 1696
Intensity: 20.75
Outermost: 15
Innermost: 14
C next to C=C: 1

C	0.87802888	0.42416259	0.05938651
H	-0.20322217	0.39462528	-0.10141651
H	1.18848446	-0.59438533	0.32948180
C	1.22238432	1.36506165	1.22911279
H	2.31318568	1.45407232	1.29819567
H	0.84687339	2.37062650	1.00186308
C	0.67728717	0.91675631	2.59710248
C	-0.85794884	0.86921657	2.62696240
H	1.05149616	-0.09865458	2.78604015
C	1.20959032	1.83166852	3.70993164
H	0.86230186	2.86006269	3.56298265
H	0.86371178	1.50095689	4.69351478
H	2.30327989	1.84702845	3.72293023
C	1.56078682	0.82795886	-1.21857088
C	0.94217032	1.19389260	-2.34015409
H	2.65053329	0.83010774	-1.19322786
H	-0.14226765	1.21081838	-2.40888609
H	1.49471120	1.48651388	-3.22657701
H	-1.27681754	1.85621394	2.40186255
H	-1.21877405	0.57198191	3.61556587
H	-1.26077090	0.15991709	1.90039293

4-methylhexene
Cas: 3769-23-1
IR stretch: 1696
Intensity: 16.94
Outermost: 15
Innermost: 14
C next to C=C: 1

C	1.13159689	0.33859428	0.11243856
H	0.05980540	0.11396003	0.13079776
H	1.65649815	-0.59565680	0.35585687
C	1.44449051	1.36944724	1.22478439
C	2.94876760	1.66127601	1.32226059
H	0.92982663	2.30234721	0.95872120
C	0.86575518	0.87568518	2.56461663
H	-0.18191426	0.59575027	2.40645228
H	1.38709426	-0.04498741	2.85648874
C	0.93987034	1.89471959	3.70784265
H	0.45161875	2.83324388	3.42688022
H	0.43904958	1.51389312	4.60193104
H	1.97154024	2.12535089	3.98367325
C	1.51560598	0.78025269	-1.27323654
C	0.65132428	1.04757185	-2.25163823
H	2.57958206	0.89119677	-1.47288937
H	-0.42075724	0.94740453	-2.10398447
H	0.98292942	1.37212659	-3.23224474
H	3.34475041	2.04706371	0.38034593
H	3.50105045	0.74860741	1.57281001
H	3.16296503	2.40433203	2.09303049

3-methylhexene
Cas: 3404-61-3
IR stretch: 1697
Intensity: 16.88
Outermost: 15
Innermost: 14
C next to C=C: 1

C	1.05270629	0.26702069	0.16189371
H	-0.03553594	0.12908084	0.13291327
C	1.70831353	-1.09675329	0.45274571
C	1.37003516	1.31461887	1.25294677
H	2.45676567	1.46543127	1.29663893
H	0.93989568	2.27370063	0.94331881
C	0.84781911	0.96406885	2.65174820
H	-0.22513497	0.74577583	2.58991485
H	1.32775348	0.04888610	3.01170464
C	1.08541212	2.09043290	3.66474225
H	0.58278978	3.01114037	3.35338543
H	0.71018850	1.82245148	4.65601816
H	2.15282229	2.31235081	3.76023286
C	1.49295892	0.77786482	-1.18698959
C	0.68926143	1.02937678	-2.21844943
H	2.56492355	0.94795113	-1.29529413
H	-0.38395894	0.87222059	-2.15196652
H	1.07267336	1.39950345	-3.16328516
H	2.79662235	-0.99420652	0.51790607
H	1.48510486	-1.80969942	-0.34426540
H	1.35246426	-1.51949496	1.39458110

4-methylpentene
Cas: 691-37-2
IR stretch 1697
Intensity 16.23
Outermost: 2
Innermost: 1
C next to C=C: 7

C	0.71187758	1.06046858	-1.80148045
C	1.61682535	0.62917720	-2.67842708
H	-0.22976203	1.46465310	-2.17356051
H	2.56718029	0.21440506	-2.35392224
H	1.44170265	0.67689964	-3.74791460
H	-0.23458577	1.45766807	2.20780108
C	0.86303977	1.03694814	-0.30611029
C	-0.22382282	0.20686175	0.41555631
C	-0.12967335	0.40341305	1.93512780
H	-0.90952788	-0.16056417	2.45455356
H	0.83870944	0.05485957	2.30990165
C	-0.13345404	-1.27947797	0.04582514
H	1.85266503	0.64735007	-0.03873240
H	0.82492542	-1.69731618	0.37348041
H	-0.20952628	-1.42884312	-1.03354369
H	-0.93017737	-1.85244664	0.52854554
H	0.81462440	2.06684899	0.07138928
H	-1.20062978	0.58281457	0.08364280

4.4'-dimethyl pen-1-tene
Cas: 762-62-9
IR stretch: 1696
Intensity: 14.2
Outermost: 2
Innermost: 1
C next to C=C: 7

C	0.73945717	1.03501855	-1.85275231
C	1.59288405	0.43167490	-2.67903241
H	-0.11524410	1.55840152	-2.27701603
H	2.46244535	-0.10168532	-2.30460999
H	1.45518552	0.45112560	-3.75488093
H	-0.01273512	1.53691197	2.21221840
C	0.86171976	1.05818192	-0.35453173
C	-0.26135825	0.30837796	0.42143392
C	0.00733218	0.48025866	1.92746913
H	-0.74978886	-0.04307815	2.51918494
H	0.98696809	0.07530246	2.19967396
C	-0.23738640	-1.18822854	0.06643935
C	-1.64271044	0.89960816	0.08508812
H	0.73083291	-1.63328234	0.31668390
H	-0.41130046	-1.34444566	-1.00084706
H	-1.01025690	-1.72794407	0.62200425
H	-1.67113090	1.97443026	0.29089408
H	-2.41940982	0.42202394	0.68954968
H	-1.90078647	0.74646280	-0.96579112
H	1.82757939	0.62935192	-0.06528818
H	0.86214094	2.10201234	-0.01389735

vinyl cyclopentane

Cas: 3742-34-5
IR stretch: 1696
Intensity: 23.36
Outermost: 10
Innermost: 14
C next to C=C: 1

C	0.86540361	0.61446827	0.03721343
H	1.02216160	-1.57807332	0.23173859
C	1.39932291	-0.67153179	0.71004639
C	1.13482904	1.67917538	1.12438621
H	2.20084922	1.93414047	1.11188540
H	0.57699284	2.60264359	0.95347234
C	0.76361023	0.97761036	2.44968888
H	-0.28446415	1.17116178	2.69434627
C	0.98310925	-0.54615430	2.19607878
C	0.84602693	1.04018523	-2.44570485
H	2.57940743	1.03848777	-1.27348663
H	-0.23293260	0.92573308	-2.50397728
H	1.36715155	1.25954055	-3.37131459
C	1.49565603	0.91653579	-1.28903168
H	1.35804304	1.34857042	3.28766506
H	0.05859882	-1.09894248	2.38225036
H	1.74138661	-0.96710588	2.86025307
H	2.49128950	-0.68737233	0.61981716
H	-0.21958673	0.51775561	-0.09656731

vinyl cyclohexane

Cas: 695-12-5
IR stretch: 1695
Intensity: 20.24
Outermost: 10
Innermost: 14
C next to C=C: 1

C	0.83075092	0.51854402	-0.12075520
H	0.85073563	-1.59285738	-0.62267480
C	1.15949541	-0.95422803	0.21043353
C	1.20575152	1.42856397	1.07022833
H	2.29652573	1.41361318	1.19442786
H	0.92965747	2.46210245	0.84029938
C	0.53874593	0.97018693	2.37515024
H	-0.54881599	1.08327652	2.28201367
C	0.86740043	-0.49621641	2.69025885
C	0.91998943	1.37748493	-2.49128943
H	2.61437062	0.92524614	-1.35091624
H	-0.16326980	1.42704685	-2.56192260
H	1.48289246	1.68311496	-3.36675666
C	1.52467762	0.96011232	-1.38032307
H	0.85137025	1.61649453	3.20147208
H	0.34893786	-0.81445878	3.60026631
H	1.94246133	-0.58933105	2.89067010
H	2.24851798	-1.05962994	0.30195871
H	-0.25318914	0.59686716	-0.27912513
C	0.49266904	-1.41179900	1.51577034
H	-0.59691152	-1.40210511	1.38556951
H	0.77280751	-2.44695296	1.73545840

vinyl cyclooctane

Cas: 61142-41-4
IR stretch 1695
Intensity 19.48
Outermost: 10
Innermost: 14
C next to C=C: 1

C	0.83300696	0.57714933	-0.54596274
H	1.12363534	-1.16912457	-1.74692600
C	0.98918175	-0.95737091	-0.68257410
C	1.17618838	1.14938765	0.84653622
H	2.23981352	0.96878344	1.04950482
H	1.06608923	2.23625404	0.77497710
C	0.34646597	0.65842323	2.04594039
H	-0.71138951	0.60401573	1.76366348
C	0.78346762	-0.67615470	2.70326260
C	1.26541688	2.07488804	-2.53545106
H	2.76926829	1.06148475	-1.49310989
H	0.20902517	2.30331855	-2.64879038
H	1.94572287	2.53785674	-3.24231244
C	1.70054889	1.26418422	-1.57300136
H	0.40391201	1.44076842	2.80899125
H	0.81754021	-0.52046950	3.78590764
H	1.81209919	-0.91579335	2.40851130
H	1.92224091	-1.26875113	-0.19825738
H	-0.21150963	0.83009423	-0.76921718
C	-0.12203468	-1.89293349	2.44711157
H	-1.16935981	-1.57772121	2.53996684
H	0.04397942	-2.62015943	3.25020096
C	0.06426515	-2.63119168	1.11555202
C	-0.19030552	-1.82329458	-0.16928115
H	1.07765357	-3.05053628	1.07376419
H	-0.61521078	-3.49127284	1.12114560
H	-1.08249266	-1.20011839	-0.03941735
H	-0.44512945	-2.53700312	-0.95821103

Allylcyclopentane

Cas: 3524-75-2
IR stretch: 1696
Intensity: 11.6
Outermost: 10
Innermost: 14
C next to C=C: 20

C	0.17366010	-0.16599289	-0.11755779
H	1.22055486	-1.96719298	0.61688448
C	1.33623776	-0.87986667	0.59807282
C	0.31696352	1.30571651	0.33927479
H	0.93428906	1.85205974	-0.37831837
H	-0.65238788	1.80892290	0.37521121
C	1.01594036	1.25710828	1.73081468
H	0.39298346	1.68328940	2.52039351
C	1.32517406	-0.24083750	1.99633184
C	1.38331724	1.07386751	-3.26065284
H	2.21550697	-0.53814094	-2.23344583
H	0.51533636	1.69348671	-3.46979339
H	2.30134455	1.32415103	-3.78160216
C	1.31827445	0.05285228	-2.40723074
H	1.94117540	1.83844782	1.71030077
H	0.52468143	-0.68961415	2.59366258
H	2.25882861	-0.38807285	2.54421430
H	2.28322584	-0.65362175	0.09619588
H	-0.75726259	-0.56507918	0.30476275
C	0.08759211	-0.36211352	-1.64713818
H	-0.11027885	-1.42324623	-1.84599455
H	-0.77550804	0.19570296	-2.02640388

Allylcyclohexane

Cas: 2114-42-3
IR stretch: 1694
Intensity: 13.13
Outermost: 10
Innermost: 14
C next to C=C: 20

C	0.37741195	-0.02995066	0.01878903
H	1.42660162	-1.89089891	0.40875122
C	1.56341043	-0.82057288	0.59973607
C	0.53502459	1.47050168	0.31685212
H	1.40747397	1.85256369	-0.22622554
H	-0.33335217	2.01730697	-0.06730509
C	0.70874413	1.73722463	1.81945704
H	-0.21264411	1.45548104	2.34519581
C	1.73108764	-0.56427384	2.10479247
C	1.23171706	1.01880996	-3.33003250
H	2.22274616	-0.45844899	-2.24234137
H	0.32179611	1.58366270	-3.51393750
H	2.08879245	1.25385457	-3.95212624
C	1.28798616	0.08029967	-2.38620391
H	0.85570546	2.80742922	1.99696028
H	0.85168051	-0.94925931	2.63672271
H	2.59576014	-1.11645479	2.48691787
H	2.48538029	-0.52285268	0.08609428
H	-0.52741967	-0.37549722	0.53831481
C	0.14627737	-0.30833543	-1.48603043
H	-0.04987353	-1.38210592	-1.60602605
H	-0.75893871	0.21823789	-1.80770735
C	1.88268264	0.93525114	2.40064569
H	1.96022742	1.10333043	3.47956719
H	2.81935551	1.29562606	1.95668589

3-butenoic acid methyl ester

Cas: 3724-55-8
IR stretch: 1706
Intensity: 13.36
Outermost: 2
Innermost: 1
C next to C=C: 7

C	0.73930990	0.94100289	-1.89573691
C	1.82083281	0.76945027	-2.65147595
H	-0.24233672	1.01400824	-2.35530855
H	2.81282778	0.67882525	-2.21762182
H	1.75131713	0.71299850	-3.73209146
O	-1.26656846	-0.28192426	-0.22697088
C	0.76681184	1.04370534	-0.39604300
C	-0.26351905	0.15329669	0.28510548
O	0.07519041	-0.06601446	1.57533850
H	0.52403423	2.06913737	-0.08247685
H	1.75746147	0.82528936	0.00830850
C	-0.85413086	-0.85477878	2.34362591
H	-0.97568671	-1.84192194	1.89584266
H	-1.82641910	-0.36181632	2.38680759
H	-0.42063701	-0.93503478	3.33795614

4-pentenoic acid methyl ester

Cas: 818-57-5
IR stretch 1701
Intensity 15.65
Outermost: 2
Innermost: 1
C next to C=C: 7

C	1.07259559	0.83146856	-1.07598248
C	1.62948417	0.15350789	-2.07763515
H	1.06117785	1.92042646	-1.11319056
H	1.65792466	-0.93261608	-2.08056718
H	2.07720642	0.65898831	-2.92630301
O	-2.29267775	-1.10089730	1.51296621
C	0.42731662	0.21101206	0.13236802
C	-1.70140673	-0.04781642	1.46248029
O	-1.47444841	0.73245927	2.54636810
H	0.91657169	0.58099872	1.04040591
H	0.55382191	-0.87500836	0.10986535
C	-1.96768321	0.22577099	3.80045605
H	-1.50895786	-0.73739720	4.02909452
H	-3.05084930	0.10208157	3.76157710
H	-1.69359124	0.96760793	4.54739893
C	-1.08156847	0.55076723	0.21697059
H	-1.21305617	1.63554889	0.23042793
H	-1.60240721	0.13963027	-0.64842145

Hex-5-en-2-one
Cas: 109-49-9
IR stretch 1699
Intensity 20.21
Outermost: 15
Innermost: 14
C next to C=C: 1

C	1.01858804	0.36225000	0.09990235
H	-0.06218487	0.20676441	0.04752774
H	1.45716247	-0.60479134	0.36758538
C	1.33945220	1.36418871	1.21604486
H	2.41893920	1.56164211	1.26269862
H	0.88056894	2.33859641	1.00909251
C	0.90261933	0.91060343	2.60544275
H	-0.28295551	0.97280214	-2.28166842
H	1.23907901	1.40693139	-3.24003926
C	1.06523887	1.93447928	3.71773194
H	0.37395508	2.76690145	3.54910560
H	0.85214212	1.47652571	4.68301993
H	2.07588173	2.35328364	3.71316260
C	1.54488399	0.81576589	-1.23368887
C	0.79806253	1.08037843	-2.30455002
H	2.62602644	0.93727620	-1.30293109
O	0.45040703	-0.19599940	2.81262865

Allylacetate
Cas: 591-87-7
IR stretch 1708
Intensity 4.31
Outermost: 2
Innermost: 1
C next to C=C: 6

C	0.92120148	0.29701860	-1.67383597
C	1.27445836	1.21050585	-2.57446767
H	1.49424657	-0.62171571	-1.56961978
H	0.71928134	2.13701517	-2.69001192
H	2.12479802	1.06273092	-3.23064865
C	-0.27156975	0.42832256	-0.77930400
O	0.17354805	0.26077106	0.59157677
C	-0.79832938	0.26659812	1.53465144
C	-0.20913936	0.08805409	2.91596501
O	-1.97222496	0.40280027	1.28254981
H	-1.01929441	-0.34182278	-0.99178602
H	-0.75398561	1.40251407	-0.88591268
H	-1.01037177	0.05308532	3.65120736
H	0.46527808	0.91890713	3.13722325
H	0.38000519	-0.83085062	2.95415905

Allylphenylether
Cas: 1746-13-0
IR stretch 1708
Intensity 5.66
Outermost: 2
Innermost: 1
C next to C=C: 6

C	0.93588061	0.35511750	-1.65177517
C	0.95426593	1.09018630	-2.76024237
H	1.56305142	-0.52912077	-1.56500533
H	0.34294679	1.98261879	-2.85979121
H	1.57715295	0.82556585	-3.60731058
C	0.06067505	0.64440094	-0.46966457
O	0.88150878	0.67161637	0.70044200
C	0.27665741	0.84423835	1.91380183
C	-1.09752652	1.04650299	2.09090149
C	-1.60896166	1.21426001	3.38238802
C	-0.77088932	1.18428137	4.49380114
C	0.60186108	0.98351094	4.30768917
C	1.12489560	0.81449858	3.03105056
H	-1.77059317	1.07752580	1.24438490
H	-2.67496813	1.37035572	3.50997269
H	-1.17606995	1.31527673	5.49066491
H	1.26796195	0.95812013	5.16362050
H	2.18579129	0.65806129	2.87218739
H	-0.69806327	-0.14312922	-0.35906020
H	-0.45728742	1.60286484	-0.59521708

allylbenzene

Cas: 300-57-2
IR stretch 1696
Intensity 16.75
Outermost: 2
Innermost: 6
C next to C=C: 1

C	0.45867605	-0.57488402	-1.43961683
C	0.55026152	1.14530892	-3.27842643
H	1.88677482	1.09425538	-1.66690088
H	-0.30928006	0.71086492	-3.78144727
H	1.00094751	2.01695561	-3.74043099
C	1.02901233	0.62784093	-2.14874248
H	1.21375637	-1.36797348	-1.40352962
H	-0.38786852	-0.96578393	-2.01413058
C	0.01717237	-0.25855429	-0.01918579
C	-0.99005296	0.68795092	0.21345839
C	-1.40243772	0.98695996	1.51101083
C	-0.80784041	0.34719587	2.60208834
C	0.19910689	-0.59247127	2.38286998
C	0.60653292	-0.89135243	1.08018474
H	-1.44591853	1.19647932	-0.63026178
H	-2.18563724	1.72018706	1.67254109
H	-1.12687659	0.58083184	3.61213073
H	0.66838943	-1.09372029	3.22288821
H	1.38990590	-1.62516679	0.91644541

Homoallylmethyl ether
Cas: 4696-30-4
IR stretch 1694
Intensity 18.8
Outermost: 15
Innermost: 14
C next to C=C: 1

C	1.01283228	0.38007797	0.12710680
H	-0.06760614	0.21562257	0.08828078
H	1.47509841	-0.55988630	0.45082891
C	1.32114009	1.44034473	1.18462396
H	2.40249559	1.64973531	1.21128343
H	0.81167528	2.38310695	0.93346321
O	0.88574258	0.96872866	2.44897217
H	1.21795468	1.26934291	-3.25740584
H	-0.29935220	0.88511888	-2.27045732
C	1.11761701	1.89619615	3.49125012
H	0.58420834	2.84099236	3.31392155
H	0.75168836	1.44959766	4.41619460
H	2.18892307	2.11822441	3.59994414
C	1.53503632	0.76981816	-1.22857548
C	0.78177760	0.98745804	-2.30522691
H	2.61565065	0.88440929	-1.30949694

pentafluoroallylbenzene

Cas: 1736-60-3
IR stretch: 1698
Intensity: 13.59
Outermost: 2
Innermost: 6
C next to C=C: 1

C	0.17127817	-0.59680027	-1.52197124
C	0.86958175	1.18810615	-3.15084895
H	2.12098154	0.44409252	-1.64134456
H	-0.09938487	1.16756431	-3.64101710
H	1.60407382	1.88409427	-3.54061092
C	1.14426663	0.39613960	-2.11807784
H	0.60328011	-1.60115565	-1.55588852
H	-0.75078994	-0.61002360	-2.10448309
C	-0.15255979	-0.26151652	-0.07849074
C	-1.26590406	0.50732976	0.26244570
C	-1.55940533	0.84483272	1.58204121
C	-0.71665481	0.41213911	2.60449207
C	0.40700054	-0.35329829	2.29735343
C	0.67131750	-0.67553008	0.96845856
F	-2.09760580	0.94127179	-0.70145791
F	-2.64002812	1.57903894	1.87442289
F	-0.98485524	0.72972743	3.87483576
F	1.21982441	-0.76980829	3.27618432
F	1.76480220	-1.41398630	0.69873690

3-buten-1-yl benzene

Cas: 768-56-9
IR stretch 1697
Intensity 19.88
Outermost: 2
Innermost: 6
C next to C=C: 1

C	-1.33741378	-0.47152910	0.03847251
C	0.06416613	-1.07206621	-1.96656678
H	-1.10818296	0.65382211	-1.84676708
H	0.41545043	-1.98861368	-1.50038553
H	0.43435141	-0.85507574	-2.96275217
C	-0.78457340	-0.25673083	-1.34258211
H	-1.00287811	-1.43569317	0.43333617
H	-2.43282173	-0.50880822	-0.00326762
C	-1.52601601	0.45731214	2.39491873
C	-0.83568509	-0.25951112	3.38049605
C	-1.40365530	-0.48323763	4.63561631
C	-2.67760215	0.00823311	4.92582012
C	-3.37620036	0.72532803	3.95256828
C	-2.80328067	0.94594283	2.69953533
H	0.15723378	-0.64201092	3.16293282
H	-0.85091691	-1.03773425	5.38681675
H	-3.11999089	-0.16226881	5.90137560
H	-4.36497032	1.11552104	4.17016251
H	-3.35157398	1.50789890	1.94890966
C	-0.92941724	0.65425758	1.01992492
H	-1.25024862	1.61757884	0.61050979
H	0.16197439	0.68510901	1.08608272

2-allyltoluene
Cas: 1587-04-8
IR stretch 1694
Intensity 18.80
Outermost: 2
Innermost: 6
C next to C=C: 1

C	0.94589735	1.11741502	-1.28361854
C	1.95992466	-0.55837045	-2.86882747
H	-0.08814135	-0.44673197	-2.46103756
H	2.96165961	-0.17650796	-2.69220035
H	1.86571937	-1.38997274	-3.55857453
C	0.89771504	-0.02877831	-2.26576348
H	0.40346649	1.97291661	-1.69922308
H	1.98407966	1.43334300	-1.15026640
C	0.35182540	0.73665316	0.06337007
C	-1.02391718	0.88444035	0.33213536
C	-1.51307904	0.48460450	1.58242255
C	-0.67241278	-0.05408797	2.55607390
C	0.68754222	-0.20180824	2.28631256
C	1.18642988	0.19231251	1.04564929
H	-1.94310242	0.92098586	-1.63657959
H	-2.57187003	0.59939027	1.79395117
H	-1.07741531	-0.35508252	3.51632389
H	1.35414381	-0.61908690	3.03342683
H	2.24384044	0.07369067	0.82872346
C	-1.96908228	1.47223132	-0.69272378
H	-1.71309323	2.51201096	-0.92169378
H	-2.99637178	1.45644606	-0.32372382

3-allyltoluene
Cas: 3333-20-8
IR stretch 1696
Intensity 16.07
Outermost: 2
Innermost: 6
C next to C=C: 1

C	0.64181910	0.97199347	-1.58054800
C	2.34129594	-0.53730015	-2.66921835
H	0.33732965	-1.06720478	-2.37109639
H	3.12909631	0.20253485	-2.55655761
H	2.61247302	-1.47599476	-3.14007810
C	1.09986519	-0.29946658	-2.25023956
H	-0.12865576	1.44973177	-2.19582436
H	1.48202518	1.67170685	-1.51962300
C	0.07343499	0.72399876	-0.19187327
C	-1.27125193	0.98561223	0.09322605
C	-1.81667611	0.75602951	1.36221225
C	-0.97775906	0.25115859	2.36369183
C	0.36468057	-0.01660069	2.09568121
C	0.88904672	0.21436922	0.82436103
H	-1.90998686	1.37995778	-0.69262735
H	-1.37775441	0.06609893	3.35623089
H	-3.37769735	1.78260466	2.45044035
H	1.00363286	-0.40889470	2.88017244
H	1.93074332	-0.00712556	0.61537771
C	-3.27338321	1.04390843	1.65008839
H	-3.79638210	0.13907734	1.97403415
H	-3.78448521	1.43025103	0.76639220

4-allyltoluene
Cas: 3333-13-9
IR stretch 1696
Intensity 18.97
Outermost: 2
Innermost: 6
C next to C=C: 1

C	0.71372088	0.95428937	-1.67100241
C	2.50167503	-0.56794594	-2.58564437
H	0.48517834	-1.10885314	-2.42351736
H	3.27297999	0.18247388	-2.43546237
H	2.81490663	-1.51662361	-3.00778466
C	1.23042122	-0.33048062	-2.26809471
H	-0.01464900	1.40520638	-2.35415105
H	1.54092770	1.66548644	-1.57274823
C	0.04777890	0.74355221	-0.32031139
C	-1.30116879	1.05379682	-0.11639902
C	-1.90501916	0.85461754	1.12493494
C	-1.18085158	0.33791769	2.20649125
C	0.16852031	0.02640074	1.99905055
C	0.77207309	0.22201697	0.75718266
H	-1.88625286	1.45755810	-0.93743380
H	-2.95416121	1.10449395	1.25420647
H	-1.13882503	-0.28429069	4.27744640
H	0.75423924	-0.37726210	2.81948933
H	1.81666764	-0.03970209	0.62000558
C	-1.84181519	0.12539837	3.54990025
H	-2.68523065	-0.56699717	3.46931552
H	-2.23187327	1.06589849	3.95064697

2-Allylanisole
Cas: 3698-28-0
IR stretch: 1695
Intensity: 19.79
Outermost: 2
Innermost: 6
C next to C=C: 1

C	1.24521336	1.15257912	-1.27393934
C	1.91153999	-0.58538545	-2.97056192
H	-0.06973818	0.01032312	-2.63047248
H	2.96371816	-0.48314597	-2.71895344
H	1.65951567	-1.30437719	-3.74250209
C	0.97569292	0.13826672	-2.35976427
H	0.92617073	2.14052879	-1.62346685
H	2.31896641	1.20121349	-1.07525607
C	0.51090443	0.82436259	0.01251045
C	-0.86753752	1.09493887	0.13709042
C	-1.55065035	0.77709479	1.31516433
C	-0.86481815	0.18177243	2.37812395
C	0.49447113	-0.09486416	2.27048527
C	1.16699541	0.22888575	1.08838267
O	-1.45998059	1.67561021	-0.95297561
H	-2.60763922	0.98641422	1.41413671
H	-1.40359508	-0.06172243	3.28755095
H	1.02919929	-0.55575368	3.09323697
H	2.22722934	0.01444386	0.99588617
C	-2.84202798	1.99478729	-0.88448898
H	-3.04699608	2.70706972	-0.07794405
H	-3.45139989	1.09670255	-0.73583949
H	-3.09634772	2.44913874	-1.84085997

3-allylanisole
Cas: 2907-1-18
IR stretch 1696
Intensity 12.10
Outermost: 2
Innermost: 6
C next to C=C: 1

C	0.79043072	1.07171383	-1.60709673
C	2.51120619	-0.46890954	-2.61509084
H	0.46212470	-0.89664097	-2.55163558
H	3.32101029	0.21545381	-2.37742744
H	2.77953508	-1.39249029	-3.11646404
C	1.24767005	-0.18377943	-2.30666361
H	0.11714691	1.63097617	-2.26566778
H	1.65597466	1.71375901	-1.41250081
C	0.06591595	0.77646814	-0.30325114
C	-1.27385694	1.11642054	-0.14076643
C	-1.94859825	0.83867451	1.05847793
C	-1.27108218	0.21307037	2.10898089
C	0.07603509	-0.12884543	1.94054826
C	0.74268021	0.14270588	0.75195118
O	-3.26141670	1.21671672	1.10285650
H	-1.76864444	-0.01031228	3.04330621
H	-3.55752797	1.48786163	3.14969861
H	0.60153721	-0.61591069	2.75533998
H	1.78283561	-0.13949422	0.63013124
C	-3.99438406	0.96300099	2.29295260
H	-4.03901639	-0.10943519	2.51255573
H	-5.00135696	1.33728425	2.11542058
H	-1.82398330	1.60529684	-0.93793431

4-allylanisole
Cas: 140-67-0
IR stretch 1696
Intensity 21.85
Outermost: 2
Innermost: 6
C next to C=C: 1

C	0.66877879	0.96033704	-1.62142274
C	2.43500682	-0.46527208	-2.71614620
H	0.45681516	-1.08672217	-2.42162792
H	3.18806219	0.30937662	-2.59953388
H	2.74953062	-1.38860188	-3.19034874
C	1.18354170	-0.28545391	-2.29761175
H	-0.12842633	1.40082366	-2.23063341
H	1.47427622	1.70100562	-1.56886385
C	0.12085267	0.68603597	-0.23032215
C	-1.21302605	0.93115864	0.09127079
C	-1.72095898	0.67818991	1.37125165
C	-0.87592479	0.16658355	2.35971800
C	0.46922397	-0.08871858	2.05067924
C	0.95227488	0.16571528	0.77510697
O	-1.26276349	-0.11552184	3.64045221
H	-2.76302925	0.88321898	1.57847948
H	-2.70779806	-0.16624101	5.04625368
H	1.11360122	-0.48798198	2.82592167
H	1.99190741	-0.04781318	0.54750431
C	-2.61590076	0.12247580	4.00037653
H	-3.30158448	-0.48143773	3.39558058
H	-2.87735895	1.18094577	3.89150351
H	-1.88058572	1.33085565	-0.66623429

3-(3.5-Dimethylphenyl)-1-propene

Cas: 77446-17-4
IR stretch 1695
Intensity 16.18
Outermost: 2
Innermost: 6
C next to C=C: 1

C	0.64769800	0.96930500	-1.58015200
C	2.32679400	-0.56705700	-2.66330500
H	0.31722000	-1.07063000	-2.35748300
H	3.12364600	0.16396700	-2.55707300
H	2.58553900	-1.51183000	-3.12899700
C	1.08929300	-0.31148600	-2.24304700
H	-0.11772500	1.45250800	-2.19741500
H	1.49653000	1.65887200	-1.52405400
C	0.07709500	0.73506800	-0.18995000
C	-1.26780900	0.98977100	0.08862400
C	-1.80251200	0.76429700	1.36353700
C	-0.95690600	0.27598600	2.36375500
C	0.39578400	0.00986800	2.11500700
C	0.89688700	0.24161600	0.83136000
H	-1.91164200	1.37205800	-0.69865300
H	-1.35840800	0.09747000	3.35833000
H	-3.36763400	1.78507500	2.45257900
C	1.28659400	-0.52009500	3.21684200
H	1.94011200	0.02811800	0.61726600
C	-3.26059400	1.04115200	1.65744900
H	-3.77387800	0.13418900	1.99080200
H	-3.77972100	1.41607900	0.77352300
H	2.30725800	-0.67413700	2.86226700
H	0.91376900	-1.47541400	3.59843700
H	1.32311100	0.17414400	4.06182400

3-(2.4.6-trimethylphenyl)-1-propene

Cas: 4810-05-3
IR stretch 1693
Intensity 21.55
Outermost: 2
Innermost: 6
C next to C=C: 1

C	1.84743050	-0.33289985	-0.15722163
C	3.35765335	-0.09955874	1.85224639
H	1.63813457	-1.28993211	1.82530919
H	4.01979918	0.58314233	1.32691642
H	3.61446776	-0.34067427	2.87794081
C	2.28250905	-0.61765278	1.26157564
H	1.92979124	-1.25213026	-0.74437732
H	2.53559181	0.38582813	-0.60771935
C	0.41737078	0.18265849	-0.21920861
C	-0.65815518	-0.71382252	-0.38991179
C	-1.96590946	-0.22249576	-0.41224786
C	-2.24572372	1.13958841	-0.26688393
C	-1.17022577	2.01117015	-0.09384887
C	0.15387014	1.55664566	-0.06453151
C	-0.42444446	-2.20105495	-0.55477724
H	-2.78708286	-0.92183693	-0.54539326
H	-3.71302642	2.72534363	-0.16612936
H	-1.36214096	3.07384886	0.02523562
C	1.27563747	2.55195418	0.13605507
C	-3.67168663	1.64214690	-0.29511021
H	-4.26684774	1.18456947	0.50107137
H	-4.15751195	1.39652684	-1.24436934
H	0.13532772	-2.42037699	-1.46986623
H	-1.37503407	-2.73465309	-0.61153936
H	0.14626062	-2.62063383	0.27830354
H	1.94919196	2.57744866	-0.72686790
H	1.88131626	2.29858729	1.01000059
H	0.87667644	3.55836936	0.27654395

3-(1-Naphthyl)-1-propene

Cas: 2489-86-3
IR stretch 1696
Intensity 14.12
Outermost: 2
Innermost: 6
C next to C=C: 1

C	0.85293200	0.76099900	-1.62047400
C	2.24575000	-0.28000800	-3.45137000
H	0.37941400	-1.01188700	-2.84793300
H	3.03780700	0.45353600	-3.32629300
H	2.39173400	-1.03167300	-4.21914700
C	1.14807800	-0.25564700	-2.69909100
H	0.02389300	1.39388100	-1.95559300
H	1.71612700	1.42041700	-1.48923300
C	0.44938100	0.12715100	-0.30027000
C	-0.87832300	0.12086900	0.07701000
C	-1.30790800	-0.47974100	1.28440800
C	-0.39554500	-1.07363300	2.12179700
C	3.28105800	-1.70932700	2.30875400
C	3.71344200	-1.11892300	1.09734900
C	2.80800400	-0.52767000	0.24508500
C	1.41988900	-0.48976900	0.55605600
C	0.98487200	-1.09228400	1.78474900
C	1.94642900	-1.69511400	2.64081900
H	-1.61383800	0.59159400	-0.56815900
H	-2.36099800	-0.46379700	1.54408300
H	-0.71396600	-1.53395700	3.05166500
H	4.00431100	-2.17258800	2.97127300
H	4.76669100	-1.13610800	0.83811200
H	3.15609100	-0.09678600	-0.68400900
H	1.60555900	-2.14586200	3.56760300

3-(2-Naphthyl)-1-propene

Cas: 2489-87-4
IR stretch 1699
Intensity 17.04
Outermost: 2
Innermost: 6
C next to C=C: 1

C	-1.77044600	1.54009900	-1.10028400
C	-1.19123900	2.12374800	-3.47920900
H	-1.59224000	0.17614400	-2.82522800
H	-1.09049900	3.17840000	-3.23823600
H	-1.02205700	1.83748800	-4.51151800
C	-1.51162900	1.22640900	-2.54917800
H	-2.79691100	1.24809400	-0.84841200
H	-1.71207800	2.62410600	-0.94561800
C	0.48817700	0.58258600	-0.45828800
C	-0.82639400	0.84119600	-0.13203100
C	-1.29677300	0.46885600	1.15792100
C	-0.46743000	-0.13354900	2.07349100
C	3.08791700	-1.27812000	2.33049100
C	3.56940300	-0.91377300	1.04809000
C	2.73331500	-0.31006600	0.13655300
C	1.37573600	-0.03926900	0.46076900
C	0.89070200	-0.40678900	1.75771800
C	1.77870400	-1.03007300	2.67530300
H	0.86411400	0.85739100	-1.43867900
H	-2.33302500	0.66509900	1.41633000
H	-0.84452300	-0.41265200	3.05242900
H	3.75702600	-1.75378700	3.03946800
H	4.60327200	-1.11371800	0.78752700
H	3.10117400	-0.03119300	-0.84587200
H	1.40655700	-1.30786400	3.65652000

Allylethylether

CAS: 557-31-3
IR stretch 1705
Intensity 4.37
Outermost: 15
Innermost: 14
C next to C=C: 1

C	1.00834798	0.45838461	0.37280304
H	-0.06423322	0.22093443	0.30836072
H	1.52988341	-0.46142137	0.68825742
O	1.23734025	1.48142584	1.33187572
H	0.58366146	3.14960487	3.29704655
H	0.84203479	1.98824129	4.61353257
C	0.84505561	1.10639478	2.64534449
H	-0.22737424	0.85775403	2.65688216
H	1.39222592	0.20132875	2.95180619
H	-0.20134893	0.51645941	-2.10932960
H	1.26041831	1.16205583	-3.04058616
H	2.20296947	2.49422444	3.59348061
C	1.13682754	2.25627579	3.59553704
C	1.52929047	0.90202051	-0.96193263
C	0.82936320	0.85955918	-2.09270022
H	2.55637252	1.26065097	-0.96430332

Allylbutylether

CAS: 3739-64-8
IR stretch 1705
Intensity 4.41
Outermost: 15
Innermost: 14
C next to C=C: 1

C	0.96715897	0.48901730	0.34597496
H	-0.12355048	0.37167144	0.25925540
H	1.36981885	-0.46118737	0.73667894
O	1.28764145	1.54029113	1.24606288
C	1.18058805	3.43278758	5.82200616
H	-0.32528627	2.16198471	4.93360900
C	0.82206213	1.29907996	2.56571357
H	-0.27398304	1.18709182	2.56228897
H	1.24350697	0.35368487	2.94357070
C	1.23168851	2.45679481	3.46434195
H	0.81746891	3.38428689	3.05455826
H	1.17399869	1.33319877	5.30933756
H	2.32199540	2.55773328	3.43251707
C	1.57273068	0.78074995	-0.99492208
C	0.90516828	0.73688893	-2.14500772
H	2.63302853	1.02414006	-0.98318574
H	-0.15642316	0.50765787	-2.17636796
H	1.39457942	0.92455788	-3.09442625
C	0.76553946	2.27038656	4.91317303
H	2.26897278	3.54314554	5.84431483
H	0.83836960	3.27860646	6.84885178
H	0.75896165	4.37779175	5.46645490

2-4-dimethylphenyl-prop-1-ene

CAS: 3840-33-3
IR stretch 1694
Intensity 19.33
Outermost: 2
Innermost: 6
C next to C=C: 1

C	0.85918000	1.00258400	-1.60221100
C	2.20334500	-0.75931800	-2.81379600
H	0.13505600	-0.87477600	-2.50977600
H	3.13073400	-0.21166900	-2.66992600
H	2.26688000	-1.70019500	-3.34951800
C	1.04305300	-0.29419600	-2.35534100
H	0.23660100	1.67483900	-2.20355000
H	1.82892500	1.49291900	-1.47876300
C	0.18031600	0.79372800	-0.25878500
C	-1.19910600	0.99822100	-0.14037600
C	-1.86901900	0.77961200	1.06062400
C	-1.16947200	0.34739200	2.19284200
C	0.20910300	0.14846500	2.07201900
C	0.89939600	0.35949400	0.87144200
H	2.77275900	-0.20565700	1.77754100
H	-2.94009500	0.94932700	1.11881200
H	-1.19413600	-0.21804400	4.28084900
H	0.76959100	-0.18369800	2.94173300
C	2.39147200	0.12534500	0.80967700
C	-1.88658200	0.10807400	3.50254800
H	-2.65828300	-0.66018500	3.39424400
H	-2.38292100	1.01841700	3.85215400
H	2.64412000	-0.63162900	0.06271800
H	-1.75743700	1.33821500	-1.00795300
H	2.92735500	1.03919600	0.53277200

2-6-dimethylphenyl-prop-1-ene

CAS: 1587-05-9
IR stretch 1694
Intensity 19.13
Outermost: 2
Innermost: 6
C next to C=C: 1

C	0.88487800	1.00580100	-1.58348000
C	2.12642100	-0.82146400	-2.80452800
H	0.05323200	-0.81267800	-2.52844200
H	3.08444200	-0.33513700	-2.64283700
H	2.13741000	-1.75826300	-3.35073700
C	0.99170400	-0.28920000	-2.35494900
H	0.34397100	1.73698200	-2.19102300
H	1.88521200	1.41377900	-1.42352100
C	0.16463600	0.81669700	-0.25643600
C	-1.23129200	0.99905200	-0.17523300
C	-1.88011500	0.79093600	1.04743700
C	-1.16669800	0.40454500	2.17887700
C	0.21074100	0.22003700	2.09337000
C	0.88966200	0.41869100	0.88581800
C	-2.04326500	1.42045400	-1.38204400
H	-2.95456000	0.93314700	1.10807300
H	2.91693900	1.12417600	0.57491300
H	0.77112500	-0.08534000	2.97148400
C	2.38566300	0.20070400	0.82767200
H	2.76089500	-0.14520400	1.79273500
H	2.65134000	-0.54183400	0.07093200
H	-1.68137900	0.24597000	3.12064500
H	-1.75812100	2.41885800	-1.72948500
H	-3.10685100	1.44592900	-1.13754900
H	-1.90973100	0.73709600	-2.22513900

4-trifluoromethylphenyl-prop-1-ene

CAS: 1587-05-9
IR stretch 1694
Intensity 19.13
Outermost: 2
Innermost: 6
C next to C=C: 1

C	0.69251296	0.94029285	-1.68013788
C	2.51325652	-0.56586757	-2.55017979
H	0.50147618	-1.13309446	-2.41849952
H	3.27146539	0.19651489	-2.39427191
H	2.84616358	-1.51323628	-2.95961542
C	1.23381472	-0.34416025	-2.25655777
H	-0.04183575	1.37102245	-2.36908378
H	1.50667209	1.66687079	-1.58590715
C	0.03202242	0.73915730	-0.32600176
C	-1.30056485	1.10391668	-0.10786701
C	-1.90002183	0.92242227	1.13773943
C	-1.16454242	0.37056069	2.18735089
C	0.16704714	-0.00270492	1.98393345
C	0.75484329	0.18006418	0.73620243
H	-1.87673953	1.53771651	-0.91866967
H	-2.93216025	1.21322813	1.29266583
F	-0.93701061	0.13972008	4.54417821
H	0.73920786	-0.43023427	2.79839548
H	1.78573929	-0.11890539	0.57961859
C	-1.82458451	0.12571903	3.52268395
F	-2.44354081	-1.08413573	3.56340765
F	-2.77197376	1.05157494	3.80250339

4-Allyl-1.2-dimethoxybenzene
CAS: 93-15-2
IR stretch 1694
Intensity 19.13
Outermost: 2
Innermost: 6
C next to C=C: 1

C	0.72872358	0.83946593	-1.51153593
C	2.02267100	-1.13269652	-2.39681670
H	-0.06880814	-1.05258157	-2.32273387
H	2.97422891	-0.64579383	-2.20139843
H	2.05925976	-2.12515970	-2.83274874
C	0.86619349	-0.53277357	-2.11995164
H	0.19011716	1.49268461	-2.20650519
H	1.72474280	1.27468852	-1.37332493
C	-0.01879579	0.82577712	-0.18678851
C	-1.16304694	1.59593593	0.00887179
C	-1.82987835	1.56836174	1.23818508
C	-1.36664425	0.78282873	2.28599668
C	-0.19974931	0.00392723	2.10168876
C	0.45202403	0.02849774	0.86800763
O	-2.01402624	0.82651128	3.49830056
H	-2.72014011	2.16484976	1.40462518
H	-3.17677108	-0.16446054	4.83366617
O	0.21716233	-0.72735365	3.17685746
H	1.33759833	-0.57355387	0.70836676
C	-2.70364255	-0.37012796	3.87378424
H	-2.01278168	-1.20978805	3.97720902
H	-3.47342987	-0.61537074	3.13314996
H	-1.54054970	2.22032690	-0.79402645
C	1.40639067	-1.49425054	3.04764063
H	2.26660098	-0.85696679	2.81643612
H	1.30582102	-2.25897600	2.26983764
H	1.56154063	-1.97609271	4.01167505

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