

-Supplementary Information-

A DFT/PCM-based methodology for predicting solvolytic reactivities of organic carbonates

Mirela Matić and Bernard Denegri*

*University of Zagreb, Faculty of Pharmacy and Biochemistry
Ante Kovačića 1, 10000 Zagreb, Croatia*

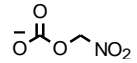
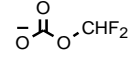
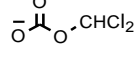
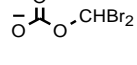
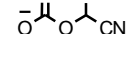
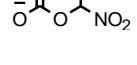
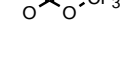
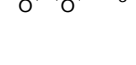
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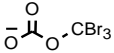
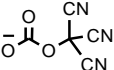
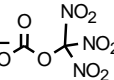
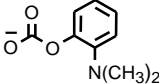
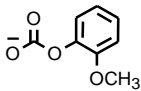
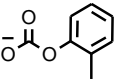
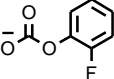
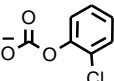
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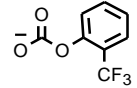
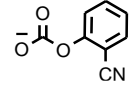
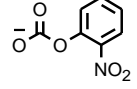
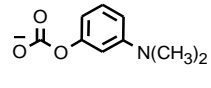
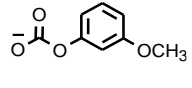
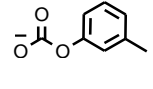
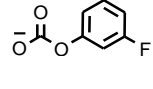
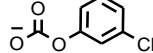
1. Tables

Table S1. Predicted solvolytic reactivities of other 4-methoxybenzhydryl aryl/alkyl carbonates and calculated nucleofugalities (N_f^{calc}) of various aryl/alkyl carbonate leaving groups along with corresponding estimated s_f values (s_f^{estim})

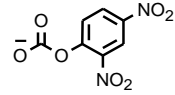
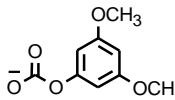
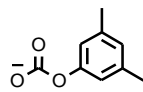
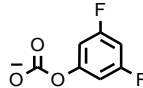
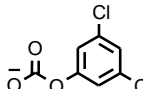
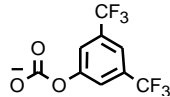
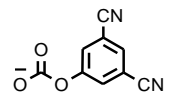
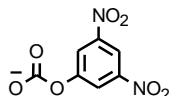
Solvent ^[a]	Ar/R Carbonate	$\Delta G^\ddagger_{\text{calc}}$ ^[b]	$\log k^{\text{calc}}$ ^[c]	s_f^{estim} ^[d]	N_f^{calc} ^[e]	Ar/R Carbonate leaving group
80E20W	hydrogen carbonate (bicarbonate)	21.63	-3.06	0.92	-1.22	
	propyl carbonate	23.25	-4.25	1.00	-2.18	
	ethenyl carbonate (vinyl carbonate)	20.49	-2.23	0.87	-0.46	
	ethynyl carbonate	16.51	0.69	0.70	3.08	
	fluoromethyl carbonate	20.18	-2.00	0.86	-0.24	
	chloromethyl carbonate	19.48	-1.48	0.83	0.30	
	bromomethyl carbonate	19.14	-1.23	0.81	0.57	
	cyanomethyl carbonate	19.56	-1.54	0.83	0.24	

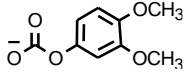
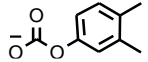
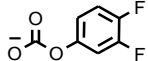
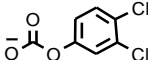
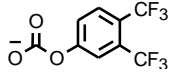
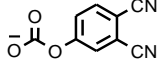
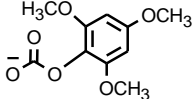
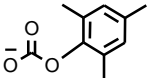
Solvent ^[a]	Ar/R Carbonate	$\Delta G^{\ddagger \text{calc}}$ ^[b]	$\log k^{\text{calc}}$ ^[c]	$s_{\text{f}}^{\text{estim}}$ ^[d]	$N_{\text{f}}^{\text{calc}}$ ^[e]	Ar/R Carbonate leaving group
	nitromethyl carbonate	17.88	-0.31	0.76	1.68	
	difluoromethyl carbonate	17.79	-0.24	0.75	1.77	
	dichloromethyl carbonate	17.27	0.13	0.73	2.27	
	dibromomethyl carbonate	17.16	0.22	0.73	2.39	
	dicyanomethyl carbonate	16.23	0.90	0.69	3.40	
	dinitromethyl carbonate	15.01	1.79	0.63	4.92	
	trifluoromethyl carbonate ^[f]	16.16	0.94	0.68	3.47	
	trichloromethyl carbonate ^[f]	16.93	0.38	0.72	2.63	

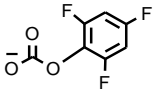
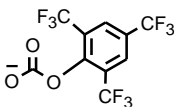
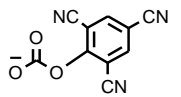
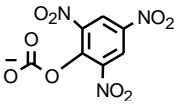
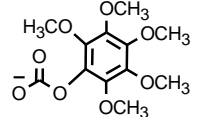
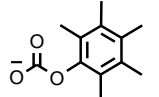
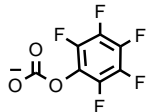
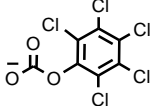
Solvent ^[a]	Ar/R Carbonate	$\Delta G^\ddagger_{\text{calc}}$ ^[b]	$\log k^{\text{calc}}$ ^[c]	$s_{\text{f}}^{\text{estim}}$ ^[d]	$N_{\text{f}}^{\text{calc}}$ ^[e]	Ar/R Carbonate leaving group
	tribromomethyl carbonate ^[f]	15.98	1.08	0.68	3.69	
	tricyanomethyl carbonate	14.82	1.92	0.62	5.18	
	trinitromethyl carbonate	11.42	4.42	0.47	11.41	
	2-(dimethylamino)phenyl carbonate	21.21	-2.75	0.91	-0.95	
	2-methoxyphenyl carbonate	21.35	-2.86	0.91	-1.04	
	2-methylphenyl carbonate	20.96	-2.57	0.89	-0.79	
	2-fluorophenyl carbonate	20.00	-1.87	0.85	-0.10	
	2-chlorophenyl carbonate	20.75	-2.42	0.89	-0.64	

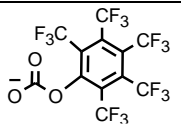
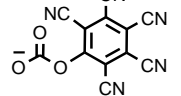

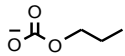
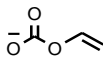
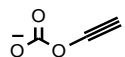
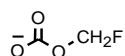
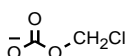
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	2-(trifluoromethyl)phenyl carbonate	19.97	-1.85	0.85	-0.08	
	2-cyanophenyl carbonate	19.36	-1.40	0.82	0.39	
	2-nitrophenyl carbonate	19.07	-1.19	0.81	0.63	
	3-(dimethylamino)phenyl carbonate	21.76	-3.16	0.93	-1.31	
	3-methoxyphenyl carbonate	21.25	-2.78	0.91	-0.98	
	3-methylphenyl carbonate	20.76	-2.43	0.89	-0.65	
	3-fluorophenyl carbonate	19.99	-1.86	0.85	-0.09	
	3-chlorophenyl carbonate	20.19	-2.00	0.86	-0.24	

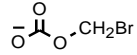
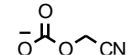
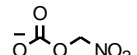
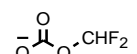
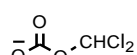
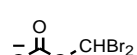
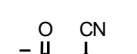
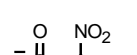
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	3-(trifluoromethyl)phenyl carbonate	20.34	-2.12	0.87	-0.35	
	3-cyanophenyl carbonate	19.85	-1.76	0.85	0.01	
	3-nitrophenyl carbonate	20.05	-1.90	0.85	-0.14	
	4-(trifluoromethyl)phenyl carbonate	20.40	-2.16	0.87	-0.39	
	2,4-dimethoxyphenyl carbonate	21.29	-2.81	0.91	-1.01	
	2,4-difluorophenyl carbonate	20.02	-1.88	0.85	-0.12	
	2,4-dichlorophenyl carbonate	19.45	-1.47	0.83	0.32	
	2,4-dicyanophenyl carbonate	17.92	-0.35	0.76	1.64	

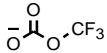
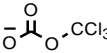
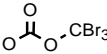
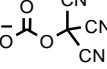
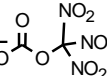
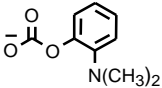
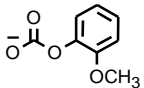
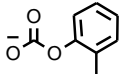
Solvent ^[a]	Ar/R Carbonate	$\Delta G^{\ddagger \text{calc}}$ ^[b]	$\log k^{\text{calc}}$ ^[c]	$s_{\text{f}}^{\text{estim}}$ ^[d]	$N_{\text{f}}^{\text{calc}}$ ^[e]	Ar/R Carbonate leaving group
	2,4-dinitrophenyl carbonate	17.39	0.05	0.74	2.15	
	3,5-dimethoxyphenyl carbonate	20.47	-2.21	0.87	-0.45	
	3,5-dimethylphenyl carbonate	20.87	-2.50	0.89	-0.72	
	3,5-difluorophenyl carbonate	19.82	-1.74	0.84	0.03	
	3,5-dichlorophenyl carbonate	19.58	-1.56	0.83	0.22	
	3,5-di(trifluoromethyl)phenyl carbonate	19.48	-1.49	0.83	0.30	
	3,5-dicyanophenyl carbonate	18.66	-0.88	0.79	0.98	
	3,5-dinitrophenyl carbonate	18.25	-0.59	0.78	1.33	

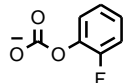
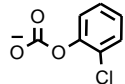
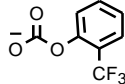
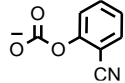
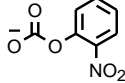
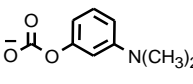
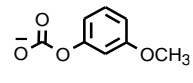
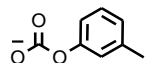
Solvent ^[a]	Ar/R Carbonate	$\Delta G^{\ddagger \text{calc}}$ ^[b]	$\log k^{\text{calc}}$ ^[c]	$s_{\text{f}}^{\text{estim}}$ ^[d]	$N_{\text{f}}^{\text{calc}}$ ^[e]	Ar/R Carbonate leaving group
	3,4-dimethoxyphenyl carbonate	21.50	-2.97	0.92	-1.14	
	3,4-dimethylphenyl carbonate	21.70	-3.12	0.93	-1.27	
	3,4-difluorophenyl carbonate	19.97	-1.85	0.85	-0.08	
	3,4-dichlorophenyl carbonate	20.20	-2.01	0.86	-0.25	
	3,4-di(trifluoromethyl)phenyl carbonate	18.93	-1.08	0.80	0.75	
	3,4-dicyanophenyl carbonate	18.37	-0.67	0.78	1.23	
	2,4,6-trimethoxyphenyl carbonate	21.52	-2.98	0.92	-1.15	
	2,4,6-trimethylphenyl carbonate	20.37	-2.14	0.87	-0.37	

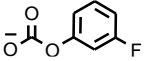
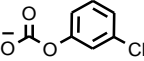
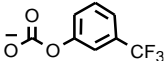
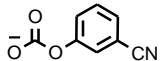
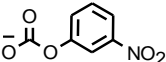
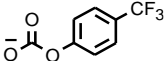
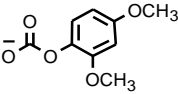
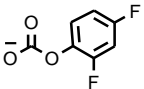
Solvent ^[a]	Ar/R Carbonate	$\Delta G^\ddagger_{\text{calc}}$ ^[b]	$\log k^{\text{calc}}$ ^[c]	$s_{\text{f}}^{\text{estim}}$ ^[d]	$N_{\text{f}}^{\text{calc}}$ ^[e]	Ar/R Carbonate leaving group
	2,4,6-trifluorophenyl carbonate	19.10	-1.20	0.81	0.61	
	2,4,6-tri(trifluoromethyl)phenyl carbonate	17.60	-0.11	0.75	1.94	
	2,4,6-tricyanophenyl carbonate	16.14	0.96	0.68	3.50	
	2,4,6-trinitrophenyl carbonate	15.33	1.56	0.65	4.50	
	pentamethoxyphenyl carbonate	21.21	-2.75	0.91	-0.95	
	pentamethylphenyl carbonate	21.15	-2.71	0.90	-0.91	
	pentafluorophenyl carbonate	17.96	-0.37	0.76	1.60	
	pentachlorophenyl carbonate	16.92	0.39	0.72	2.64	

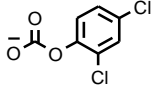
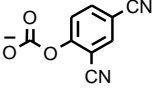
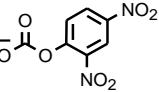
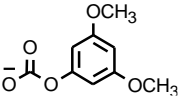
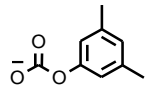
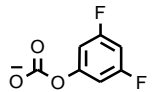
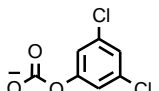
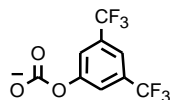
Solvent ^[a]	Ar/R Carbonate	$\Delta G^\ddagger_{\text{calc}}$ ^[b]	$\log k^{\text{calc}}$ ^[c]	$s_{\text{f}}^{\text{estim}}$ ^[d]	$N_{\text{f}}^{\text{calc}}$ ^[e]	Ar/R Carbonate leaving group
	penta(trifluoromethyl)phenyl carbonate	16.41	0.77	0.69	3.20	
	pentacyanophenyl carbonate	14.13	2.44	0.59	6.20	
60E40W	hydrogen carbonate (bicarbonate)	20.89	-2.52	0.87	-0.82	
	propyl carbonate	22.50	-3.70	0.92	-1.91	
	ethenyl carbonate (vinyl carbonate)	19.77	-1.69	0.82	0.04	
	ethynyl carbonate	15.82	1.20	0.68	3.85	
	fluoromethyl carbonate	19.46	-1.47	0.81	0.28	
	chloromethyl carbonate	18.76	-0.96	0.79	0.88	

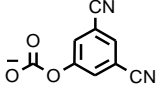
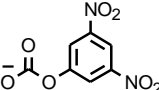
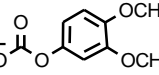
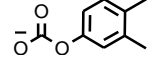
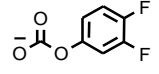
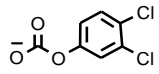
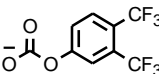
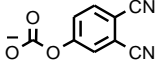
Solvent ^[a]	Ar/R Carbonate	$\Delta G^{\ddagger \text{calc}}$ ^[b]	$\log k^{\text{calc}}$ ^[c]	$s_{\text{f}}^{\text{estim}}$ ^[d]	$N_{\text{f}}^{\text{calc}}$ ^[e]	Ar/R Carbonate leaving group
	bromomethyl carbonate	18.42	-0.71	0.78	1.18	
	cyanomethyl carbonate	18.84	-1.01	0.79	0.81	
	nitromethyl carbonate	17.17	0.20	0.73	2.37	
	difluoromethyl carbonate	17.08	0.27	0.73	2.46	
	dichloromethyl carbonate	16.57	0.65	0.71	3.00	
	dibromomethyl carbonate	16.46	0.73	0.70	3.12	
	dicyanomethyl carbonate	15.54	1.40	0.67	4.18	
	dinitromethyl carbonate	14.34	2.28	0.63	5.74	

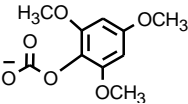
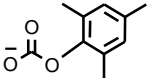
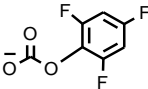
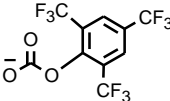
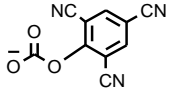
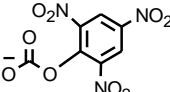
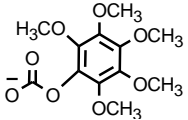
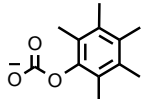
Solvent ^[a]	Ar/R Carbonate	$\Delta G^\ddagger_{\text{calc}}$ ^[b]	$\log k^{\text{calc}}$ ^[c]	$s_{\text{f}}^{\text{estim}}$ ^[d]	$N_{\text{f}}^{\text{calc}}$ ^[e]	Ar/R Carbonate leaving group
	trifluoromethyl carbonate ^[f]	15.51	1.43	0.67	4.23	
	trichloromethyl carbonate ^[f]	16.26	0.87	0.70	3.34	
	tribromomethyl carbonate ^[f]	15.32	1.56	0.66	4.45	
	tricyanomethyl carbonate	14.15	2.42	0.62	6.01	
	trinitromethyl carbonate	10.78	4.89	0.50	11.97	
	2-(dimethylamino)phenyl carbonate	20.47	-2.21	0.85	-0.51	
	2-methoxyphenyl carbonate	20.61	-2.31	0.86	-0.61	
	2-methylphenyl carbonate	20.23	-2.04	0.84	-0.33	

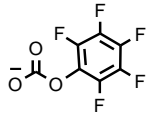
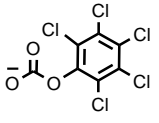
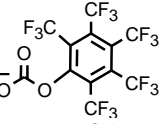
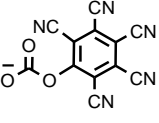

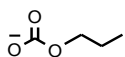
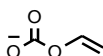
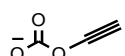
Solvent ^[a]	Ar/R Carbonate	$\Delta G^\ddagger_{\text{calc}}$ ^[b]	$\log k^{\text{calc}}$ ^[c]	$s_{\text{f}}^{\text{estim}}$ ^[d]	$N_{\text{f}}^{\text{calc}}$ ^[e]	Ar/R Carbonate leaving group
	2-fluorophenyl carbonate	19.27	-1.33	0.81	0.44	
	2-chlorophenyl carbonate	20.02	-1.88	0.83	-0.16	
	2-(trifluoromethyl)phenyl carbonate	19.25	-1.32	0.81	0.46	
	2-cyanophenyl carbonate	18.64	-0.87	0.78	0.98	
	2-nitrophenyl carbonate	18.36	-0.66	0.77	1.23	
	3-(dimethylamino)phenyl carbonate	21.02	-2.61	0.87	-0.91	
	3-methoxyphenyl carbonate	20.51	-2.24	0.85	-0.54	
	3-methylphenyl carbonate	20.03	-1.89	0.83	-0.18	

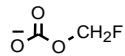
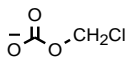
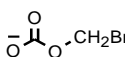
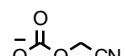
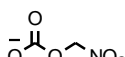
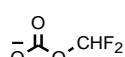
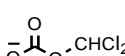
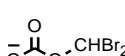
Solvent ^[a]	Ar/R Carbonate	$\Delta G^{\ddagger \text{calc}}$ ^[b]	$\log k^{\text{calc}}$ ^[c]	$s_{\text{f}}^{\text{estim}}$ ^[d]	$N_{\text{f}}^{\text{calc}}$ ^[e]	Ar/R Carbonate leaving group
	3-fluorophenyl carbonate	19.27	-1.33	0.81	0.44	
	3-chlorophenyl carbonate	19.46	-1.47	0.81	0.28	
	3-(trifluoromethyl)phenyl carbonate	19.61	-1.58	0.82	0.16	
	3-cyanophenyl carbonate	19.13	-1.23	0.80	0.56	
	3-nitrophenyl carbonate	19.32	-1.37	0.81	0.39	
	4-(trifluoromethyl)phenyl carbonate	19.67	-1.63	0.82	0.11	
	2,4-dimethoxyphenyl carbonate	20.56	-2.27	0.85	-0.57	
	2,4-difluorophenyl carbonate	19.29	-1.35	0.81	0.42	

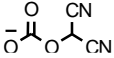
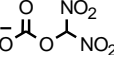
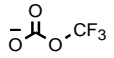
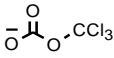
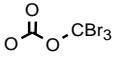
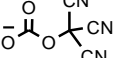
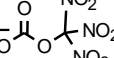
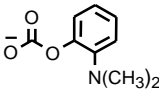
Solvent ^[a]	Ar/R Carbonate	$\Delta G^\ddagger_{\text{calc}}$ ^[b]	$\log k^{\text{calc}}$ ^[c]	s_f^{estim} ^[d]	N_f^{calc} ^[e]	Ar/R Carbonate leaving group
	2,4-dichlorophenyl carbonate	18.73	-0.94	0.79	0.90	
	2,4-dicyanophenyl carbonate	17.22	0.17	0.73	2.32	
	2,4-dinitrophenyl carbonate	16.69	0.56	0.71	2.87	
	3,5-dimethoxyphenyl carbonate	19.74	-1.68	0.82	0.05	
	3,5-dimethylphenyl carbonate	20.13	-1.96	0.84	-0.25	
	3,5-difluorophenyl carbonate	19.10	-1.21	0.80	0.58	
	3,5-dichlorophenyl carbonate	18.86	-1.03	0.79	0.79	
	3,5-di(trifluoromethyl)phenyl carbonate	18.76	-0.96	0.79	0.87	

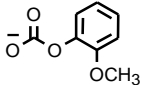
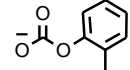
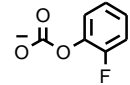
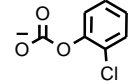
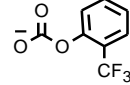
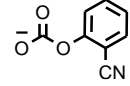
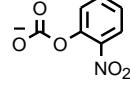
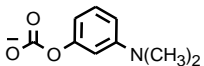
Solvent ^[a]	Ar/R Carbonate	$\Delta G^{\ddagger \text{calc}}$ ^[b]	$\log k^{\text{calc}}$ ^[c]	$s_{\text{f}}^{\text{estim}}$ ^[d]	$N_{\text{f}}^{\text{calc}}$ ^[e]	Ar/R Carbonate leaving group
	3,5-dicyanophenyl carbonate	17.95	-0.36	0.76	1.61	
	3,5-dinitrophenyl carbonate	17.54	-0.07	0.74	2.00	
	3,4-dimethoxyphenyl carbonate	20.76	-2.43	0.86	-0.73	
	3,4-dimethylphenyl carbonate	20.96	-2.57	0.87	-0.87	
	3,4-difluorophenyl carbonate	19.25	-1.32	0.81	0.46	
	3,4-dichlorophenyl carbonate	19.47	-1.48	0.81	0.27	
	3,4-di(trifluoromethyl)phenyl carbonate	18.21	-0.56	0.77	1.36	
	3,4-dicyanophenyl carbonate	17.66	-0.15	0.75	1.89	

Solvent ^[a]	Ar/R Carbonate	$\Delta G^\ddagger_{\text{calc}}$ ^[b]	$\log k^{\text{calc}}$ ^[c]	$s_{\text{f}}^{\text{estim}}$ ^[d]	$N_{\text{f}}^{\text{calc}}$ ^[e]	Ar/R Carbonate leaving group
	2,4,6-trimethoxyphenyl carbonate	20.78	-2.44	0.86	-0.74	
	2,4,6-trimethylphenyl carbonate	19.64	-1.60	0.82	0.14	
	2,4,6-trifluorophenyl carbonate	18.38	-0.68	0.77	1.21	
	2,4,6-tri(trifluoromethyl)phenyl carbonate	16.90	0.40	0.72	2.65	
	2,4,6-tricyanophenyl carbonate	15.45	1.47	0.67	4.29	
	2,4,6-trinitrophenyl carbonate	14.65	2.06	0.64	5.31	
	pentamethoxyphenyl carbonate	20.47	-2.21	0.85	-0.51	
	pentamethylphenyl carbonate	20.41	-2.17	0.85	-0.47	

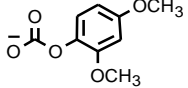
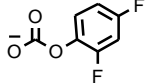
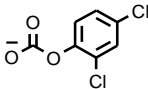
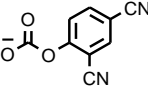
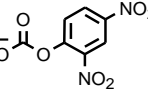
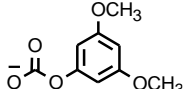
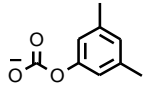
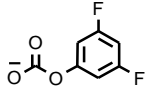
Solvent ^[a]	Ar/R Carbonate	$\Delta G^\ddagger_{\text{calc}}$ ^[b]	$\log k^{\text{calc}}$ ^[c]	$s_{\text{f}}^{\text{estim}}$ ^[d]	$N_{\text{f}}^{\text{calc}}$ ^[e]	Ar/R Carbonate leaving group
	pentafluorophenyl carbonate	17.26	0.14	0.73	2.29	
	pentachlorophenyl carbonate	16.22	0.90	0.69	3.39	
	penta(trifluoromethyl)phenyl carbonate	15.72	1.27	0.68	3.97	
	pentacyanophenyl carbonate	13.46	2.93	0.59	7.02	
60A40W	hydrogen carbonate (bicarbonate)	22.10	-3.41	0.87	-1.84	
	propyl carbonate	23.79	-4.65	0.92	-2.98	
	ethenyl carbonate (vinyl carbonate)	20.92	-2.54	0.83	-0.97	
	ethynyl carbonate	16.78	0.49	0.71	2.78	

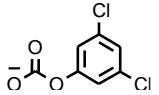
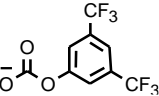
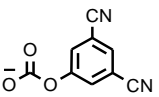
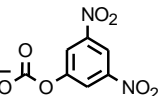
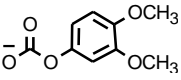
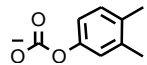
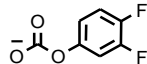
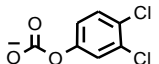
Solvent ^[a]	Ar/R Carbonate	$\Delta G^{\ddagger \text{calc}}$ ^[b]	$\log k^{\text{calc}}$ ^[c]	$s_{\text{f}}^{\text{estim}}$ ^[d]	$N_{\text{f}}^{\text{calc}}$ ^[e]	Ar/R Carbonate leaving group
	fluoromethyl carbonate	20.60	-2.31	0.82	-0.72	
	chloromethyl carbonate	19.87	-1.77	0.80	-0.12	
	bromomethyl carbonate	19.51	-1.51	0.79	0.18	
	cyanomethyl carbonate	19.95	-1.83	0.80	-0.19	
	nitromethyl carbonate	18.20	-0.55	0.75	1.36	
	difluoromethyl carbonate	18.11	-0.48	0.75	1.45	
	dichloromethyl carbonate	17.57	-0.09	0.73	1.97	
	dibromomethyl carbonate	17.45	0.00	0.73	2.09	

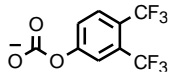
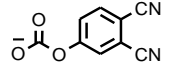
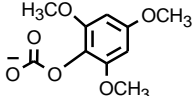
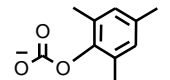
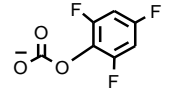
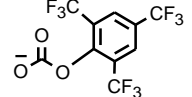
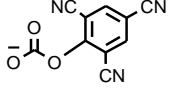
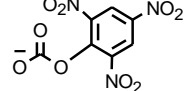
Solvent ^[a]	Ar/R Carbonate	$\Delta G^{\ddagger \text{calc}}$ ^[b]	$\log k^{\text{calc}}$ ^[c]	$s_{\text{f}}^{\text{estim}}$ ^[d]	$N_{\text{f}}^{\text{calc}}$ ^[e]	Ar/R Carbonate leaving group
	dicyanomethyl carbonate	16.49	0.71	0.70	3.10	
	dinitromethyl carbonate	15.23	1.63	0.66	4.54	
	trifluoromethyl carbonate ^[f]	16.42	0.76	0.70	3.17	
	trichloromethyl carbonate ^[f]	17.21	0.18	0.72	2.33	
	tribromomethyl carbonate ^[f]	16.23	0.90	0.69	3.39	
	tricyanomethyl carbonate	15.02	1.78	0.66	4.79	
	trinitromethyl carbonate	11.49	4.37	0.56	9.97	
	2-(dimethylamino)phenyl carbonate	21.66	-3.09	0.85	-1.53	

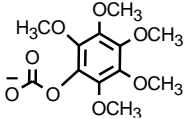
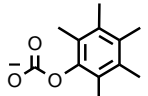
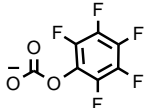
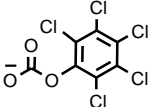
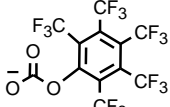
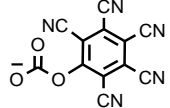


Solvent ^[a]	Ar/R Carbonate	$\Delta G^\ddagger_{\text{calc}}$ ^[b]	$\log k^{\text{calc}}$ ^[c]	$s_{\text{f}}^{\text{estim}}$ ^[d]	$N_{\text{f}}^{\text{calc}}$ ^[e]	Ar/R Carbonate leaving group
	2-methoxyphenyl carbonate	21.81	-3.20	0.86	-1.63	
	2-methylphenyl carbonate	21.41	-2.90	0.85	-1.34	
	2-fluorophenyl carbonate	20.41	-2.17	0.82	-0.56	
	2-chlorophenyl carbonate	21.19	-2.74	0.84	-1.17	
	2-(trifluoromethyl)phenyl carbonate	20.38	-2.15	0.82	-0.54	
	2-cyanophenyl carbonate	19.74	-1.68	0.80	-0.02	
	2-nitrophenyl carbonate	19.45	-1.46	0.79	0.24	
	3-(dimethylamino)phenyl carbonate	22.24	-3.51	0.87	-1.94	

Solvent ^[a]	Ar/R Carbonate	$\Delta G^{\ddagger \text{calc}}$ ^[b]	$\log k^{\text{calc}}$ ^[c]	$s_{\text{f}}^{\text{estim}}$ ^[d]	$N_{\text{f}}^{\text{calc}}$ ^[e]	Ar/R Carbonate leaving group
	3-methoxyphenyl carbonate	21.71	-3.12	0.85	-1.56	
	3-methylphenyl carbonate	21.21	-2.75	0.84	-1.18	
	3-fluorophenyl carbonate	20.40	-2.16	0.82	-0.56	
	3-chlorophenyl carbonate	20.60	-2.31	0.82	-0.72	
	3-(trifluoromethyl)phenyl carbonate	20.76	-2.43	0.83	-0.84	
	3-cyanophenyl carbonate	20.25	-2.05	0.81	-0.44	
	3-nitrophenyl carbonate	20.46	-2.20	0.82	-0.60	
	4-(trifluoromethyl)phenyl carbonate	20.82	-2.47	0.83	-0.89	

Solvent ^[a]	Ar/R Carbonate	$\Delta G^{\ddagger \text{calc}}$ ^[b]	$\log k^{\text{calc}}$ ^[c]	$s_{\text{f}}^{\text{estim}}$ ^[d]	$N_{\text{f}}^{\text{calc}}$ ^[e]	Ar/R Carbonate leaving group
	2,4-dimethoxyphenyl carbonate	21.75	-3.15	0.86	-1.59	
	2,4-difluorophenyl carbonate	20.43	-2.18	0.82	-0.58	
	2,4-dichlorophenyl carbonate	19.84	-1.75	0.80	-0.10	
	2,4-dicyanophenyl carbonate	18.25	-0.59	0.75	1.31	
	2,4-dinitrophenyl carbonate	17.70	-0.18	0.74	1.85	
	3,5-dimethoxyphenyl carbonate	20.90	-2.53	0.83	-0.95	
	3,5-dimethylphenyl carbonate	21.31	-2.83	0.84	-1.26	
	3,5-difluorophenyl carbonate	20.23	-2.03	0.81	-0.42	

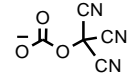
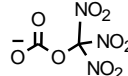
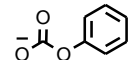
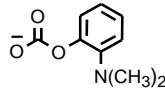
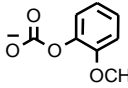
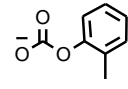
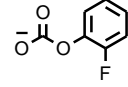
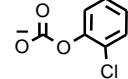
Solvent ^[a]	Ar/R Carbonate	$\Delta G^{\ddagger \text{calc}}$ ^[b]	$\log k^{\text{calc}}$ ^[c]	$s_{\text{f}}^{\text{estim}}$ ^[d]	$N_{\text{f}}^{\text{calc}}$ ^[e]	Ar/R Carbonate leaving group
	3,5-dichlorophenyl carbonate	19.97	-1.85	0.80	-0.21	
	3,5-di(trifluoromethyl)phenyl carbonate	19.87	-1.77	0.80	-0.12	
	3,5-dicyanophenyl carbonate	19.01	-1.14	0.78	0.62	
	3,5-dinitrophenyl carbonate	18.59	-0.84	0.76	1.00	
	3,4-dimethoxyphenyl carbonate	21.97	-3.31	0.86	-1.75	
	3,4-dimethylphenyl carbonate	22.18	-3.47	0.87	-1.90	
	3,4-difluorophenyl carbonate	20.38	-2.15	0.82	-0.54	
	3,4-dichlorophenyl carbonate	20.61	-2.32	0.82	-0.73	

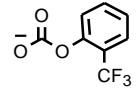
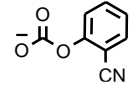
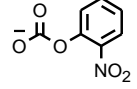
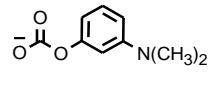
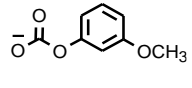
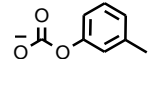
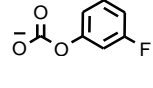
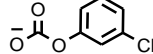
Solvent ^[a]	Ar/R Carbonate	$\Delta G^{\ddagger \text{calc}}$ ^[b]	$\log k^{\text{calc}}$ ^[c]	$s_{\text{f}}^{\text{estim}}$ ^[d]	$N_{\text{f}}^{\text{calc}}$ ^[e]	Ar/R Carbonate leaving group
	3,4-di(trifluoromethyl)phenyl carbonate	19.30	-1.35	0.78	0.37	
	3,4-dicyanophenyl carbonate	18.71	-0.92	0.77	0.89	
	2,4,6-trimethoxyphenyl carbonate	21.99	-3.33	0.86	-1.76	
	2,4,6-trimethylphenyl carbonate	20.79	-2.45	0.83	-0.87	
	2,4,6-trifluorophenyl carbonate	19.47	-1.48	0.79	0.22	
	2,4,6-tri(trifluoromethyl)phenyl carbonate	17.92	-0.34	0.74	1.63	
	2,4,6-tricyanophenyl carbonate	16.40	0.77	0.70	3.20	
	2,4,6-trinitrophenyl carbonate	15.55	1.39	0.67	4.16	

Solvent ^[a]	Ar/R Carbonate	$\Delta G^\ddagger_{\text{calc}}$ ^[b]	$\log k^{\text{calc}}$ ^[c]	s_f^{estim} ^[d]	N_f^{calc} ^[e]	Ar/R Carbonate leaving group
	pentamethoxyphenyl carbonate	21.67	-3.09	0.85	-1.53	
	pentamethylphenyl carbonate	21.60	-3.04	0.85	-1.48	
	pentafluorophenyl carbonate	18.29	-0.61	0.75	1.28	
	pentachlorophenyl carbonate	17.21	0.18	0.72	2.34	
	penta(trifluoromethyl)phenyl carbonate	16.67	0.57	0.71	2.90	
	pentacyanophenyl carbonate	14.31	2.31	0.64	5.71	
60AN40W	hydrogen carbonate (bicarbonate)	21.80	-3.18	0.86	-1.62	
	methyl carbonate	22.99	-4.06	0.89	-2.46	

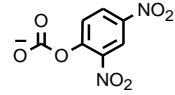
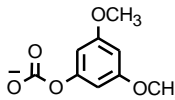
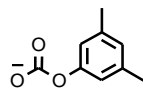
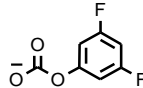
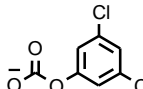
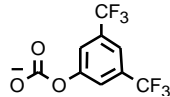
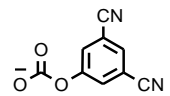
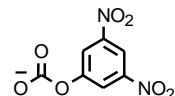
Solvent ^[a]	Ar/R Carbonate	$\Delta G^{\ddagger \text{calc}}$ ^[b]	$\log k^{\text{calc}}$ ^[c]	$s_{\text{f}}^{\text{estim}}$ ^[d]	$N_{\text{f}}^{\text{calc}}$ ^[e]	Ar/R Carbonate leaving group
	propyl carbonate	23.46	-4.40	0.91	-2.77	
	ethenyl carbonate (vinyl carbonate)	20.64	-2.34	0.82	-0.75	
	ethynyl carbonate	16.58	0.64	0.70	3.00	
	fluoromethyl carbonate	20.33	-2.11	0.81	-0.50	
	chloromethyl carbonate	19.61	-1.58	0.79	0.10	
	bromomethyl carbonate	19.26	-1.32	0.78	0.40	
	cyanomethyl carbonate	19.69	-1.64	0.80	0.03	
	nitromethyl carbonate	17.98	-0.38	0.75	1.58	

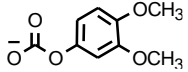
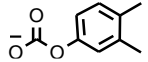
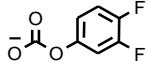
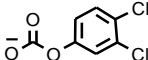
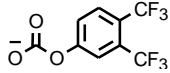
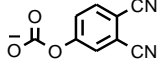
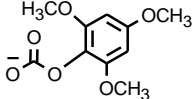
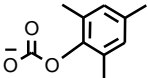
Solvent ^[a]	Ar/R Carbonate	$\Delta G^{\ddagger \text{calc}}$ ^[b]	$\log k^{\text{calc}}$ ^[c]	$s_{\text{f}}^{\text{estim}}$ ^[d]	$N_{\text{f}}^{\text{calc}}$ ^[e]	Ar/R Carbonate leaving group
	difluoromethyl carbonate	17.88	-0.32	0.74	1.67	
	dichloromethyl carbonate	17.36	0.07	0.73	2.19	
	dibromomethyl carbonate	17.24	0.16	0.72	2.30	
	dicyanomethyl carbonate	16.29	0.85	0.70	3.31	
	dinitromethyl carbonate	15.06	1.76	0.66	4.75	
	trifluoromethyl carbonate ^[f]	16.17	0.94	0.69	3.45	
	trichloromethyl carbonate ^[f]	16.95	0.37	0.72	2.61	
	tribromomethyl carbonate ^[f]	15.98	1.08	0.69	3.66	

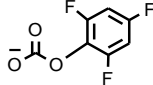
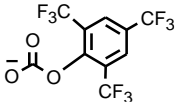
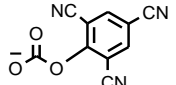
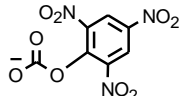
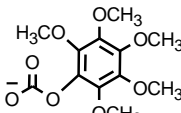
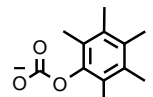
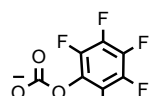
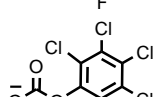
Solvent ^[a]	Ar/R Carbonate	$\Delta G^{\ddagger \text{calc}}$ ^[b]	$\log k^{\text{calc}}$ ^[c]	$s_{\text{f}}^{\text{estim}}$ ^[d]	$N_{\text{f}}^{\text{calc}}$ ^[e]	Ar/R Carbonate leaving group
	tricyanomethyl carbonate	14.86	1.90	0.65	5.00	
	trinitromethyl carbonate	11.39	4.45	0.55	10.14	
	phenyl carbonate	21.24	-2.78	0.84	-1.21	
	2-(dimethylamino)phenyl carbonate	21.37	-2.87	0.84	-1.31	
	2-methoxyphenyl carbonate	21.52	-2.98	0.85	-1.42	
	2-methylphenyl carbonate	21.12	-2.69	0.84	-1.12	
	2-fluorophenyl carbonate	20.14	-1.97	0.81	-0.34	
	2-chlorophenyl carbonate	20.91	-2.53	0.83	-0.95	

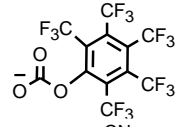
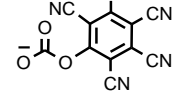
Solvent ^[a]	Ar/R Carbonate	$\Delta G^{\ddagger \text{calc}}$ ^[b]	$\log k^{\text{calc}}$ ^[c]	$s_{\text{f}}^{\text{estim}}$ ^[d]	$N_{\text{f}}^{\text{calc}}$ ^[e]	Ar/R Carbonate leaving group
	2-(trifluoromethyl)phenyl carbonate	20.11	-1.95	0.81	-0.32	
	2-cyanophenyl carbonate	19.49	-1.49	0.79	0.20	
	2-nitrophenyl carbonate	19.19	-1.28	0.78	0.46	
	3-(dimethylamino)phenyl carbonate	21.93	-3.28	0.86	-1.72	
	3-methoxyphenyl carbonate	21.41	-2.90	0.85	-1.34	
	3-methylphenyl carbonate	20.92	-2.54	0.83	-0.97	
	3-fluorophenyl carbonate	20.13	-1.96	0.81	-0.34	
	3-chlorophenyl carbonate	20.33	-2.11	0.81	-0.50	

Solvent ^[a]	Ar/R Carbonate	$\Delta G^{\ddagger \text{calc}}$ ^[b]	$\log k^{\text{calc}}$ ^[c]	$s_{\text{f}}^{\text{estim}}$ ^[d]	$N_{\text{f}}^{\text{calc}}$ ^[e]	Ar/R Carbonate leaving group
	3-(trifluoromethyl)phenyl carbonate	20.49	-2.22	0.82	-0.62	
	3-cyanophenyl carbonate	19.99	-1.86	0.80	-0.22	
	3-nitrophenyl carbonate	20.19	-2.01	0.81	-0.39	
	4-(trifluoromethyl)phenyl carbonate	20.55	-2.27	0.82	-0.67	
	2,4-dimethoxyphenyl carbonate	21.46	-2.94	0.85	-1.37	
	2,4-difluorophenyl carbonate	20.16	-1.98	0.81	-0.36	
	2,4-dichlorophenyl carbonate	19.58	-1.56	0.79	0.12	
	2,4-dicyanophenyl carbonate	18.02	-0.42	0.75	1.53	

Solvent ^[a]	Ar/R Carbonate	$\Delta G^{\ddagger \text{calc}}$ ^[b]	$\log k^{\text{calc}}$ ^[c]	$s_{\text{f}}^{\text{estim}}$ ^[d]	$N_{\text{f}}^{\text{calc}}$ ^[e]	Ar/R Carbonate leaving group
	2,4-dinitrophenyl carbonate	17.48	-0.02	0.73	2.06	
	3,5-dimethoxyphenyl carbonate	20.62	-2.32	0.82	-0.73	
	3,5-dimethylphenyl carbonate	21.02	-2.62	0.83	-1.05	
	3,5-difluorophenyl carbonate	19.96	-1.84	0.80	-0.20	
	3,5-dichlorophenyl carbonate	19.71	-1.65	0.80	0.01	
	3,5-di(trifluoromethyl)phenyl carbonate	19.61	-1.58	0.79	0.09	
	3,5-dicyanophenyl carbonate	18.77	-0.97	0.77	0.83	
	3,5-dinitrophenyl carbonate	18.36	-0.66	0.76	1.21	

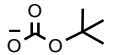
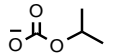
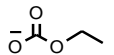
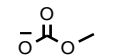
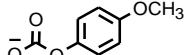
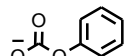
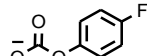
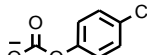
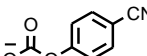
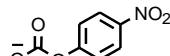
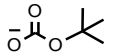
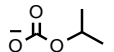
Solvent ^[a]	Ar/R Carbonate	$\Delta G^{\ddagger \text{calc}}$ ^[b]	$\log k^{\text{calc}}$ ^[c]	$s_{\text{f}}^{\text{estim}}$ ^[d]	$N_{\text{f}}^{\text{calc}}$ ^[e]	Ar/R Carbonate leaving group
	3,4-dimethoxyphenyl carbonate	21.67	-3.09	0.85	-1.53	
	3,4-dimethylphenyl carbonate	21.88	-3.24	0.86	-1.68	
	3,4-difluorophenyl carbonate	20.11	-1.95	0.81	-0.32	
	3,4-dichlorophenyl carbonate	20.34	-2.12	0.81	-0.51	
	3,4-di(trifluoromethyl)phenyl carbonate	19.05	-1.17	0.78	0.59	
	3,4-dicyanophenyl carbonate	18.47	-0.75	0.76	1.11	
	2,4,6-trimethoxyphenyl carbonate	21.69	-3.11	0.85	-1.55	
	2,4,6-trimethylphenyl carbonate	20.51	-2.24	0.82	-0.65	

Solvent ^[a]	Ar/R Carbonate	$\Delta G^{\ddagger \text{calc}}$ ^[b]	$\log k^{\text{calc}}$ ^[c]	$s_{\text{f}}^{\text{estim}}$ ^[d]	$N_{\text{f}}^{\text{calc}}$ ^[e]	Ar/R Carbonate leaving group
	2,4,6-trifluorophenyl carbonate	19.22	-1.29	0.78	0.44	
	2,4,6-tri(trifluoromethyl)phenyl carbonate	17.69	-0.18	0.74	1.85	
	2,4,6-tricyanophenyl carbonate	16.20	0.92	0.69	3.41	
	2,4,6-trinitrophenyl carbonate	15.38	1.52	0.67	4.37	
	pentamethoxyphenyl carbonate	21.37	-2.87	0.84	-1.31	
	pentamethylphenyl carbonate	21.31	-2.83	0.84	-1.26	
	pentafluorophenyl carbonate	18.06	-0.45	0.75	1.49	
	pentachlorophenyl carbonate	17.00	0.33	0.72	2.56	

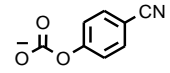
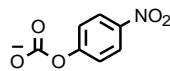
Solvent ^[a]	Ar/R Carbonate	$\Delta G^\ddagger_{\text{calc}}$ ^[b]	$\log k^{\text{calc}}$ ^[c]	s_f^{estim} ^[d]	N_f^{calc} ^[e]	Ar/R Carbonate leaving group
	penta(trifluoromethyl)phenyl carbonate	16.47	0.72	0.70	3.11	
	pentacyanophenyl carbonate	14.15	2.42	0.63	5.91	

^[a] Binary solvents are v/v at 25 °C. E = ethanol, A = acetone, AN = acetonitrile, W = water. ^[b] in kcal mol⁻¹. Obtained from plots of experimental solvolysis ΔG^\ddagger (25 °C) for 4-methoxybenzhydryl aryl/alkyl carbonates *versus* heterolytic ΔG^\ddagger (25 °C) for 2-oxyethyl aryl/alkyl carbonates calculated at the IEFPCM-M06-2X/6-311+G(2d,p) level of theory unless otherwise noted (Figures 2, S7, S9 and S11). ^[c] Logarithms of solvolytic first-order rate constants at 25 °C obtained from $\Delta G^\ddagger_{\text{calc}}$. ^[d] s_f values estimated from correlation plots of s_f *versus* $\log k$ (25 °C) for solvolysis of 4-methoxybenzhydryl aryl/alkyl carbonates in a corresponding solvent using $\log k^{\text{calc}}$ values. The correlation plots are presented in Figures S13-S16. ^[e] N_f^{calc} value for Ar/R carbonate leaving group is obtained from $\log k^{\text{calc}}$ of 4-methoxybenzhydryl Ar/R carbonate in a given solvent and corresponding s_f^{estim} by using $\log k = s_f(E_f + N_f)$. E_f value for the 4-methoxybenzhydryl electrofuge is -2.09 (ref 1). ^[f] Obtained from plots of experimental solvolysis ΔG^\ddagger (25 °C) for 4-methoxybenzhydryl aryl/alkyl carbonates *versus* heterolytic ΔG^\ddagger (25 °C) for 2-oxyethyl aryl/alkyl carbonates calculated at the IEFPCM-M06-2X/AUG-cc-pVDZ level of theory (Figures S3, S8, S10 and S12).

Table S2. Predicted solvolytic reactivities of reference 4-methoxybenzhydryl aryl/alkyl carbonates obtained from ΔG^\ddagger (4-methoxybenzhydryl aryl/alkyl carbonates) versus $\Delta G^\ddagger_{\text{model}}$ [2-oxyethyl aryl/alkyl carbonate; IEFPCM-M06-2X/6-311+G(2d,p)] plots, and corresponding calculated nucleofugalities (N_f^{calc}) of aryl/alkyl carbonate leaving groups along with corresponding estimated s_f values (s_f^{estim})

Solvent ^[a]	Ar/R Carbonate	$\Delta G^\ddagger_{\text{calc}}$ ^[b,f]	$\log k^{\text{calc}}$ ^[c,f]	s_f^{estim} ^[d,f]	N_f^{calc} ^[e,f]	Ar/R Carbonate leaving group
60E40W	tert-butyl carbonate	23.57 (+0.05)	-4.49 (-0.04)	0.96 (+0.07)	-2.49 (+0.42)	
	iso-propyl carbonate	22.61 (-0.07)	-3.78 (+0.05)	0.93 (\pm 0.00)	-2.04 (-0.01)	
	ethyl carbonate	22.10 (-0.20)	-3.41 (+0.15)	0.91 (-0.01)	-1.87 (-0.07)	
	methyl carbonate	22.04 (+0.11)	-3.36 (-0.08)	0.91 (+0.02)	-1.72 (-0.13)	
	4-methoxyphenyl carbonate	20.19 (-0.28)	-2.00 (+0.21)	0.84 (+0.02)	-0.57 (\pm 0.00)	
	phenyl carbonate	20.35 (+0.09)	-2.12 (-0.06)	0.85 (+0.04)	-0.43 (-0.03)	
	4-fluorophenyl carbonate	19.81 (-0.20)	-1.73 (+0.14)	0.83 (-0.01)	0.04 (+0.12)	
	4-chlorophenyl carbonate	19.72 (-0.05)	-1.66 (+0.04)	0.82 (+0.02)	-0.01 (-0.01)	
	4-cyanophenyl carbonate	18.97 (+0.13)	-1.11 (-0.10)	0.80 (\pm 0.00)	0.78 (-0.04)	
	4-nitrophenyl carbonate	18.62 (+0.03)	-0.85 (-0.02)	0.78 (-0.02)	0.84 (-0.21)	
60A40W	tert-butyl carbonate	24.92 (+0.14)	-5.47 (-0.10)	0.95 (+0.01)	-3.57 (+0.05)	
	iso-propyl carbonate	23.91 (-0.09)	-4.73 (+0.07)	0.92 (-0.05)	-3.10 (-0.24)	

Solvent ^[a]	Ar/R Carbonate	$\Delta G^\ddagger_{\text{calc}}$ ^[b,f]	$\log k^{\text{calc}}$ ^[c,f]	s_f^{estim} ^[d,f]	N_f^{calc} ^[e,f]	Ar/R Carbonate leaving group
	ethyl carbonate	23.38 (-0.12)	-4.34 (+0.09)	0.90 (-0.03)	-2.92 (-0.20)	
	methyl carbonate	23.31 (+0.25)	-4.29 (-0.18)	0.90 (+0.02)	-2.76 (-0.20)	
	4-methoxyphenyl carbonate	21.37 (-0.23)	-2.87 (+0.17)	0.84 (\pm 0.00)	-1.56 (-0.04)	
	phenyl carbonate	21.54 (+0.16)	-2.99 (-0.11)	0.85 (+0.02)	-1.42 (-0.03)	
	4-fluorophenyl carbonate	20.97 (-0.06)	-2.58 (+0.04)	0.83 (-0.04)	-0.94 (\pm 0.00)	
	4-chlorophenyl carbonate	20.88 (+0.10)	-2.51 (-0.07)	0.83 (-0.01)	-0.99 (-0.19)	
	4-cyanophenyl carbonate	20.09 (+0.18)	-1.93 (-0.13)	0.81 (-0.02)	-0.18 (-0.15)	
	4-nitrophenyl carbonate	19.72 (+0.03)	-1.66 (-0.02)	0.80 (-0.01)	-0.13 (-0.25)	
60AN40W	tert-butyl carbonate	24.56 (+0.08)	-5.21 (-0.05)	0.94 (-0.02)	-3.33 (-0.05)	
	iso-propyl carbonate	23.57 (+0.12)	-4.48 (-0.08)	0.91 (+0.03)	-2.85 (+0.09)	
	ethyl carbonate	23.05 (-0.11)	-4.10 (+0.08)	0.89 (-0.01)	-2.67 (-0.13)	
	4-methoxyphenyl carbonate	21.08 (-0.06)	-2.66 (+0.04)	0.84 (+0.03)	-1.30 (-0.06)	
	4-fluorophenyl carbonate	20.69 (+0.02)	-2.37 (-0.01)	0.82 (+0.01)	-0.68 (+0.11)	
	4-chlorophenyl carbonate	20.60 (+0.16)	-2.31 (-0.12)	0.82 (+0.03)	-0.73 (-0.11)	

Solvent ^[a]	Ar/R Carbonate	$\Delta G^\ddagger_{\text{calc}}$ ^[b,f]	$\log k^{\text{calc}}$ ^[c,f]	s_f^{estim} ^[d,f]	N_f^{calc} ^[e,f]	Ar/R Carbonate leaving group
	4-cyanophenyl carbonate	19.83 (+0.12)	-1.74 (-0.09)	0.80 (± 0.00)	0.08 (-0.02)	
	4-nitrophenyl carbonate	19.47 (-0.04)	-1.47 (+0.04)	0.79 (-0.01)	0.14 (-0.13)	

^[a] Binary solvents are v/v at 25 °C. E = ethanol, A = acetone, AN = acetonitrile, W = water. ^[b] in kcal mol⁻¹. Obtained from ΔG^\ddagger (4-methoxybenzhydryl aryl/alkyl carbonates) *versus* $\Delta G^\ddagger_{\text{model}}$ [2-oxyethyl aryl/alkyl carbonate; IEFPCM-M06-2X/6-311+G(2d,p) level] plots given in (Figures 2, S7, S9 and S11). Deviations from experimental values ($\Delta G^\ddagger_{\text{calc}} - \Delta G^\ddagger$) are given in parentheses. ^[c] Logarithms of solvolytic first-order rate constants at 25 °C obtained from $\Delta G^\ddagger_{\text{calc}}$. Deviations from experimental values ($\log k^{\text{calc}} - \log k$) are given in parentheses. ^[d] s_f values estimated from the correlation plots of s_f *versus* $\log k$ (25 °C) for solvolysis of 4-methoxybenzhydryl aryl/alkyl carbonates in a corresponding solvent. The correlation plots are presented in Figures S13-S16. Deviations from experimental s_f values ($s_f^{\text{estim}} - s_f$) are given in parentheses.

^[e] N_f^{calc} value for Ar/R carbonate leaving group is obtained from $\log k^{\text{calc}}$ of 4-methoxybenzhydryl Ar/R carbonate in a given solvent and corresponding s_f^{estim} by using $\log k = s_f (E_f + N_f)$. E_f value for the 4-methoxybenzhydryl electrofuge is -2.09 (ref 1). Deviations from experimental values ($N_f^{\text{calc}} - N_f$) are given in parentheses. ^[f] Experimental data and references are given in Table S5.

Table S3. Activation energies (in kcal mol⁻¹) for heterolysis of 2-oxyethyl aryl/alkyl carbonates (OEt aryl/alkyl carbonates) calculated by the M06-2X method in combination with various basis sets and solvation models

Solvation model	Basis Set	OEt aryl/alkyl carbonate	$\Delta E^{\ddagger\text{model [a]}}$	$\Delta H^{\ddagger\text{model [b]}}$	$\Delta G^{\ddagger\text{model [c]}}$
<i>Reference Carbonates</i>					
IEFPCM (water)	AUG-cc-pVDZ	OEt tert-butyl carbonate	22.33	22.47	21.64
		OEt isopropyl carbonate	21.55	21.69	20.92
		OEt ethyl carbonate	21.34	21.46	20.66
		OEt methyl carbonate	21.07	21.17	20.42
		OEt 4-methoxyphenyl carbonate	19.39	19.52	18.80
		OEt phenyl carbonate	19.12	19.24	18.62
		OEt 4-fluorophenyl carbonate	18.85	19.00	18.03
		OEt 4-chlorophenyl carbonate	18.59	18.73	18.09
		OEt 4-cyanophenyl carbonate	17.86	17.99	17.15
		OEt 4-nitrophenyl carbonate	17.56	17.66	17.09
	AUG-cc-pVTZ	OEt tert-butyl carbonate	21.78	21.90	21.32
		OEt isopropyl carbonate	21.04	21.15	20.49
		OEt ethyl carbonate	20.81	20.93	20.05
		OEt methyl carbonate	20.51	20.64	19.56
		OEt 4-methoxyphenyl carbonate	18.85	19.01	17.99
		OEt phenyl carbonate	18.62	18.77	17.72
		OEt 4-fluorophenyl carbonate	18.41	18.54	17.93
		OEt 4-chlorophenyl carbonate	18.14	18.28	17.54
		OEt 4-cyanophenyl carbonate	17.40	17.54	16.44
		OEt 4-nitrophenyl carbonate	17.12	17.25	16.53
	6-31+G(d)	OEt tert-butyl carbonate	22.84	22.98	22.20

Solvation model	Basis Set	OEt aryl/alkyl carbonate	$\Delta E^{\ddagger\text{model [a]}}$	$\Delta H^{\ddagger\text{model [b]}}$	$\Delta G^{\ddagger\text{model [c]}}$
		OEt isopropyl carbonate	22.08	22.20	21.51
		OEt ethyl carbonate	21.88	21.99	21.25
		OEt methyl carbonate	21.60	21.71	20.85
		OEt 4-methoxyphenyl carbonate	19.93	20.09	19.16
		OEt phenyl carbonate	19.74	19.87	19.07
		OEt 4-fluorophenyl carbonate	19.46	19.60	18.91
		OEt 4-chlorophenyl carbonate	19.22	19.35	18.74
		OEt 4-cyanophenyl carbonate	18.54	18.68	17.69
		OEt 4-nitrophenyl carbonate	18.17	18.31	17.52
	6-311+G(2d,p)	OEt tert-butyl carbonate	22.24	22.37	21.79
		OEt isopropyl carbonate	21.44	21.57	20.83
		OEt ethyl carbonate	21.18	21.33	20.32
		OEt methyl carbonate	20.95	21.07	20.26
		OEt 4-methoxyphenyl carbonate	19.27	19.44	18.41
		OEt phenyl carbonate	19.07	19.19	18.57
		OEt 4-fluorophenyl carbonate	18.78	18.94	18.03
		OEt 4-chlorophenyl carbonate	18.52	18.65	17.94
		OEt 4-cyanophenyl carbonate	17.80	17.94	17.19
		OEt 4-nitrophenyl carbonate	17.45	17.60	16.84
	6-311+G(3df,2p)	OEt tert-butyl carbonate	22.45	22.57	22.02
		OEt isopropyl carbonate	21.68	21.80	21.13
		OEt ethyl carbonate	21.43	21.57	20.58
		OEt methyl carbonate	21.20	21.32	20.44
		OEt 4-methoxyphenyl carbonate	19.49	19.64	18.71

Solvation model	Basis Set	OEt aryl/alkyl carbonate	$\Delta E^{\ddagger\text{model [a]}}$	$\Delta H^{\ddagger\text{model [b]}}$	$\Delta G^{\ddagger\text{model [c]}}$
SMD (water)	AUG-cc-pVDZ	OEt phenyl carbonate	19.27	19.38	19.12
		OEt 4-fluorophenyl carbonate	19.04	19.17	18.49
		OEt 4-chlorophenyl carbonate	18.72	18.84	18.41
		OEt 4-cyanophenyl carbonate	17.97	18.11	17.07
		OEt 4-nitrophenyl carbonate	17.70	17.83	17.06
		OEt tert-butyl carbonate	24.81	24.94	24.18
		OEt isopropyl carbonate	23.93	24.13	23.22
		OEt ethyl carbonate	23.77	23.84	23.35
		OEt methyl carbonate	23.80	23.74	23.88
		OEt 4-methoxyphenyl carbonate	–	–	–
SMD (water)	6-311+G(2d,p)	OEt phenyl carbonate	21.79	21.90	21.40
		OEt 4-fluorophenyl carbonate	21.60	21.73	20.89
		OEt 4-chlorophenyl carbonate	21.45	21.56	20.68
		OEt 4-cyanophenyl carbonate	21.16	21.25	20.81
		OEt 4-nitrophenyl carbonate	20.77	20.87	20.30
		OEt tert-butyl carbonate	24.78	24.92	23.98
		OEt isopropyl carbonate	23.90	24.12	23.10
		OEt ethyl carbonate	23.76	23.82	23.43
		OEt methyl carbonate	23.76	23.73	23.78
		OEt 4-methoxyphenyl carbonate	–	–	–
OEt phenyl carbonate	21.78	21.91	21.32		
OEt 4-fluorophenyl carbonate	21.62	21.76	20.84		
OEt 4-chlorophenyl carbonate	–	–	–		
OEt 4-cyanophenyl carbonate	21.12	21.25	20.45		

Solvation model	Basis Set	OEt aryl/alkyl carbonate	$\Delta E^{\ddagger\text{model [a]}}$	$\Delta H^{\ddagger\text{model [b]}}$	$\Delta G^{\ddagger\text{model [c]}}$
		OEt 4-nitrophenyl carbonate	20.88	20.98	20.54
		<i>Other Carbonates</i>			
IEFPCM (water)	AUG-cc-pVDZ	OEt trifluoromethyl carbonate	14.67	14.82	13.86
		OEt trichloromethyl carbonate	14.69	14.84	14.60
		OEt tribromomethyl carbonate	14.39	14.56	13.68
	6-311+G(2d,p)	OEt hydrogen carbonate	19.85	20.01	19.11
		OEt propyl carbonate	21.29	21.41	20.72
		OEt ethenyl carbonate	18.63	18.78	17.99
		OEt ethynyl carbonate	14.66	14.80	14.04
		OEt fluoromethyl carbonate	18.24	18.36	17.68
		OEt chloromethyl carbonate	17.77	17.93	16.98
		OEt bromomethyl carbonate	17.45	17.62	16.64
		OEt cyanomethyl carbonate	17.73	17.86	17.06
		OEt nitromethyl carbonate	16.52	16.71	15.39
		OEt difluoromethyl carbonate	16.04	16.20	15.30
		OEt dichloromethyl carbonate	15.63	15.80	14.79
		OEt dibromomethyl carbonate	15.34	15.52	14.68
		OEt dicyanomethyl carbonate	14.76	14.91	13.76
		OEt dinitromethyl carbonate	13.06	13.16	12.56
		OEt tricyanomethyl carbonate	12.42	12.45	12.37
		OEt trinitromethyl carbonate	9.68	9.84	9.00
		OEt 2-(dimethylamino)phenyl carbonate	19.52	19.65	18.69
		OEt 2-methoxyphenyl carbonate	19.28	19.36	18.83
		OEt 2-methylphenyl carbonate	19.11	19.23	18.45

Solvation model	Basis Set	OEt aryl/alkyl carbonate	$\Delta E^{\ddagger\text{model [a]}}$	$\Delta H^{\ddagger\text{model [b]}}$	$\Delta G^{\ddagger\text{model [c]}}$
		OEt 2-fluorophenyl carbonate	18.16	18.28	17.49
		OEt 2-chlorophenyl carbonate	18.21	18.26	18.24
		OEt 2-(trifluoromethyl)phenyl carbonate	17.91	18.01	17.47
		OEt 2-cyanophenyl carbonate	17.29	17.39	16.86
		OEt 2-nitrophenyl carbonate	16.93	17.03	16.58
		OEt 3-(dimethylamino)phenyl carbonate	19.53	19.61	19.24
		OEt 3-methoxyphenyl carbonate	19.06	19.17	18.73
		OEt 3-methylphenyl carbonate	19.20	19.35	18.25
		OEt 3-fluorophenyl carbonate	18.51	18.64	17.49
		OEt 3-chlorophenyl carbonate	18.42	18.56	17.68
		OEt 3-(trifluoromethyl)phenyl carbonate	18.19	18.32	17.83
		OEt 3-cyanophenyl carbonate	18.00	18.14	17.35
		OEt 3-nitrophenyl carbonate	17.84	17.95	17.54
		OEt 4-(trifluoromethyl)phenyl carbonate	18.18	18.27	17.89
		OEt 2,4-dimethoxyphenyl carbonate	19.41	19.53	18.78
		OEt 2,4-difluorophenyl carbonate	17.93	18.03	17.51
		OEt 2,4-dichlorophenyl carbonate	17.62	17.77	16.95
		OEt 2,4-dicyanophenyl carbonate	16.04	16.18	15.44
		OEt 2,4-dinitrophenyl carbonate	15.35	15.45	14.91
		OEt 3,5-dimethoxyphenyl carbonate	18.92	19.10	17.96
		OEt 3,5-dimethylphenyl carbonate	19.25	19.42	18.35
		OEt 3,5-difluorophenyl carbonate	17.91	18.05	17.32
		OEt 3,5-dichlorophenyl carbonate	17.76	17.89	17.08
		OEt 3,5-di(trifluoromethyl)phenyl carbonate	17.28	17.40	16.98

Solvation model	Basis Set	OEt aryl/alkyl carbonate	$\Delta E^{\ddagger\text{model [a]}}$	$\Delta H^{\ddagger\text{model [b]}}$	$\Delta G^{\ddagger\text{model [c]}}$
		OEt 3,5-dicyanophenyl carbonate	16.85	17.00	16.17
		OEt 3,5-dinitrophenyl carbonate	16.45	16.60	15.76
		OEt 3,4-dimethoxyphenyl carbonate	19.32	19.43	18.98
		OEt 3,4-dimethylphenyl carbonate	19.44	19.54	19.18
		OEt 3,4-difluorophenyl carbonate	18.27	18.41	17.47
		OEt 3,4-dichlorophenyl carbonate	18.04	18.17	17.69
		OEt 3,4-di(trifluoromethyl)phenyl carbonate	17.29	17.45	16.43
		OEt 3,4-dicyanophenyl carbonate	16.76	16.90	15.88
		OEt 2,4,6-trimethoxyphenyl carbonate	19.45	19.59	19.00
		OEt 2,4,6-trimethylphenyl carbonate	19.26	19.46	17.86
		OEt 2,4,6-trifluorophenyl carbonate	16.99	17.09	16.60
		OEt 2,4,6-tri(trifluoromethyl)phenyl carbonate	15.73	15.89	15.12
		OEt 2,4,6-tricyanophenyl carbonate	14.31	14.44	13.67
		OEt 2,4,6-trinitrophenyl carbonate	13.62	13.77	12.87
		OEt pentamethoxyphenyl carbonate	18.70	18.75	18.69
		OEt pentamethylphenyl carbonate	19.60	19.80	18.63
		OEt pentafluorophenyl carbonate	15.93	16.04	15.48
		OEt pentachlorophenyl carbonate	15.95	16.14	14.44
		OEt penta(trifluoromethyl)phenyl carbonate	14.69	14.85	13.94
		OEt pentacyanophenyl carbonate	12.45	12.57	11.68

^[a] Zero-point correction is added to total energy. ^[b] Thermal correction to enthalpy is added to total energy. ^[c] Thermal correction to free energy is added to total energy.

Table S4. Standard free energies (in kcal mol⁻¹) for heterolysis of reference 2-oxyethyl aryl/alkyl carbonates (OEt aryl/alkyl carbonates) calculated at the M06-2X/6-311+G(2d,p) level with the IEFPCM solvation model (water)

OEt aryl/alkyl carbonate	$\Delta E^{\text{omodel [a]}}$	$\Delta H^{\text{omodel [b]}}$	$\Delta G^{\text{omodel [c]}}$
OEt tert-butyl carbonate	-3.45	-3.28	-14.42
OEt isopropyl carbonate	-4.56	-4.38	-15.88
OEt ethyl carbonate	-4.94	-4.76	-16.20
OEt methyl carbonate	-5.38	-5.21	-16.40
OEt 4-methoxyphenyl carbonate	-8.32	-8.13	-19.77
OEt phenyl carbonate	-8.78	-8.61	-20.37
OEt 4-fluorophenyl carbonate	-9.22	-9.03	-20.50
OEt 4-chlorophenyl carbonate	-9.67	-9.51	-20.76
OEt 4-cyanophenyl carbonate	-11.14	-10.97	-22.33
OEt 4-nitrophenyl carbonate	-11.84	-11.62	-23.36

^[a] Zero-point correction is added to total energy. ^[b] Thermal correction to enthalpy is added to total energy. ^[c] Thermal correction to free energy is added to total energy.

Table S5. Literature rate constants and free energies of activation for solvolysis of 4-methoxybenzhydryl aryl/alkyl carbonates at 25 °C in different solvents along with nucleofuge-specific parameters (N_f and s_f) of corresponding aryl/alkyl leaving groups

Solvent ^[a]	Aryl/alkyl carbonate	k / s^{-1}	$\Delta G^\ddagger / kcal mol^{-1}$	N_f	s_f	Reference
80E20W	4-nitrophenyl carbonate	3.78×10^{-2}	19.39	0.31	0.80	2 and 3
	4-cyanophenyl carbonate	2.73×10^{-2}	19.59	0.24	0.84	2 and 3
	4-chlorophenyl carbonate	7.14×10^{-3}	20.38	-0.46	0.84	2 and 3
	4-fluorophenyl carbonate	4.59×10^{-3}	20.64	-0.49	0.90	2 and 3
	phenyl carbonate	2.71×10^{-3}	20.96	-0.74	0.90	1
	4-methoxyphenyl carbonate	1.91×10^{-3}	21.16	-0.88	0.91	2 and 3
	methyl carbonate	1.39×10^{-4}	22.72	-1.96	0.95	1
	ethyl carbonate	7.84×10^{-5}	23.05	-2.04	0.99	2 and 3
	<i>iso</i> -propyl carbonate	4.28×10^{-5}	23.41	-2.26	1.00	2 and 3
	<i>tert</i> -butyl carbonate	$9.96 \times 10^{-6 [b]}$	24.28	-3.12	0.96	1
60E40W	4-nitrophenyl carbonate	$1.47 \times 10^{-1 [b]}$	18.59	1.05	0.80	3
	4-cyanophenyl carbonate	$9.64 \times 10^{-2 [b]}$	18.84	0.82	0.80	3
	4-chlorophenyl carbonate	1.99×10^{-2}	19.77	0.00	0.80	3
	4-fluorophenyl carbonate	1.34×10^{-2}	20.01	-0.08	0.84	3
	phenyl carbonate	8.76×10^{-3}	20.26	-0.40	0.81	1
	4-methoxyphenyl carbonate	6.12×10^{-3}	20.47	-0.57	0.82	3
	methyl carbonate	5.22×10^{-4}	21.93	-1.59	0.89	1
	ethyl carbonate	2.78×10^{-4}	22.30	-1.80	0.92	3
	<i>iso</i> -propyl carbonate	1.48×10^{-4}	22.68	-2.03	0.93	3
	<i>tert</i> -butyl carbonate	$3.55 \times 10^{-5 [b]}$	23.52	-2.91	0.89	1
60A40W	4-nitrophenyl carbonate	2.27×10^{-2}	19.70	0.12	0.81	3

Solvent ^[a]	Aryl/alkyl carbonate	k / s^{-1}	$\Delta G^\ddagger / \text{kcal mol}^{-1}$	N_f	s_f	Reference
60AN40W	4-cyanophenyl carbonate	1.57×10^{-2}	19.91	-0.03	0.83	3
	4-chlorophenyl carbonate	3.64×10^{-3}	20.78	-0.80	0.84	3
	4-fluorophenyl carbonate	2.40×10^{-3}	21.03	-0.94	0.87	3
	phenyl carbonate	1.33×10^{-3}	21.38	-1.39	0.83	1
	4-methoxyphenyl carbonate	9.11×10^{-4}	21.60	-1.52	0.84	3
	methyl carbonate	7.78×10^{-5}	23.06	-2.56	0.88	1
	ethyl carbonate	3.73×10^{-5}	23.49	-2.72	0.93	3
	<i>iso</i> -propyl carbonate	1.59×10^{-5}	24.00	-2.86	0.97	3
	<i>tert</i> -butyl carbonate	$4.29 \times 10^{-6 [b]}$	24.78	-3.62	0.94	1
	4-nitrophenyl carbonate	3.11×10^{-2}	19.51	0.27	0.80	3
	4-cyanophenyl carbonate	2.23×10^{-2}	19.71	0.10	0.80	3
	4-chlorophenyl carbonate	6.48×10^{-3}	20.44	-0.62	0.79	3
	4-fluorophenyl carbonate	4.41×10^{-3}	20.67	-0.79	0.81	3
	4-methoxyphenyl carbonate	1.99×10^{-3}	21.14	-1.24	0.81	3
	ethyl carbonate	6.59×10^{-5}	23.16	-2.54	0.90	3
	<i>iso</i> -propyl carbonate	3.99×10^{-5}	23.45	-2.94	0.88	3
	<i>tert</i> -butyl carbonate	$7.00 \times 10^{-6 [b]}$	24.49	-3.28	0.96	1

^[a] Binary solvents are v/v at 25 °C. E = ethanol, A = acetone, AN = acetonitrile, W = water. ^[b] Calculated from N_f , s_f and E_f values by using eq.

$\log k = s_f (N_f + E_f)$.

2. Correlations

2.1. ΔG^\ddagger (4-methoxybenzhydryl aryl/alkyl carbonates) vs. ΔG^\ddagger ^{model} (2-oxyethyl aryl/alkyl carbonates)

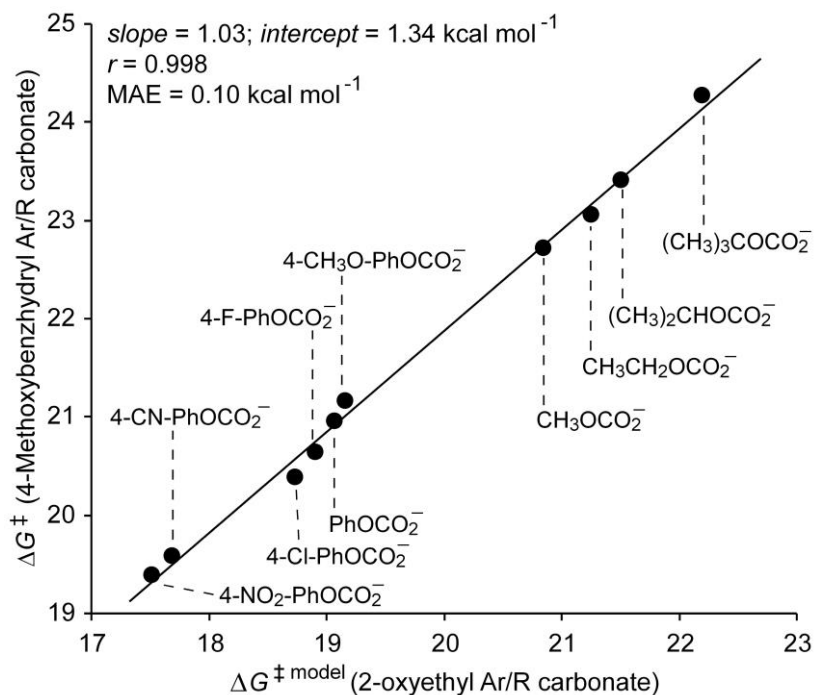


Figure S1. Correlation of experimental free energies of activation (in kcal mol⁻¹) for solvolyses of 4-methoxybenzhydryl aryl/alkyl carbonates in **80% ethanol** (Table S5) versus free energies of activation (in kcal mol⁻¹) for heterolysis of 2-oxyethyl aryl/alkyl carbonates calculated at the **M06-2X/6-31+G(d)** level of theory in the presence of the **IEFPCM** solvation model (solvent = water, Table S3).

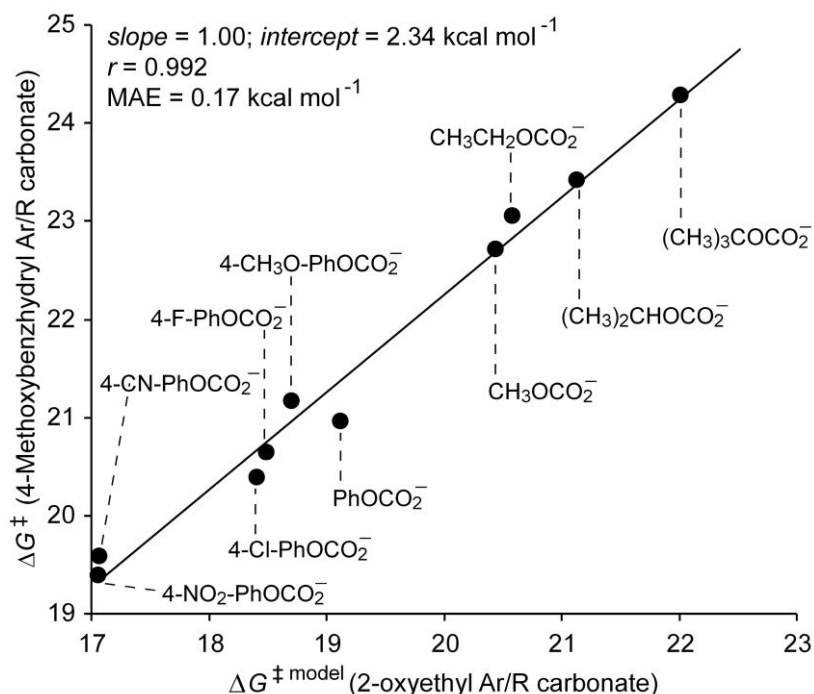


Figure S2. Correlation of experimental free energies of activation (in kcal mol⁻¹) for solvolyses of 4-methoxybenzhydryl aryl/alkyl carbonates in **80% ethanol** (Table S5) versus free energies of activation (in kcal mol⁻¹) for heterolysis of 2-oxyethyl aryl/alkyl carbonates calculated at the **M06-2X/6-311+G(3df,2p)** level of theory in the presence of the **IEFPCM** solvation model (solvent = water, Table S3).

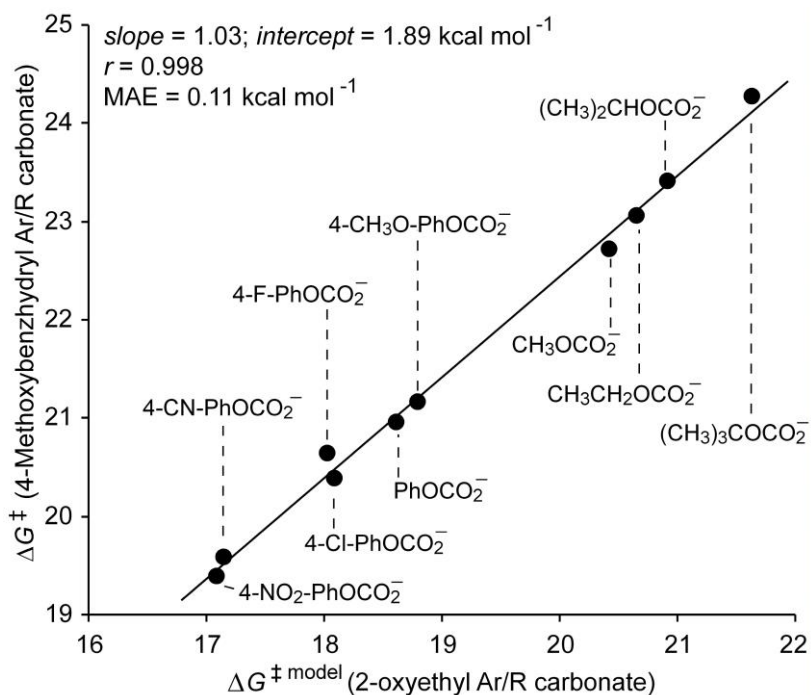


Figure S3. Correlation of experimental free energies of activation (in kcal mol⁻¹) for solvolyses of 4-methoxybenzhydryl aryl/alkyl carbonates in **80% ethanol** (Table S5) versus free energies of activation (in kcal mol⁻¹) for heterolysis of 2-oxyethyl aryl/alkyl carbonates calculated at the **M06-2X/AUG-cc-pVDZ** level of theory in the presence of the **IEFPCM** solvation model (solvent = water, Table S3).

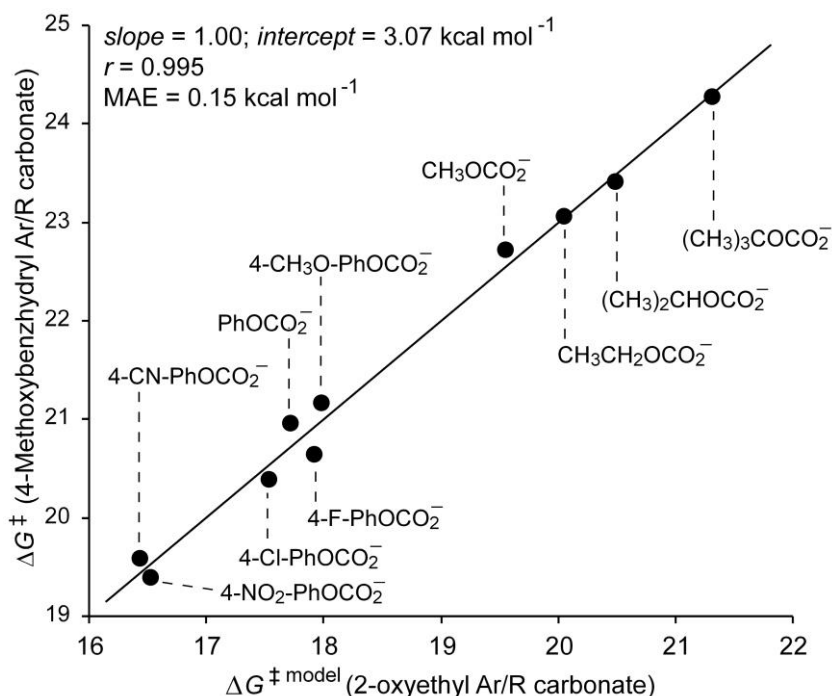


Figure S4. Correlation of experimental free energies of activation (in kcal mol⁻¹) for solvolyses of 4-methoxybenzhydryl aryl/alkyl carbonates in **80% ethanol** (Table S5) versus free energies of activation (in kcal mol⁻¹) for heterolysis of 2-oxyethyl aryl/alkyl carbonates calculated at the **M06-2X/AUG-cc-pVTZ** level of theory in the presence of the **IEFPCM** solvation model (solvent = water, Table S3).

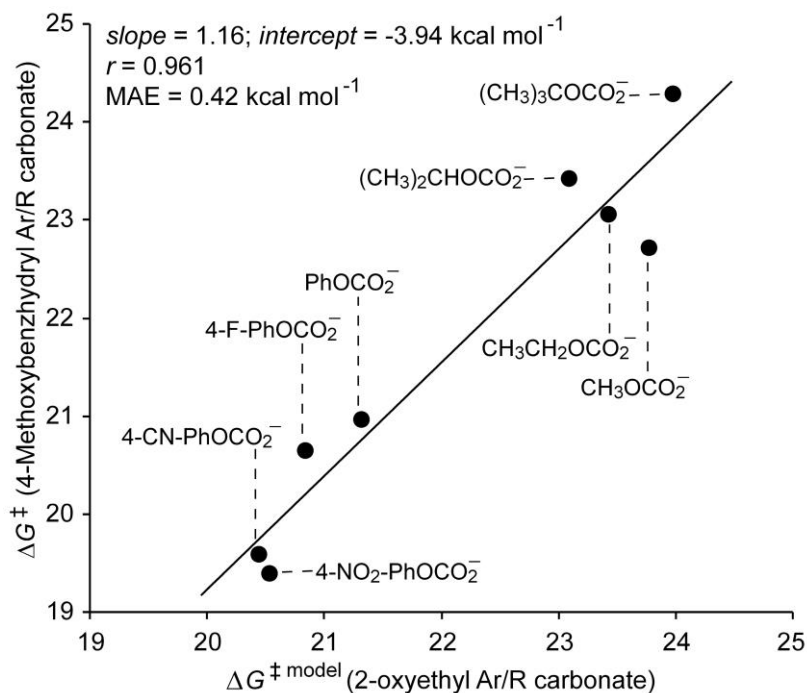


Figure S5. Correlation of experimental free energies of activation (in kcal mol⁻¹) for solvolyses of 4-methoxybenzhydryl aryl/alkyl carbonates in **80% ethanol** (Table S5) versus free energies of activation (in kcal mol⁻¹) for heterolysis of 2-oxyethyl aryl/alkyl carbonates calculated at the **M06-2X/6-311+G(2d,p)** level of theory in the presence of the **SMD** solvation model (solvent = water, Table S3).

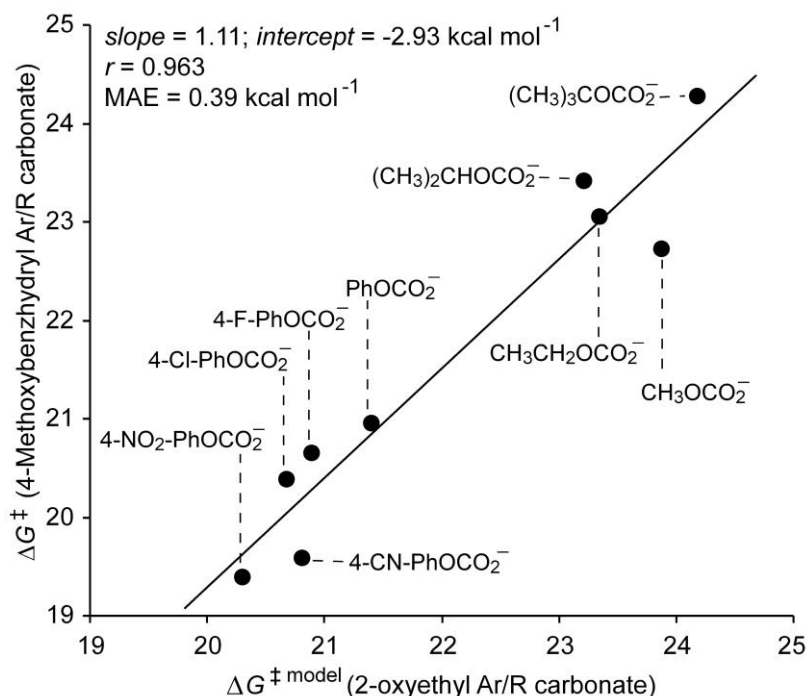


Figure S6. Correlation of experimental free energies of activation (in kcal mol⁻¹) for solvolyses of 4-methoxybenzhydryl aryl/alkyl carbonates in **80% ethanol** (Table S5) versus free energies of activation (in kcal mol⁻¹) for heterolysis of 2-oxyethyl aryl/alkyl carbonates calculated at the **M06-2X/AUG-cc-pVDZ** level of theory in the presence of the **SMD** solvation model (solvent = water, Table S3).

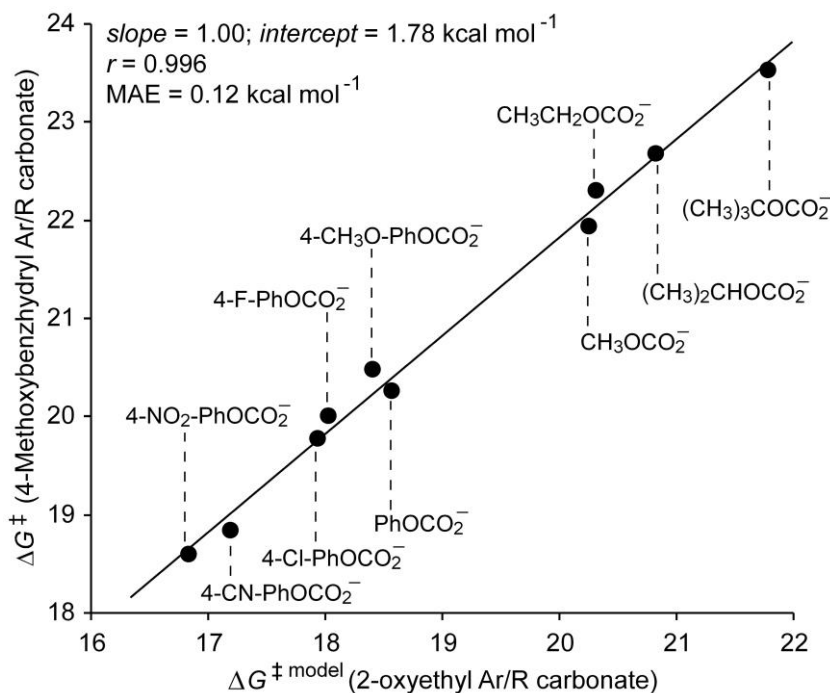


Figure S7. Correlation of experimental free energies of activation (in kcal mol⁻¹) for solvolyses of 4-methoxybenzhydryl aryl/alkyl carbonates in **60% ethanol** (Table S5) versus free energies of activation (in kcal mol⁻¹) for heterolysis of 2-oxyethyl aryl/alkyl carbonates calculated at the **M06-2X/6-311+G(2d,p)** level of theory in the presence of the **IEFPCM** solvation model (solvent = water, Table S3).

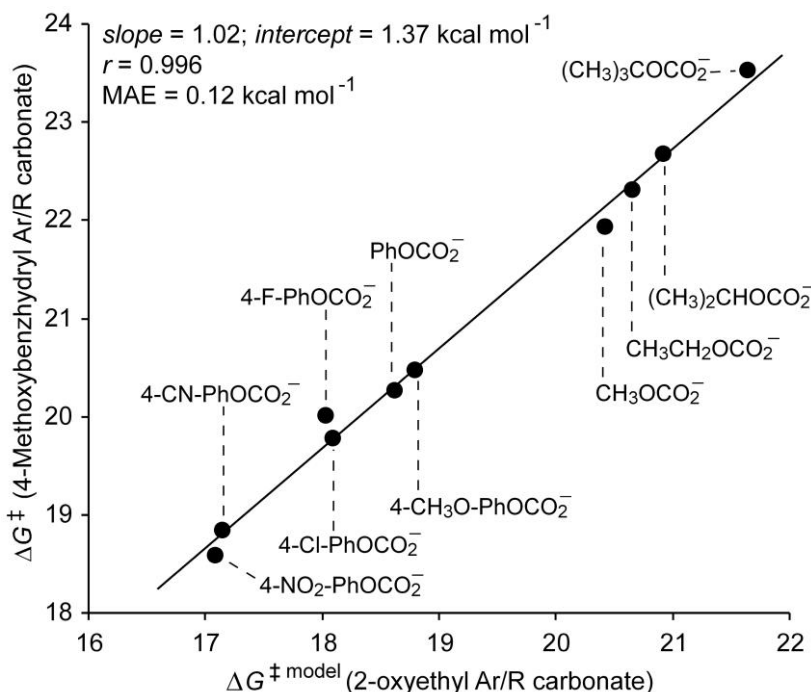


Figure S8. Correlation of experimental free energies of activation (in kcal mol⁻¹) for solvolyses of 4-methoxybenzhydryl aryl/alkyl carbonates in **60% ethanol** (Table S5) versus free energies of activation (in kcal mol⁻¹) for heterolysis of 2-oxyethyl aryl/alkyl carbonates calculated at the **M06-2X/AUG-cc-pVDZ** level of theory in the presence of the **IEFPCM** solvation model (solvent = water, Table S3).

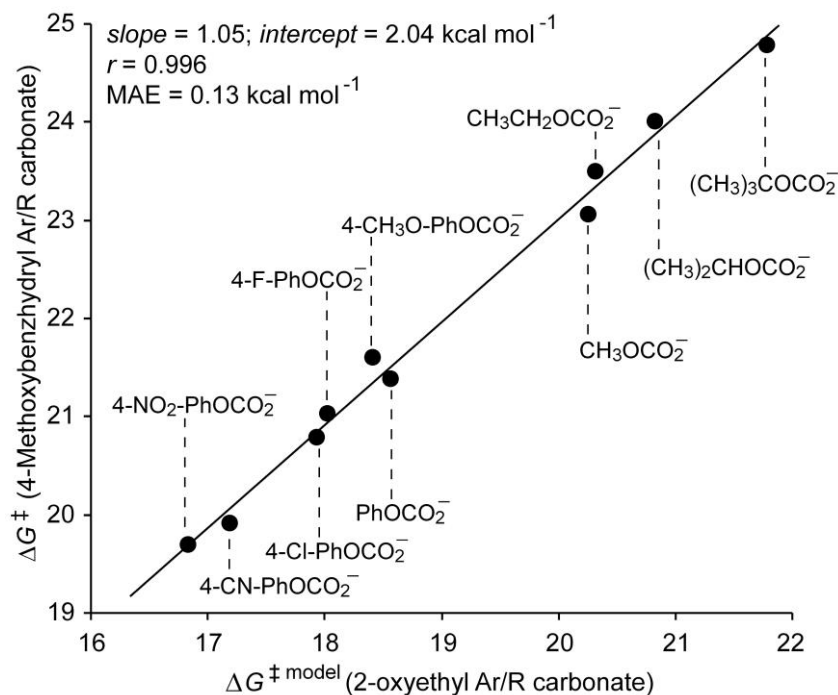


Figure S9. Correlation of experimental free energies of activation (in kcal mol⁻¹) for solvolyses of 4-methoxybenzhydryl aryl/alkyl carbonates in 60% acetone (Table S5) versus free energies of activation (in kcal mol⁻¹) for heterolysis of 2-oxyethyl aryl/alkyl carbonates calculated at the M06-2X/6-311+G(2d,p) level of theory in the presence of the IEFPCM solvation model (solvent = water, Table S3).

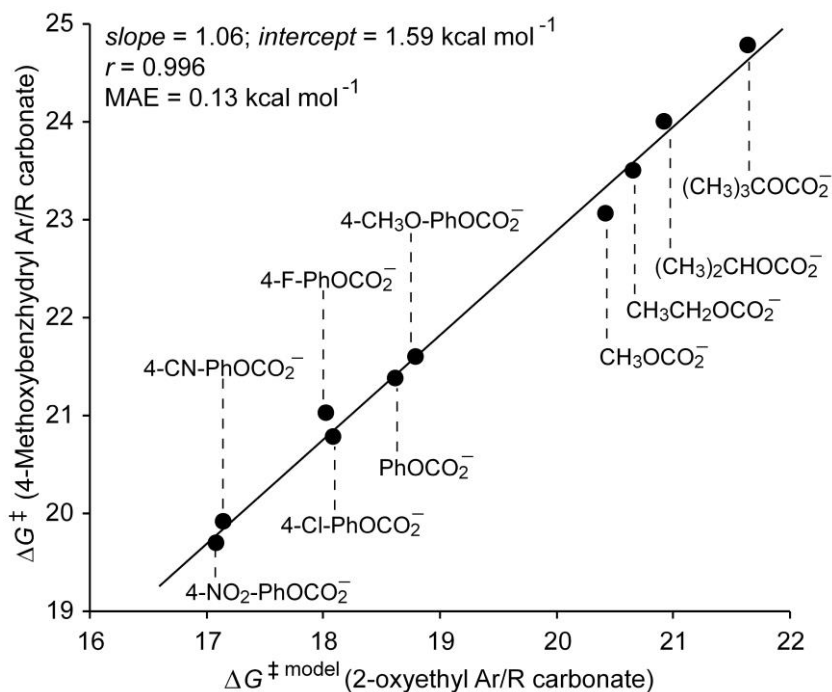


Figure S10. Correlation of experimental free energies of activation (in kcal mol⁻¹) for solvolyses of 4-methoxybenzhydryl aryl/alkyl carbonates in 60% acetone (Table S5) versus free energies of activation (in kcal mol⁻¹) for heterolysis of 2-oxyethyl aryl/alkyl carbonates calculated at the M06-2X/AUG-cc-pVDZ level of theory in the presence of the IEFPCM solvation model (solvent = water, Table S3).

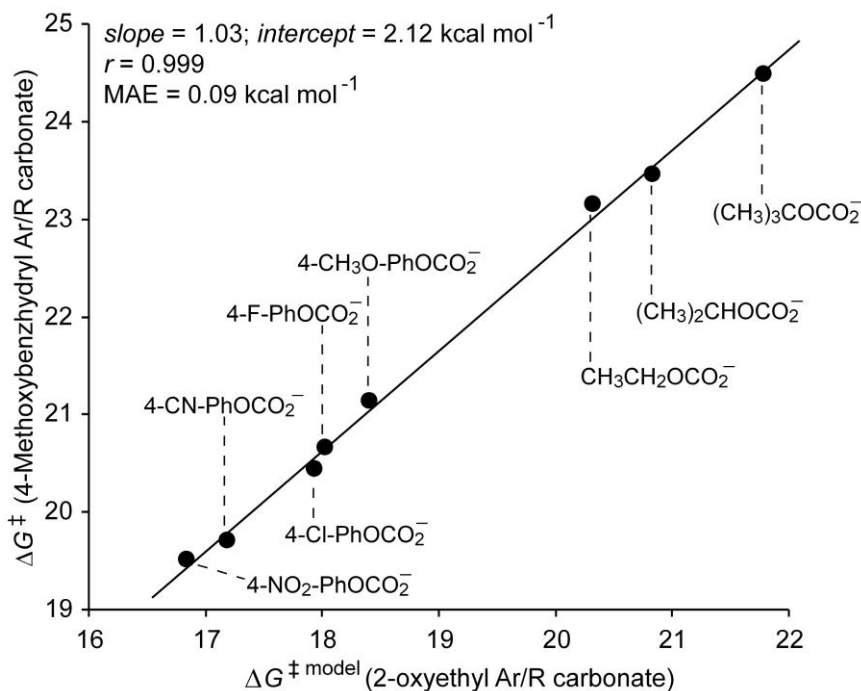


Figure S11. Correlation of experimental free energies of activation (in kcal mol⁻¹) for solvolyses of 4-methoxybenzhydryl aryl/alkyl carbonates in **60% acetonitrile** (Table S5) *versus* free energies of activation (in kcal mol⁻¹) for heterolysis of 2-oxyethyl aryl/alkyl carbonates calculated at the **M06-2X/6-311+G(2d,p)** level of theory in the presence of the **IEFPCM** solvation model (solvent = water, Table S3).

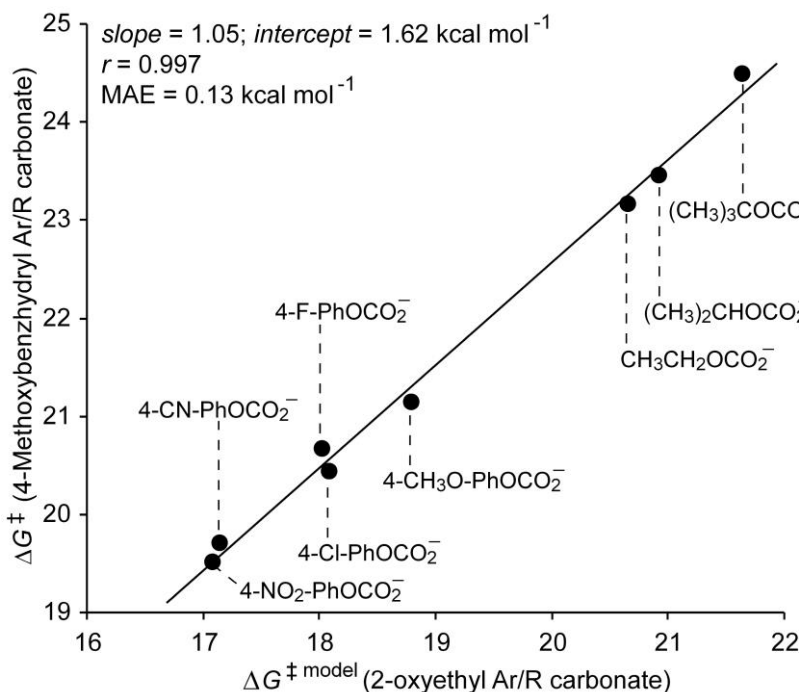


Figure S12. Correlation of experimental free energies of activation (in kcal mol⁻¹) for solvolyses of 4-methoxybenzhydryl aryl/alkyl carbonates in **60% acetonitrile** (Table S5) *versus* free energies of activation (in kcal mol⁻¹) for heterolysis of 2-oxyethyl aryl/alkyl carbonates calculated at the **M06-2X/AUG-cc-pVDZ** level of theory in the presence of the **IEFPCM** solvation model (solvent = water, Table S3).

2.2. s_f (aryl/alkyl carbonate leaving groups) vs. $\log k$ (4-methoxybenzhydryl aryl/alkyl carbonates)

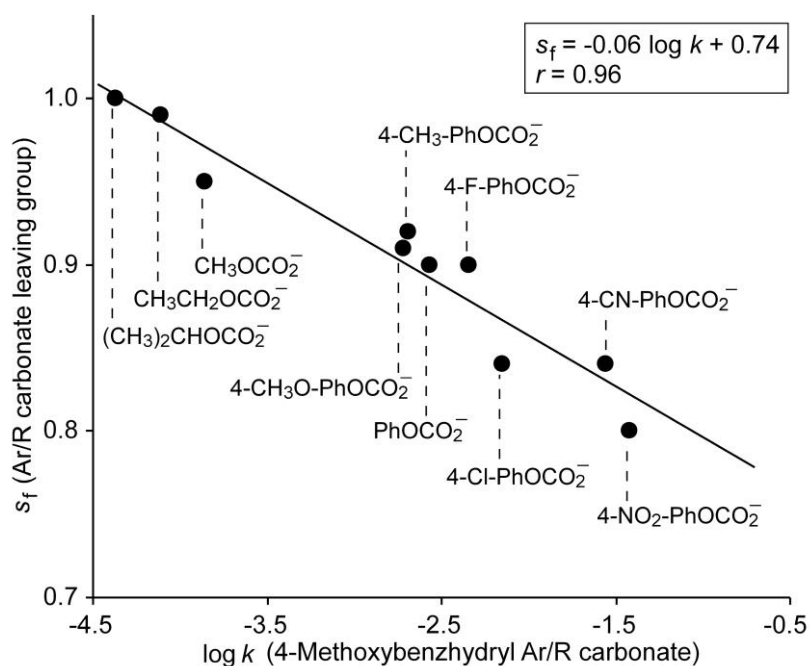


Figure S13. Correlation of s_f values of aryl/alkyl carbonate leaving groups against $\log k$ (25 °C) for solvolysis of corresponding 4-methoxybenzhydryl aryl/alkyl carbonates in **80% ethanol**. The values of $\log k$ and s_f , along with corresponding references are given in Table S5.

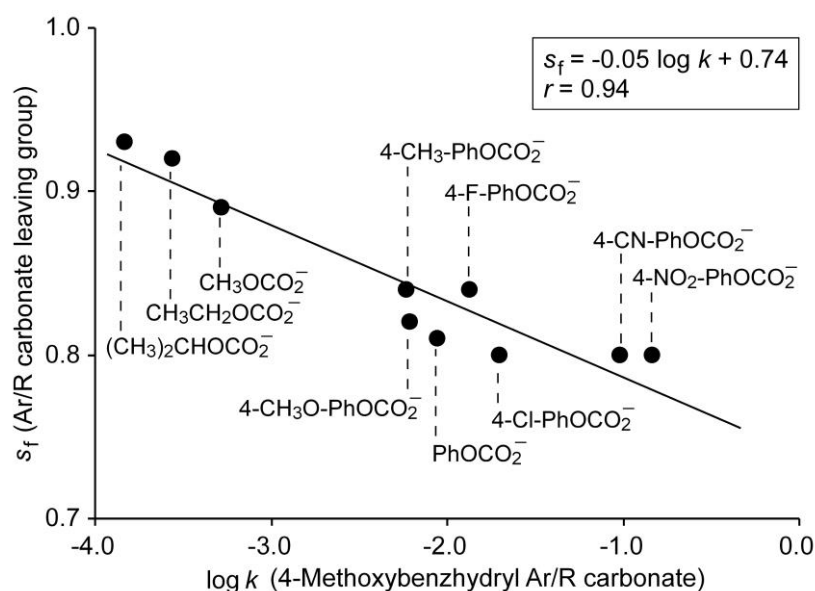


Figure S14. Correlation of s_f values of aryl/alkyl carbonate leaving groups against $\log k$ (25 °C) for solvolysis of corresponding 4-methoxybenzhydryl aryl/alkyl carbonates in **60% ethanol**. The values of $\log k$ and s_f , along with corresponding references are given in Table S5.

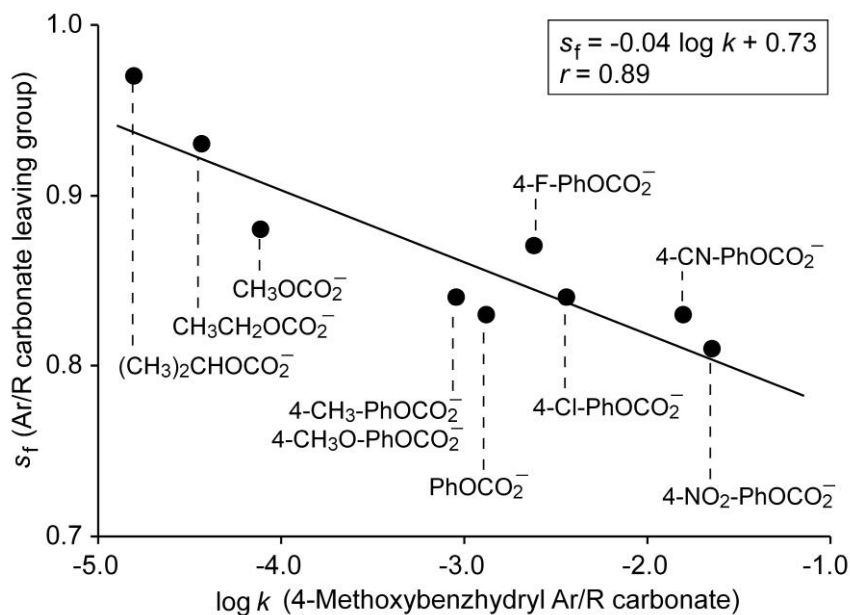


Figure S15. Correlation of s_f values of aryl/alkyl carbonate leaving groups against $\log k$ (25 °C) for solvolysis of corresponding 4-methoxybenzhydryl aryl/alkyl carbonates in **60% acetone**. The values of $\log k$ and s_f , along with corresponding references are given in Table S5.

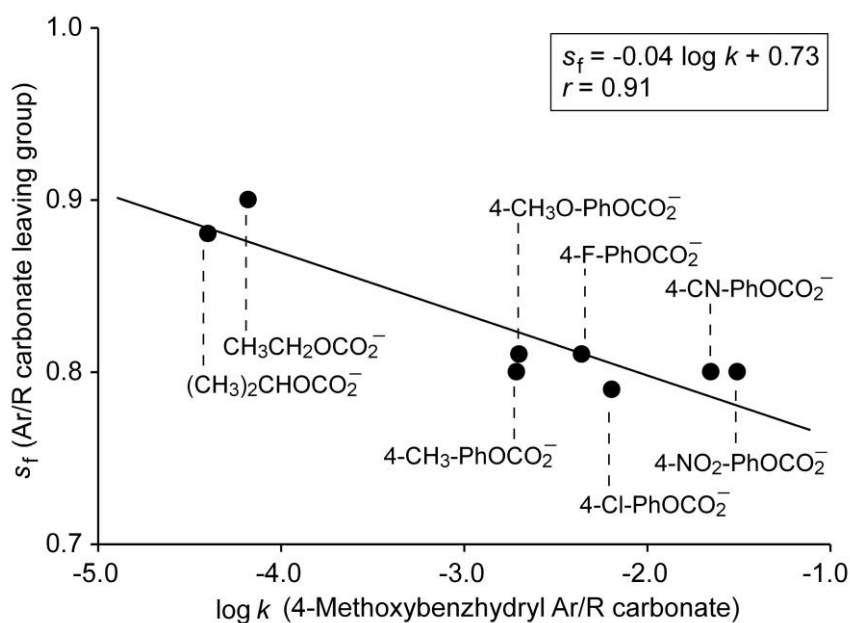


Figure S16. Correlation of s_f values of aryl/alkyl carbonate leaving groups against $\log k$ (25 °C) for solvolysis of corresponding 4-methoxybenzhydryl aryl/alkyl carbonates in **60% acetonitrile**. The values of $\log k$ and s_f , along with corresponding references are given in Table S5.

**3. Geometries of reference 2-oxyethyl aryl/alkyl carbonates
and geometries of corresponding heterolytic transition
states optimized at the IEFPCM-M06-2X/6-311+G(2d,p)
level**

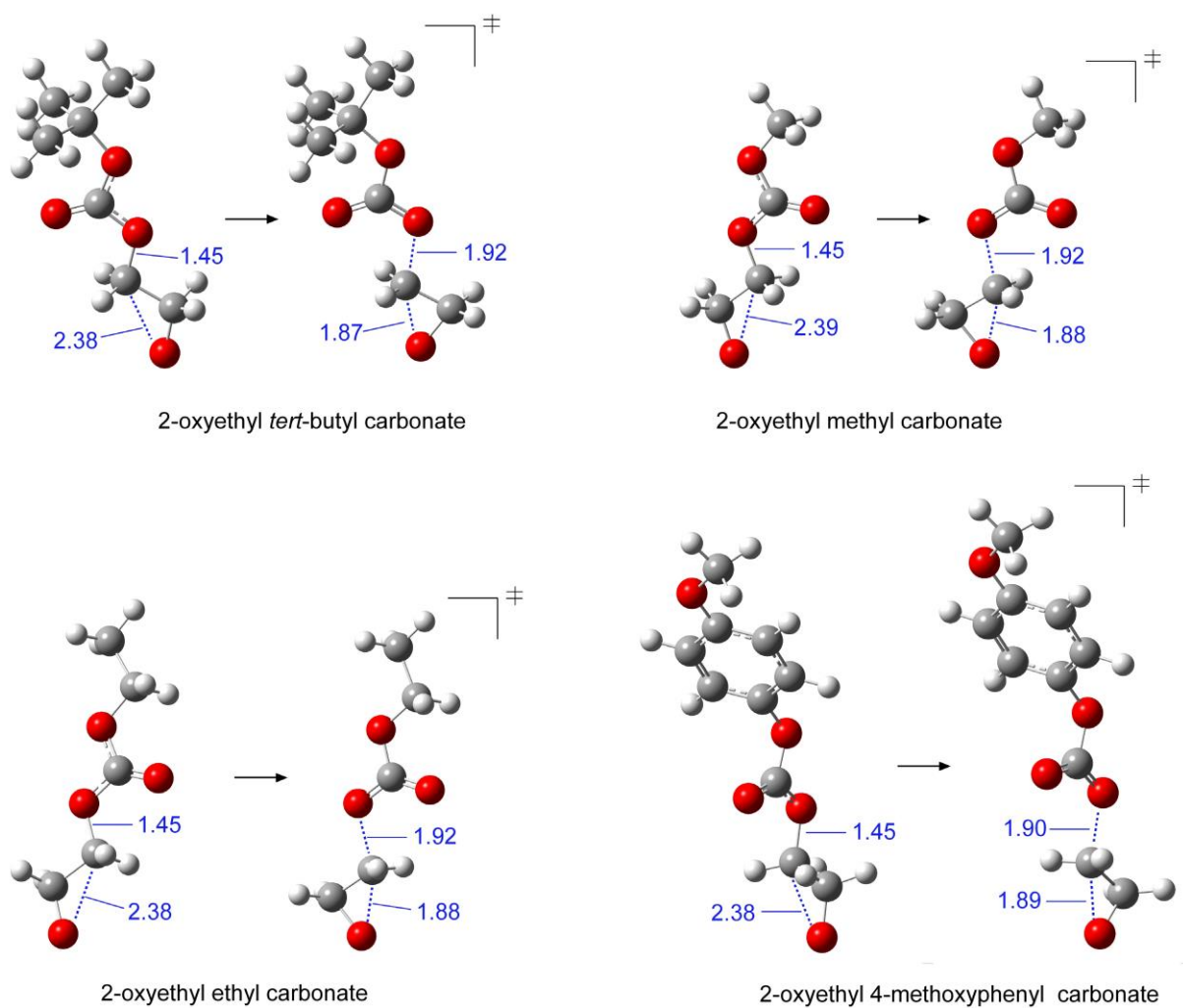


Figure S17. Geometries of reference 2-oxyethyl aryl/alkyl carbonates and geometries of corresponding heterolytic transition states optimized at the IEFPCM-M06-2X/6-311+G(2d,p) level.

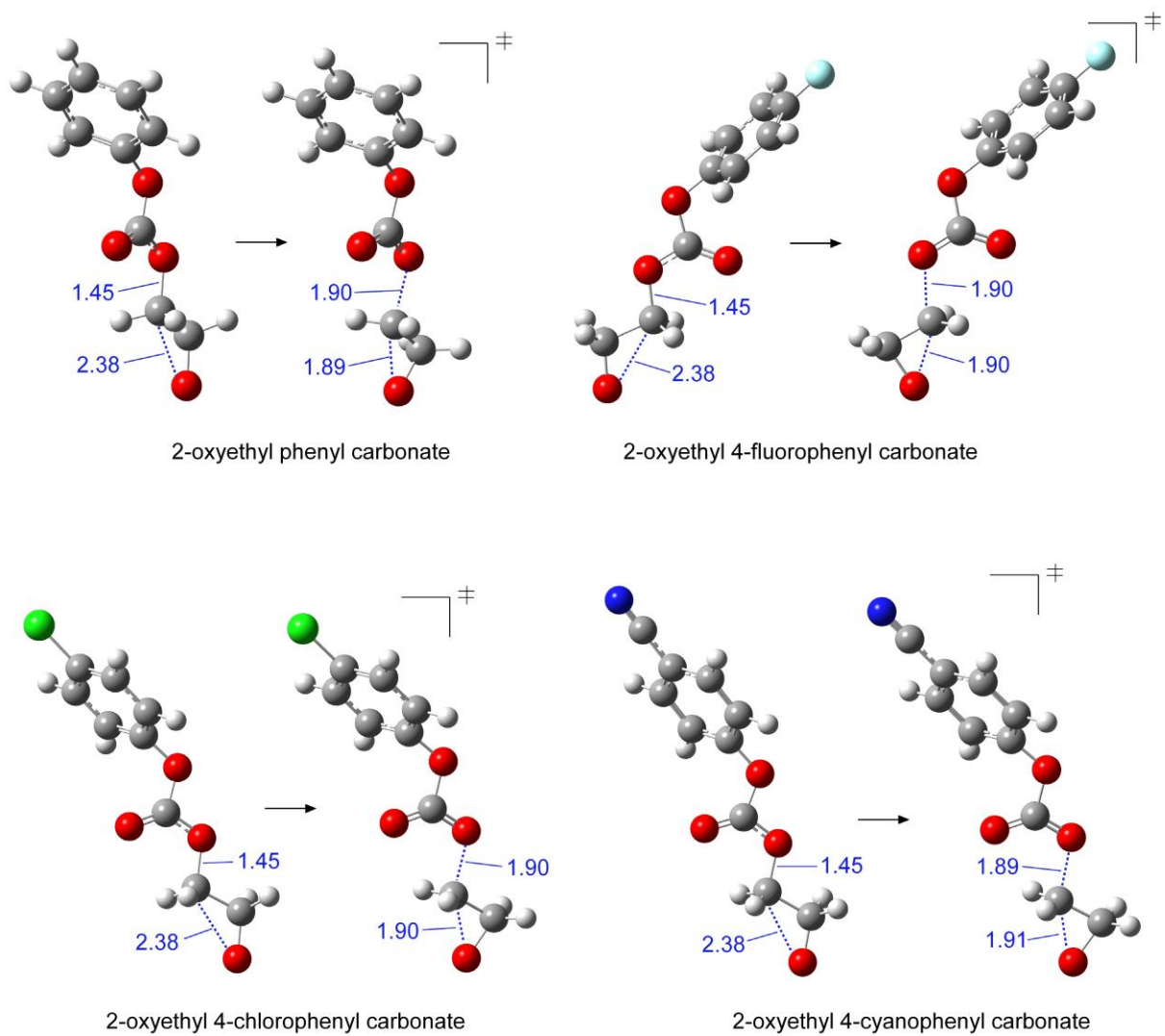


Figure S17. (Continued)

4. Coordinates and energies

Reference

2-oxyethyl alkyl/aryl carbonates (OEt alkyl/aryl carbonates)

M06-2X/AUG-cc-pVDZ IEFPCM, Solvent = Water

Substrates

OEt methyl carbonate

E (total electronic) = -457.534806

E (total electronic) + ZPVE = -457.419400

Internal Thermal Energy = -457.410635

Enthalpy = -457.409690

Gibbs Free Energy = -457.454045

O,0,2.1835137526,-0.1086864634,0.6686119617
C,0,0.9463930633,0.3611516126,0.6637912424
O,0,-0.0726004344,-0.2957425854,0.6613553966
O,0,0.9960642711,1.6965407532,0.6619918021
C,0,-0.2813886947,2.3472871052,0.6567679791
C,0,2.3165632656,-1.553891577,0.6711783281
C,0,3.8037023215,-1.9086021672,0.676645694
O,0,3.987925443,-3.2618157794,0.6792457227
H,0,-0.0632587099,3.4162761303,0.6559254592
H,0,-0.8487229307,2.0706710623,1.5509420024
H,0,-0.8427388066,2.068038317,-0.2403596573
H,0,1.8225840749,-1.9509548071,-0.2245882542
H,0,1.8166326088,-1.9483249846,1.5648025973
H,0,4.2444078179,-1.3864614083,1.5642116592
H,0,4.2503069574,-1.3890662083,-0.2094989336

OEt ethyl carbonate

E (total electronic) = -496.8365807

E (total electronic) + ZPVE = -496.692946

Internal Thermal Energy = -496.682892

Enthalpy = -496.681948

Gibbs Free Energy = -496.729489

O,0,0.1663495682,-0.5025112597,-0.0000070781
C,0,-1.0021963122,0.1211902808,0.0000013957
O,0,-1.1724294264,1.3219893579,0.0000080379
O,0,-1.9760287379,-0.7921320344,-0.0000040498
C,0,-3.3178593042,-0.2616227761,-0.000000102
C,0,1.3412942463,0.3485172533,-0.0000051014
C,0,2.5899383136,-0.533703802,-0.0000133915
O,0,3.7254673914,0.225482137,-0.000013201
H,0,-3.4435968729,0.3647338063,-0.8902821971
H,0,-3.4435983557,0.364716481,0.8902940033
H,0,1.3123724981,0.983943685,0.8943303189
H,0,1.312368105,0.9839539022,-0.8943331471
H,0,2.493499267,-1.2108258615,-0.8868730252
H,0,2.4935048441,-1.210834612,0.8868401676
C,0,-4.2653582484,-1.4386079634,-0.0000122302
H,0,-4.1153925086,-2.0563737532,0.8925667407
H,0,-5.2970705807,-1.0697349032,-0.000009536
H,0,-4.1153909667,-2.0563565082,-0.8926028847

OEt isopropyl carbonate

E (total electronic) = -536.1392653

E (total electronic) + ZPVE = -535.967683

Internal Thermal Energy = -535.956385

Enthalpy = -535.955441

Gibbs Free Energy = -536.005588

O,0,0.3466963452,-0.9113272668,0.0514451576
C,0,0.3508738683,0.3797077461,0.3532837449
O,0,0.4556366322,0.8484341259,1.4672078833
O,0,0.2127810915,1.0803062778,-0.7742992851
C,0,0.2405725736,2.5269658565,-0.6442527649
C,0,0.48885322,-1.8250334396,1.1687019543
C,0,0.4677693219,-3.2598663731,0.6412700521
O,0,0.6088407285,-4.1580408908,1.6610476941
C,0,-0.4372941172,3.0652845322,-1.8878887121
C,0,1.6767123272,2.9972803222,-0.4995267273
H,0,-0.336166445,2.7856093405,0.2505314953
H,0,-0.3393100663,-1.6544154968,1.8682778448
H,0,1.438007735,-1.610421813,1.6758383637
H,0,1.2735473472,-3.3194112377,-0.134279293
H,0,-0.487989386,-3.3678742521,0.0675401007
H,0,-1.4646443952,2.6928074881,-1.9622149253
H,0,-0.4626009185,4.1598850747,-1.8430011123
H,0,0.1187458394,2.7645587813,-2.7844778692
H,0,2.1411102502,2.5632103194,0.3917483547
H,0,2.2558466176,2.7126789427,-1.3868512491
H,0,1.6948254304,4.0894319626,-0.4050157073

OEt tert-butyl carbonate

E (total electronic) = -575.438765

E (total electronic) + ZPVE = -575.239712

Internal Thermal Energy = -575.227031

Enthalpy = -575.226087

Gibbs Free Energy = -575.279416

O,0,0.1752824393,-0.4295325562,-0.0299941131
C,0,-0.9641533521,0.2553919292,-0.0253674442
O,0,-1.0524355889,1.4649288279,-0.0229595335
O,0,-1.9694351927,-0.6193582199,-0.0231912194
C,0,-3.3598891722,-0.1508567935,-0.0020374965
C,0,1.3903259469,0.3596042682,-0.0266039682
C,0,2.5922796982,-0.5836694841,0.0296613658
O,0,3.7656409332,0.1157500825,0.0456174817
H,0,1.37622307,1.0222350831,0.8477904079
H,0,1.4149803164,0.9699730482,-0.9386498622
H,0,2.4867803071,-1.2774464709,-0.843371896
H,0,2.4360600152,-1.2325359762,0.9291422989
C,0,-3.6275325606,0.6350613766,1.2761660791
H,0,-3.0922692455,1.5877636107,1.2795582669
H,0,-4.7033626199,0.8339794339,1.3472802699
H,0,-3.3277594906,0.0446373549,2.1503034535
C,0,-3.6615514304,0.6569250023,-1.258812032
H,0,-3.3840390861,0.0825199692,-2.1507726245
H,0,-4.7392337124,0.8548740364,-1.2980997432
H,0,-3.127946717,1.6104671938,-1.2595139854
C,0,-4.146918284,-1.4546319993,-0.0028691676
H,0,-3.8951052143,-2.0531471853,0.880323503
H,0,-5.2200165988,-1.2344403717,0.0143478567
H,0,-3.9203848409,-2.0366758296,-0.9037422073

OEt phenyl carbonate

E (total electronic) = -649.2287727

E (total electronic) + ZPVE = -649.061009

Internal Thermal Energy = -649.049207

Enthalpy = -649.048263

Gibbs Free Energy = -649.102038

C,0,3.0182116803,0.0000073054,0.3946656326
C,0,4.2876190023,-0.0000168196,-0.4572531369
O,0,5.4033474324,0.0000033391,0.3295901462
O,0,1.8635587157,-0.0000156296,-0.4896351018
C,0,0.6850741534,0.000002766,0.0999975698
O,0,0.4623955914,0.0000322509,1.2871621929
O,0,-0.2627550701,-0.0000252232,-0.8655070857
C,0,-1.5906930953,-0.0000106598,-0.4291587792

C,0,-2.2397841319,1.2154881847,-0.2511409018
C,0,-3.5847760093,1.2091934445,0.1202442625
C,0,-4.2573375082,0.0000144291,0.3058584261
C,0,-3.5847819313,-1.2091772591,0.1203055166
C,0,-2.2397900489,-1.2154973109,-0.2510794903
H,0,2.969495693,-0.8951791086,1.0269568766
H,0,2.9694973525,0.8952280719,1.0269083673
H,0,4.2070230273,0.8869883091,-1.13618372
H,0,4.2070213702,-0.8870582079,-1.1361361062
H,0,-1.696212176,2.1459834714,-0.4051709631
H,0,-4.1079429785,2.1534559598,0.2619437857
H,0,-5.307343026,0.0000242758,0.5933340016
H,0,-4.107953452,-2.1534300716,0.2620529375
H,0,-1.6962225909,-2.1460030281,-0.4050624301

OEt 4-nitrophenyl carbonate

E (total electronic) = -853.7045577
E (total electronic) + ZPVE = -853.533787
Internal Thermal Energy = -853.519518
Enthalpy = -853.518574
Gibbs Free Energy = -853.578263

C,0,-0.0699593562,-3.437262298,1.0004725726
C,0,-0.127581573,-4.7902906329,0.2918336372
O,0,-0.2554030432,-5.8045097918,1.196538578
O,0,0.0533591103,-2.3895399671,-0.004224926
C,0,0.0848828764,-1.1581551716,0.452072254
O,0,0.0258368511,-0.7951259372,1.6000100936
O,0,0.2174355408,-0.3303928381,-0.621200883
C,0,0.1785619634,1.0352109716,-0.4129868488
C,0,1.1880777934,1.7817479459,-1.0161084093
C,0,1.1607777021,3.167795315,-0.9174942059
C,0,0.1181158351,3.7603400645,-0.2124985647
C,0,-0.8981227487,3.0221579256,0.3888537815
C,0,-0.8690790139,1.6374868259,0.2846533012
N,0,0.0844859742,5.2232319802,-0.1031849538
O,0,0.9754212068,5.8583647282,-0.6383425985
O,0,-0.8325450094,5.7308912974,0.5172172168
H,0,-0.9862914004,-3.2554172691,1.5748401222
H,0,0.7983405462,-3.3767442292,1.6681682499
H,0,0.7953833864,-4.8524377012,-0.3390677037
H,0,-0.9707031946,-4.7212769589,-0.4417020818
H,0,1.980578083,1.2721098717,-1.5586796334
H,0,1.932031596,3.7803836824,-1.3749557353
H,0,-1.6981675771,3.5275077217,0.9218698183
H,0,-1.6503265487,1.032061465,0.735401919

OEt 4-cyanophenyl carbonate

E (total electronic) = -741.4642456
E (total electronic) + ZPVE = -741.297632
Internal Thermal Energy = -741.284134
Enthalpy = -741.283190
Gibbs Free Energy = -741.340153

C,0,0.1063783887,-3.6806182575,-0.8651279111
C,0,0.1627330482,-4.5358933181,-2.1306163703
O,0,0.0636283154,-5.8622419789,-1.8227261963
O,0,0.2032307787,-2.2780488576,-1.2451107416
C,0,0.1308222888,-1.410392579,-0.2604523483
O,0,-0.0039358075,-1.6410222451,0.9154045318
O,0,0.2520840088,-0.1682842334,-0.8017213272
C,0,0.1172202323,0.9275823344,0.0340807639
C,0,1.1274788165,1.8829173144,-0.0202963587
C,0,1.0044980699,3.0443850937,0.7337223202
C,0,-0.1293988655,3.2290223619,1.5337655614
C,0,-1.1421656648,2.260899772,1.5764993387
C,0,-1.0208900173,1.1026835976,0.819729435
C,0,-0.2597272305,4.4292677078,2.3187164182
N,0,-0.3647567948,5.3945438176,2.9497763571
H,0,-0.841718469,-3.8278251278,-0.3339573589
H,0,0.9417573395,-3.9131985817,-0.1930987603
H,0,1.112089607,-4.2568907461,-2.6546895365

H,0,-0.6532501305,-4.1579900831,-2.7977687564
H,0,1.9950591186,1.7117970223,-0.65330436
H,0,1.782945358,3.8032283233,0.7044026443
H,0,-2.0216401083,2.4200932664,2.1962075124
H,0,-1.7997002819,0.3448793968,0.8356741426

OEt 4-methoxyphenyl carbonate

E (total electronic) = -763.726691
E (total electronic) + ZPVE = -763.525966
Internal Thermal Energy = -763.511753
Enthalpy = -763.510809
Gibbs Free Energy = -763.569494

C,0,-0.252426993,-3.9637025852,-0.9142446806
C,0,-0.2825069197,-4.8883750832,-2.1310007644
O,0,-0.3303221415,-6.1978145229,-1.7464978804
O,0,-0.2038984433,-2.5859387496,-1.3758238832
C,0,-0.1558753285,-1.6634369723,-0.434971036
O,0,-0.1477442593,-1.841845349,0.7596849197
O,0,-0.1130993266,-0.4552156249,-1.0410080551
C,0,-0.0812615868,0.6635794118,-0.2028003816
C,0,-1.2498419574,1.1001840976,0.4180493178
C,0,-1.215782407,2.2507250902,1.1926512755
C,0,-0.0182812239,2.96647736,1.343249024
C,0,1.1466851763,2.5213730188,0.7119840836
C,0,1.107502039,1.358469696,-0.0643197702
O,0,-0.0895339653,4.0813569745,2.1187385229
C,0,1.1064422603,4.8291193059,2.2923779698
H,0,-1.1535714096,-4.0917149728,-0.3015921771
H,0,0.6354173405,-4.1547694556,-0.2988841375
H,0,0.6160764416,-4.6245029609,-2.7449376425
H,0,-1.1564819769,-4.5610640575,-2.7500540594
H,0,-2.1744830154,0.5397565685,0.2914152195
H,0,-2.1124013456,2.6158475642,1.6898747113
H,0,2.0846891662,3.0597011628,0.8101568057
H,0,2.0042624526,0.9983501375,-0.5650038376
H,0,0.8443023199,5.6700314352,2.9373651834
H,0,1.4762601011,5.2031284352,1.3282669234
H,0,1.8814030022,4.2192150758,2.775665349

OEt 4-chlorophenyl carbonate

E (total electronic) = -1108.8225931
E (total electronic) + ZPVE = -1108.664375
Internal Thermal Energy = -1108.651437
Enthalpy = -1108.650492
Gibbs Free Energy = -1108.706941

C,0,3.7357858678,-0.2939366775,0.3214031564
C,0,5.0215636129,0.2739966007,-0.278941651
O,0,6.1193374193,-0.3087164696,0.2850785292
O,0,2.5991607766,0.3518126365,-0.3174972036
C,0,1.4102419927,-0.0331988602,0.0960814561
O,0,1.1601844347,-0.8565714713,0.9422753226
O,0,0.4848234859,0.673329101,-0.5994765341
C,0,-0.854941618,0.3914143955,-0.34854851
C,0,-1.6432589038,1.4135289515,0.1643036607
C,0,-3.0078331062,1.1954702666,0.3525232995
C,0,-3.542470893,-0.0460692367,0.0239760585
C,0,-2.7528224397,-1.0721090594,-0.4910182025
C,0,-1.3917941534,-0.8480091298,-0.6823808411
H,0,3.6634102154,-1.3740240229,0.1440656194
H,0,3.6844829441,-0.0971041392,1.3993643539
H,0,4.9680391196,1.3835282007,-0.1371301614
H,0,4.9410185069,0.1239950193,-1.3857711037
H,0,-1.1922999488,2.3731859326,0.4078749292
H,0,-3.6450879034,1.9820422249,0.7499665652
H,0,-3.1967620315,-2.0321167877,-0.7441065304
H,0,-0.7534646516,-1.6297518406,-1.0885536812
Cl,0,-5.2554813763,-0.3267192043,0.2586630682

OEt 4-fluorophenyl carbonate

E (total electronic) = -748.4531684
E (total electronic) + ZPVE = -748.293568
Internal Thermal Energy = -748.281022
Enthalpy = -748.280077
Gibbs Free Energy = -748.335229

C,0,0.1799041937,-2.6556716636,-1.6107267039
C,0,-0.0848571541,-3.1805040252,-3.0215537465
O,0,0.2237374908,-4.5075210502,-3.112148655
O,0,-0.1656403119,-1.2432219602,-1.5657435008
C,0,0.006895147,-0.6446836079,-0.4054676441
O,0,0.4164391383,-1.1369782823,0.6181863821
O,0,-0.3581007258,0.6520967671,-0.5489821188
C,0,-0.2537477562,1.4528132309,0.5894097316
C,0,0.8603242796,2.2712714168,0.7281849234
C,0,0.9454907259,3.125411447,1.8273123558
C,0,-0.0936114897,3.1214862396,2.7461361576
C,0,-1.2116792303,2.3090146967,2.6181419421
C,0,-1.2904227638,1.4601251013,1.5157447681
F,0,-0.016190685,3.9498475508,3.8138667089
H,0,-0.4353590103,-3.185580346,-0.8731682262
H,0,1.2389661163,-2.7609153082,-1.3445827941
H,0,0.5030960004,-2.5255208258,-3.7138375986
H,0,-1.1560818667,-2.9434169335,-3.2460823019
H,0,1.6500683985,2.2418059283,-0.0196709873
H,0,1.7990674504,3.7840505626,1.9713348912
H,0,-2.0013017711,2.3461261113,3.3653131117
H,0,-2.1503831759,0.8087329507,1.3731673047

Transition states

TS-OEt methyl carbonate

E (total electronic) = -457.4988527
E (total electronic) + ZPVE = -457.385827
Internal Thermal Energy = -457.376901
Enthalpy = -457.375957
Gibbs Free Energy = -457.421510

O,0,0.0167530523,-0.7310649309,-0.0000009239
C,0,-1.0142473348,0.0186008,0.0000010241
O,0,-1.0601726768,1.2515616317,0.0000075257
O,0,-2.1752861659,-0.7135580822,-0.0000053462
C,0,-3.380630576,0.0466785005,-0.0000034229
C,0,1.6530713651,0.2572168961,0.0000020294
C,0,2.7738204384,-0.6758958377,-0.0000067233
O,0,3.5143146803,0.5091543632,-0.000000787
H,0,-4.1948615216,-0.6825325734,-0.0000098896
H,0,-3.4417653517,0.6793805973,-0.8927611828
H,0,-3.4417695939,0.6793693921,0.8927620009
H,0,1.4176180369,0.7623954815,0.9289581606
H,0,1.4176137014,0.7624076641,-0.9289463742
H,0,2.8740176504,-1.3000933439,-0.9029743116
H,0,2.8740220458,-1.3001051785,0.9029521981

TS-OEt ethyl carbonate

E (total electronic) = -496.800183
E (total electronic) + ZPVE = -496.658940
Internal Thermal Energy = -496.648694
Enthalpy = -496.647750
Gibbs Free Energy = -496.696570

O,0,0.5009375379,-0.6435219726,0.0214762556
C,0,-0.4725248254,0.1801702529,0.0163474358
O,0,-0.4249768422,1.4136262206,0.0177013637
O,0,-1.6833185848,-0.46435407,0.007560485
C,0,-2.8423343784,0.3761518385,0.0035556573
C,0,2.210301643,0.2137846966,-0.0166125022
C,0,3.2536868474,-0.804197719,0.0188305367

O,0,4.0838389467,0.3187844197,-0.034414921
C,0,-4.0588454505,-0.5241391095,-0.0282490204
H,0,-2.8085587914,1.033890046,-0.8736209476
H,0,-2.834433161,1.0064068189,0.9015587887
H,0,2.0193945061,0.7729510295,0.8912522604
H,0,2.0096647771,0.6964284492,-0.9654708216
H,0,3.2981012521,-1.4721634756,-0.8568773351
H,0,3.3111434297,-1.395475406,0.9473315403
H,0,-4.9686056095,0.0874507494,-0.030051079
H,0,-4.0562995063,-1.1464600382,-0.9309788935
H,0,-4.0807879505,-1.1778250903,0.8517487169

TS-OEt isopropyl carbonate

E (total electronic) = -536.1024033
E (total electronic) + ZPVE = -535.933333
Internal Thermal Energy = -535.921827
Enthalpy = -535.920883
Gibbs Free Energy = -535.972256

O,0,0.4487935095,-1.1121408323,-0.5920337748
C,0,0.499260852,0.1399964142,-0.3532652896
O,0,1.0719865585,0.7090643021,0.5803728852
O,0,-0.1998720194,0.8600857049,-1.289591833
C,0,-0.1595400838,2.2948741767,-1.1818409921
C,0,1.4078125184,-2.1622816638,0.6905475653
C,0,1.2693541291,-3.5717332603,0.3443080964
O,0,2.0671319353,-3.7298586533,1.4808891302
C,0,1.1493896282,2.8226178149,-1.7476102099
C,0,-1.3690057385,2.8109298841,-1.9399207065
H,0,-0.2371470483,2.5577616533,-0.1206931181
H,0,0.8251754788,-1.7869807293,1.5230023175
H,0,2.3510770172,-1.678167524,0.4681230501
H,0,1.7318513232,-3.8766493858,-0.608552658
H,0,0.2492839411,-3.982825104,0.4171364654
H,0,1.1807037222,3.9159188672,-1.6623811909
H,0,1.9998255662,2.4040878797,-1.199475087
H,0,1.2344489805,2.5525752463,-2.8083891361
H,0,-1.3111176449,2.5155179248,-2.9954923314
H,0,-2.2947202659,2.4108525537,-1.5109868755
H,0,-1.4018913595,3.9055127309,-1.8861293073

TS-OEt tert-butyl carbonate

E (total electronic) = -575.4007269
E (total electronic) + ZPVE = -575.204121
Internal Thermal Energy = -575.191229
Enthalpy = -575.190285
Gibbs Free Energy = -575.244938

O,0,0.9418560573,0.6422111775,-0.0020710138
C,0,-0.0757150465,-0.1303097521,-0.0008221351
O,0,-0.0761659733,-1.3642825802,0.0004994426
O,0,-1.2404021423,0.5934142884,-0.0011132888
C,0,-2.5375683225,-0.0598444194,0.0001056994
C,0,-3.5091081821,1.1168070012,-0.0007588797
C,0,-2.7280538174,-0.8902341417,1.266741723
C,0,-2.7290732054,-0.8929354442,-1.2646012101
H,0,-3.3563912018,1.7360353917,-0.8929755418
H,0,-3.3556661995,1.7379438534,0.8900055936
H,0,-4.5418168842,0.7491937944,0.000546555
H,0,-2.0680659368,-1.7606208061,1.2703442211
H,0,-2.5219958014,-0.2747449209,2.151433607
H,0,-3.7698023748,-1.2302851468,1.319904716
H,0,-3.7708686981,-1.2330820726,-1.3162089312
H,0,-2.5237102857,-0.2793404434,-2.15076936
H,0,-2.0691006355,-1.7633382581,-1.2668703367
C,0,2.6064556776,-0.3129237914,-0.0016769166
C,0,3.702693499,0.6477967927,-0.0030735421
O,0,4.4646621224,-0.5244538867,-0.0021295747
H,0,2.3778352866,-0.8214484658,-0.9301392308
H,0,2.3785056377,-0.819513815,0.9280068908

H,0,3.7913828501,1.2739337903,0.8994923916
H,0,3.7907295764,1.2720548549,-0.9070039794

TS-OEt phenyl carbonate

E (total electronic) = -649.1958407
E (total electronic) + ZPVE = -649.030545
Internal Thermal Energy = -649.018542
Enthalpy = -649.017598
Gibbs Free Energy = -649.072369

C,0,-4.1692660195,-0.33205363,-0.3103057919
C,0,-5.4175918589,0.1750788375,0.2514844271
O,0,-5.9876160069,-0.7839709455,-0.587017954
O,0,-2.7113830185,0.6135997465,0.4505352333
C,0,-1.5842714164,0.1963813646,0.0427601242
O,0,-1.3284814264,-0.6908475918,-0.7645182932
O,0,-0.5487649465,0.917002937,0.6434843665
C,0,0.7512514854,0.5289710006,0.3740117816
C,0,1.5838125178,1.4290567017,-0.2849252723
C,0,2.9239537081,1.0960917002,-0.4942029115
C,0,3.4212336346,-0.1294375681,-0.0511450272
C,0,2.5736280947,-1.0238433648,0.608403146
C,0,1.2363266878,-0.697603883,0.8265007618
H,0,-3.8182179019,-1.2956631757,0.0401132157
H,0,-3.9221179943,-0.0398980313,-1.3242790654
H,0,-5.6539478801,1.2238815155,0.0064609121
H,0,-5.5521582137,0.0040314606,1.3325134711
H,0,1.1783087753,2.3817884128,-0.6216342112
H,0,3.5791897742,1.7994597991,-1.0062542664
H,0,2.9575331621,-1.9807942855,0.959373666
H,0,0.5655699483,-1.3836012144,1.3407927951
H,0,4.4661032348,-0.3875050861,-0.2157943475

TS-OEt 4-nitrophenyl carbonate

E (total electronic) = -853.6741587
E (total electronic) + ZPVE = -853.505802
Internal Thermal Energy = -853.491370
Enthalpy = -853.490426
Gibbs Free Energy = -853.551035

C,0,4.4730776823,-0.3573988138,0.2485293632
C,0,5.7073359736,0.2089206525,-0.2903858745
O,0,6.3159344397,-0.8042006802,0.4500800136
O,0,2.9961172853,0.6216394637,-0.3976678494
C,0,1.889778626,0.170698035,0.0196652635
O,0,1.6508240846,-0.7758719574,0.7559585212
O,0,0.8320710885,0.9631625073,-0.4717363722
C,0,-0.4599681463,0.5641882574,-0.2749978442
C,0,-0.8897888386,-0.7403572985,-0.5463399955
C,0,-2.2335188646,-1.0579971297,-0.4073291304
C,0,-3.1228340635,-0.0637288354,-0.0031149176
C,0,-2.7125909522,1.2399367517,0.26108403
C,0,-1.3660722215,1.550977016,0.1235694749
N,0,-4.538818059,-0.4009324248,0.1434102283
O,0,-4.8845559232,-1.5481453286,-0.0830364298
O,0,-5.3087957285,0.4805477825,0.4855400833
H,0,4.131775798,-1.2965787154,-0.1715933587
H,0,4.2477215896,-0.1581457529,1.2900862969
H,0,5.9318841667,1.238516253,0.0353183211
H,0,5.8186930867,0.1325219851,-1.3850812011
H,0,-0.1751244232,-1.4934455665,-0.864229956
H,0,-2.5958722368,-2.0609096167,-0.6143439369
H,0,-3.4350603028,1.9894621247,0.5710029213
H,0,-1.0025506609,2.5572314912,0.3188469491

TS-OEt 4-cyanophenyl carbonate

E (total electronic) = -741.4333591
E (total electronic) + ZPVE = -741.269174

Internal Thermal Energy = -741.255463
Enthalpy = -741.254519
Gibbs Free Energy = -741.312822

C,0,-0.1007351006,-3.846662324,-1.5252429546
C,0,-0.1011939137,-4.5022460193,-2.8306546699
O,0,-0.2956757791,-5.6590416146,-2.0758817417
O,0,0.1486360566,-1.9889849463,-1.7540710764
C,0,0.1216383776,-1.3520462057,-0.6600031418
O,0,-0.0348574345,-1.7585556346,0.483372889
O,0,0.3365512757,0.0188690425,-0.8950570058
C,0,0.2063524448,0.9058529601,0.1409262312
C,0,1.2180022768,1.8560310583,0.2895777952
C,0,1.1054296573,2.8384137579,1.2659480433
C,0,-0.0232995981,2.8610020498,2.094371008
C,0,-1.0395777214,1.907071717,1.9387045883
C,0,-0.926806888,0.9292193889,0.9600672392
C,0,-0.1442831627,3.8725157057,3.1102184723
N,0,-0.2420534947,4.6870773933,3.928319226
H,0,-1.0552910007,-3.7330588815,-1.0245279411
H,0,0.7829667577,-3.9659254115,-0.9087590297
H,0,0.8516232899,-4.4480725149,-3.3835072616
H,0,-0.934468647,-4.2211448244,-3.4962980594
H,0,2.0839700381,1.8175315714,-0.367643143
H,0,1.8885591926,3.5833045108,1.389357143
H,0,-1.9164218611,1.9388311082,2.5819318927
H,0,-1.7084977657,0.1866991129,0.8271384966

TS-OEt 4-methoxyphenyl carbonate

E (total electronic) = -763.6933683
E (total electronic) + ZPVE = -763.495060
Internal Thermal Energy = -763.480646
Enthalpy = -763.479702
Gibbs Free Energy = -763.539541

C,0,-4.1609291475,0.1184159917,0.4613252225
C,0,-5.4266099251,-0.1875930016,-0.1983561239
O,0,-5.9678307524,0.3396269241,0.9755169426
H,0,-3.856258565,1.1574174664,0.503224817
H,0,-3.8445869519,-0.5362818156,1.2648123578
H,0,-5.6210607579,-1.2586116395,-0.3740114924
H,0,-5.6313015824,0.3859684,-1.1175412248
O,0,-2.7213448618,-0.3774354675,-0.6732389764
C,0,-1.5861092286,-0.1105975878,-0.1706859281
O,0,-1.3173694264,0.3870181258,0.9187102014
O,0,-0.5614668639,-0.4706119351,-1.046311063
C,0,0.738285256,-0.2009541747,-0.6446386071
C,0,1.2523295408,1.0931026149,-0.7466491458
C,0,2.575890843,1.3369241448,-0.4080533412
C,0,3.397226511,0.2884474954,0.0321890065
C,0,2.8815192605,-1.0061641396,0.1299427813
C,0,1.5443667733,-1.241857943,-0.2099730498
O,0,4.6814978175,0.6284725749,0.3369111211
C,0,5.5377993512,-0.413296887,0.7817296349
H,0,0.6090574007,1.9012025572,-1.0913459262
H,0,2.9964596844,2.3384211074,-0.4806089572
H,0,3.4969604907,-1.8363145269,0.4646097959
H,0,1.1294169631,-2.2459890882,-0.1401878647
H,0,6.5069969017,0.0526824571,0.9708238071
H,0,5.6442851173,-1.1883909949,0.0106486409
H,0,5.1571141517,-0.8639386584,1.7083133716

TS-OEt 4-chlorophenyl carbonate

E (total electronic) = -1108.7905229
E (total electronic) + ZPVE = -1108.634745
Internal Thermal Energy = -1108.621595
Enthalpy = -1108.620651
Gibbs Free Energy = -1108.678107

C,0,0.0372411325,-3.6617884922,-0.7602981015
C,0,0.056121958,-4.568010244,-1.9048525287
O,0,-0.0745385422,-5.5490493129,-0.9210316494
O,0,0.1931090355,-1.8762916058,-1.3725166291
C,0,0.1453363783,-1.0257508992,-0.4333386535
O,0,0.0255676578,-1.1997640817,0.7739169943
O,0,0.2679814378,0.2726327683,-0.9452094919
C,0,0.1571547343,1.3291752877,-0.0656791476
C,0,1.2398178286,2.1951793043,0.0577947081
C,0,1.1387293525,3.3234594189,0.8722814442
C,0,-0.0507262731,3.5563507361,1.5538438156
C,0,-1.1404558274,2.6957742736,1.4372234739
C,0,-1.0337882229,1.575457521,0.6175439051
Cl,0,-0.1856999377,4.9709033669,2.582180128
H,0,-0.9168105183,-3.488028545,-0.2762990308
H,0,0.9321887643,-3.6080624157,-0.1511080542
H,0,0.9996291612,-4.5871959706,-2.4753976451
H,0,-0.7968186592,-4.4699946897,-2.5969675217
H,0,2.1573215617,1.9867108799,-0.4891493931
H,0,1.9758333307,4.0103659954,0.9753933099
H,0,-2.0620410072,2.9020080299,1.9771328127
H,0,-1.871641345,0.8903256747,0.5078582547

TS-OEt 4-fluorophenyl carbonate

E (total electronic) = -748.4206429
E (total electronic) + ZPVE = -748.263529
Internal Thermal Energy = -748.250737
Enthalpy = -748.249793
Gibbs Free Energy = -748.306499

C,0,-3.518535193,-0.2561740771,-0.3983283159
C,0,-4.7557139334,0.1508352054,0.2611523526
O,0,-5.3494784669,-0.5029209906,-0.8197191945
H,0,-3.2314796204,-1.2984931128,-0.3233418797
H,0,-3.2233573131,0.2889226335,-1.2873036787
H,0,-4.9266421682,1.2389643989,0.3128388336
H,0,-4.9346408691,-0.3031014119,1.2500259876
O,0,-2.0367059413,0.3512829488,0.6161772662
C,0,-0.9221155509,0.0419337132,0.0953508007
O,0,-0.6888190914,-0.5811308688,-0.9352908685
O,0,0.1351455496,0.525202142,0.8723013604
C,0,1.4173759739,0.2461250068,0.4330201348
C,0,2.1423775364,1.2459569463,-0.208990646
C,0,3.4612027318,1.0063027158,-0.5964537532
C,0,4.0097197655,-0.2383298586,-0.3275677227
C,0,3.3047077506,-1.2487428714,0.3114997114
C,0,1.9894752666,-0.996642786,0.6972150061
F,0,5.2911967882,-0.4782820256,-0.7013083111
H,0,1.6732308097,2.2093113914,-0.3996400308
H,0,4.0554129023,1.7677583136,-1.0972241945
H,0,3.7809020136,-2.2081497895,0.5026208629
H,0,1.4027300595,-1.7615776235,1.2024392792

M06-2X/AUG-cc-pVTZ IEFPCM, Solvent = Water

Substrates

OEt methyl carbonate

E (total electronic) = -457.6520897
E (total electronic) + ZPVE = -457.536080
Internal Thermal Energy = -457.527345
Enthalpy = -457.526401
Gibbs Free Energy = -457.570691

O,0,2.1767213722,-0.1118247932,0.668589274
C,0,0.9455685498,0.3591733,0.6637906241

O,0,-0.0691739251,-0.2945089559,0.6613667231
O,0,0.9926871976,1.6898141902,0.6619883381
C,0,-0.2785161332,2.3460650395,0.6567806419
C,0,2.3170131159,-1.5533884932,0.6711759825
C,0,3.8016061558,-1.9056683989,0.67663605
O,0,3.9869933333,-3.2544583058,0.6792357869
H,0,-0.0603912203,3.4080126288,0.6559442954
H,0,-0.8453437986,2.0752731616,1.5443319286
H,0,-0.8394114782,2.0726543519,-0.2337316225
H,0,1.8274163696,-1.952722736,-0.2174104059
H,0,1.8215070885,-1.9501126956,1.5576534759
H,0,4.2384245728,-1.3846512304,1.557246997
H,0,4.2442827997,-1.3872380633,-0.2025750893

OEt ethyl carbonate

E (total electronic) = -496.964022
E (total electronic) + ZPVE = -496.819716
Internal Thermal Energy = -496.809678
Enthalpy = -496.808734
Gibbs Free Energy = -496.856299

O,0,0.1621765879,-0.495441728,-0.0000038747
C,0,-1.0028431182,0.1238813774,-0.000001091
O,0,-1.1720056665,1.319469995,0.0000039634
O,0,-1.9754493927,-0.7837454466,-0.0000040792
C,0,-3.3170446047,-0.2608711967,-0.0000013443
C,0,1.3397338575,0.3470222053,-0.0000017995
C,0,2.5843858877,-0.5355137316,-0.0000145839
O,0,3.7177774526,0.2193008797,-0.000015048
H,0,-3.4459186561,0.3627806913,-0.8834006381
H,0,-3.445920352,0.3627671781,0.8834071407
H,0,1.3157520893,0.9805790481,0.8871906253
H,0,1.3157448358,0.9805934535,-0.8871837353
H,0,2.4857886127,-1.2090030432,-0.8798946771
H,0,2.4857979277,-1.2090157814,0.8798569791
C,0,-4.2593597407,-1.4375994377,-0.0000113598
H,0,-4.1078588062,-2.0525712255,0.8855361684
H,0,-5.2870268576,-1.0782525849,-0.000009507
H,0,-4.1078571366,-2.0525572229,-0.8855684191

OEt isopropyl carbonate

E (total electronic) = -536.2765565
E (total electronic) + ZPVE = -536.104211
Internal Thermal Energy = -536.092924
Enthalpy = -536.091980
Gibbs Free Energy = -536.142207

O,0,0.3498342006,-0.9061604115,0.0586017716
C,0,0.3547872896,0.3801982209,0.3581270917
O,0,0.4559306551,0.845308582,1.4681158282
O,0,0.2232012657,1.0819884419,-0.7638305777
C,0,0.2438763581,2.5266876214,-0.6408006755
C,0,0.484437768,-1.8256611562,1.1682685004
C,0,0.4658323098,-3.2561300886,0.6376829915
O,0,0.5987428834,-4.1550570497,1.6522529363
C,0,-0.4365726216,3.0579137002,-1.8820631063
C,0,1.675545917,3.0030306854,-0.505336757
H,0,-0.3269193243,2.786315519,0.249392696
H,0,-0.3408433247,-1.660631887,1.8616840737
H,0,1.4235021933,-1.6172790675,1.6817415982
H,0,1.2700619746,-3.3123246407,-0.1288300049
H,0,-0.4789603538,-3.3594780761,0.0595754166
H,0,-1.4551454297,2.6816348011,-1.9576331357
H,0,-0.4682102425,4.1456504783,-1.8423137291
H,0,0.1172846242,2.7602381517,-2.7725816824
H,0,2.1469564771,2.5730042828,0.3760848324
H,0,2.2467684285,2.7221961716,-1.3906313658
H,0,1.6927029518,4.0883257211,-0.4124217023

OEt tert-butyl carbonate

E (total electronic) = -575.5854468

E (total electronic) + ZPVE = -575.385690
Internal Thermal Energy = -575.373002
Enthalpy = -575.372058
Gibbs Free Energy = -575.425774

O,0,0.1729786787,-0.4200560702,-0.0226632573
C,0,-0.9627621627,0.2610396116,-0.0190626644
O,0,-1.0502748281,1.4652682784,-0.0177409921
O,0,-1.967134549,-0.607509751,-0.016695493
C,0,-3.3579633764,-0.149876252,-0.001020979
C,0,1.3909591544,0.3591698786,-0.0199401674
C,0,2.5874212472,-0.5868903908,0.0215000991
O,0,3.7599788988,0.1054638202,0.0336104419
H,0,1.3880043945,1.0128072997,0.8527724105
H,0,1.4161589875,0.9744743209,-0.9201688458
H,0,2.4717405503,-1.2705342299,-0.8485922099
H,0,2.4344539319,-1.2380566551,0.9105008806
C,0,-3.6352163345,0.6364800599,1.2710458763
H,0,-3.1022085694,1.5830715993,1.2776511247
H,0,-4.7046889842,0.8358519653,1.3345826926
H,0,-3.343533971,0.0518819296,2.1437158489
C,0,-3.6607330815,0.6521153331,-1.2574013929
H,0,-3.3843071358,0.0795237428,-2.1428850698
H,0,-4.7317418642,0.8493478015,-1.2980651107
H,0,-3.1302275024,1.6000552231,-1.2619482635
C,0,-4.1392302574,-1.4534765197,-0.0012645495
H,0,-3.8900750267,-2.0456628272,0.8785421243
H,0,-5.206731571,-1.2389045147,0.011823009
H,0,-3.9093366291,-2.0337836535,-0.8941355127

OEt phenyl carbonate

E (total electronic) = -649.3817102
E (total electronic) + ZPVE = -649.213241
Internal Thermal Energy = -649.201536
Enthalpy = -649.200592
Gibbs Free Energy = -649.253827

C,0,0.0946455998,-2.6491361466,-1.3828132754
C,0,0.0409114301,-3.216866553,-2.7978100175
O,0,0.0987021595,-4.5764598169,-2.7797834634
O,0,0.0153810232,-1.2020997405,-1.4567929999
C,0,0.0412624432,-0.5545003031,-0.3152992764
O,0,0.1262152777,-1.0299372946,0.7856713121
O,0,-0.0378487643,0.7643829497,-0.5834408823
C,0,-0.068462839,1.6411123504,0.4985662186
C,0,1.0250456697,2.461778614,0.7010118398
C,0,0.9832590583,3.3926400912,1.7313490937
C,0,-0.1399334416,3.4881912846,2.5414406115
C,0,-1.2287086639,2.65285133,2.3203658558
C,0,-1.199829816,1.7228281309,1.2914428267
H,0,-0.7432632276,-3.0122944042,-0.7873543226
H,0,1.027765769,-2.9208515972,-0.888830059
H,0,0.8717202401,-2.732025707,-3.3563862555
H,0,-0.8837027055,-2.8053351365,-3.2593418583
H,0,1.8875794961,2.3697390504,0.0559484738
H,0,1.8312195633,4.0421313558,1.8981868653
H,0,-0.1693570488,4.213470359,3.3423909318
H,0,-2.1059902783,2.7267271018,2.9478022712
H,0,-2.0380989451,1.0669918344,1.10102011

OEt 4-nitrophenyl carbonate

E (total electronic) = -853.8986846
E (total electronic) + ZPVE = -853.727420
Internal Thermal Energy = -853.713237
Enthalpy = -853.712293
Gibbs Free Energy = -853.771710

C,0,-0.0582834455,-3.4284378368,0.999443512
C,0,-0.1114827224,-4.781114047,0.2968296414
O,0,-0.175355192,-5.7927674276,1.2041460237

O,0,0.0182137385,-2.3795056829,-0.0043795342
C,0,0.0642675871,-1.1503885209,0.4420063041
O,0,0.0415638252,-0.7842679425,1.5847302376
O,0,0.1620881316,-0.3263671756,-0.6309741808
C,0,0.1439957325,1.0372043078,-0.4262811558
C,0,1.1692104058,1.7684613427,-1.0049290376
C,0,1.1615689463,3.1472935243,-0.8971524982
C,0,0.1229415182,3.7490665766,-0.2083354117
C,0,-0.9080011048,3.0259952076,0.3695333264
C,0,-0.8984472042,1.6487434169,0.2564727709
N,0,0.1106990748,5.2109922726,-0.0889862724
O,0,1.0179886803,5.8323273833,-0.6018981647
O,0,-0.8060059391,5.7259660483,0.5166027387
H,0,-0.9530059212,-3.2654260112,1.5999698844
H,0,0.8211608512,-3.3564664323,1.6393348311
H,0,0.7792623603,-4.8188664586,-0.3682028417
H,0,-0.9784102275,-4.7345602388,-0.3983861188
H,0,1.9577641665,1.253302626,-1.5331599927
H,0,1.9441037909,3.7466721538,-1.3349028405
H,0,-1.7022147025,3.5363181366,0.8912209264
H,0,-1.6885133503,1.0539617778,0.6887828525

OEt 4-cyanophenyl carbonate

E (total electronic) = -741.6344004
E (total electronic) + ZPVE = -741.467214
Internal Thermal Energy = -741.453730
Enthalpy = -741.452786
Gibbs Free Energy = -741.509956

C,0,0.1113664107,-3.6739834667,-0.8625624813
C,0,0.1678409567,-4.5275353613,-2.1254447192
O,0,0.0834424854,-5.8505185081,-1.8179474532
O,0,0.1918310748,-2.272107655,-1.2378312563
C,0,0.1261405483,-1.4042277081,-0.2597432536
O,0,0.009303173,-1.6319087106,0.9131804088
O,0,0.2289993777,-0.1657415816,-0.7996795531
C,0,0.102761494,0.931447373,0.0301110688
C,0,1.1160262301,1.8740268278,-0.0179526939
C,0,1.0017693071,3.0278658894,0.7363182082
C,0,-0.1265124563,3.219773046,1.5310482751
C,0,-1.142087451,2.2639342701,1.5675892924
C,0,-1.0293412597,1.1134793308,0.8104882463
C,0,-0.2475665175,4.4132884837,2.3166599695
N,0,-0.3449040115,5.3688975219,2.9458680232
H,0,-0.8246702908,-3.8335481404,-0.3277519339
H,0,0.9461838925,-3.9010883385,-0.1993794154
H,0,1.1042012664,-4.2397023783,-2.652182103
H,0,-0.6489661634,-4.1581708979,-2.7837829294
H,0,1.9781643325,1.6975352303,-0.6443146278
H,0,1.7813792296,3.7750417522,0.7120665979
H,0,-2.0150009905,2.4268508608,2.1826958019
H,0,-1.8076186377,0.3652861605,0.821655528

OEt 4-methoxyphenyl carbonate

E (total electronic) = -763.9086778
E (total electronic) + ZPVE = -763.707103
Internal Thermal Energy = -763.692972
Enthalpy = -763.692028
Gibbs Free Energy = -763.750402

C,0,-0.2548416078,-3.9593345177,-0.9144599476
C,0,-0.2836857295,-4.8794842697,-2.1307906931
O,0,-0.3332281363,-6.1857303372,-1.7506315478
O,0,-0.201603616,-2.5815936025,-1.3663218792
C,0,-0.1555419676,-1.6616993814,-0.4299409028
O,0,-0.1534921227,-1.8405195859,0.7593138538
O,0,-0.1064136288,-0.4562907591,-1.0292869282
C,0,-0.0765683753,0.6643966463,-0.1989456722
C,0,-1.2390756423,1.0986063198,0.420010521
C,0,-1.2071862286,2.2438188649,1.1899250487
C,0,-0.0171026132,2.9596030185,1.3392315264
C,0,1.1415057866,2.5167085241,0.7104633086

C,0,1.1045267019,1.3586640057,-0.0613490379
O,0,-0.0865765602,4.0725927516,2.111542128
C,0,1.1013630042,4.8255072555,2.2865999997
H,0,-1.1508980006,-4.0898957106,-0.3073307684
H,0,0.6236477687,-4.1568987526,-0.300037187
H,0,0.6092775675,-4.6150317939,-2.7390198887
H,0,-1.1493464363,-4.5504441515,-2.7470309768
H,0,-2.1558947429,0.5387299134,0.2962039167
H,0,-2.0979242753,2.6051366483,1.6845124551
H,0,2.0720157396,3.053805515,0.8086065613
H,0,1.9961932245,1.001297832,-0.5574354773
H,0,0.8390272458,5.6613929421,2.9267855395
H,0,1.4710495609,5.1993892875,1.3303905095
H,0,1.8763010837,4.2262083379,2.7673365383

OEt 4-chlorophenyl carbonate

E (total electronic) = -1108.9918417
E (total electronic) + ZPVE = -1108.832997
Internal Thermal Energy = -1108.820128
Enthalpy = -1108.819183
Gibbs Free Energy = -1108.875396

C,0,3.7316596052,-0.2929691667,0.3207992667
C,0,5.0135211137,0.2768729769,-0.278166758
O,0,6.1094451462,-0.3009156244,0.2842881077
O,0,2.5922249175,0.3450627965,-0.3141310547
C,0,1.4066923593,-0.0362453554,0.0966641323
O,0,1.1580118498,-0.8538060224,0.9413958714
O,0,0.4823037024,0.6630334822,-0.597012777
C,0,-0.8565801712,0.3881998156,-0.3510732162
C,0,-1.6398220346,1.4053626895,0.161020809
C,0,-2.9975168999,1.1896980547,0.3497417138
C,0,-3.5348043812,-0.0438387892,0.0236630456
C,0,-2.7487746349,-1.064070585,-0.4902061139
C,0,-1.3945233251,-0.8435554685,-0.6825760009
H,0,3.6663540587,-1.3672149269,0.1478926999
H,0,3.6836359157,-0.0998367853,1.3925120466
H,0,4.9559315691,1.3789644347,-0.1390895445
H,0,4.9326575025,0.1289391682,-1.377644958
H,0,-1.1895353816,2.3570720858,0.4043609874
H,0,-3.628492068,1.9716035193,0.7460559715
H,0,-3.1911796877,-2.0170389368,-0.7407047924
H,0,-0.7609001529,-1.6206200101,-1.0857296028
Cl,0,-5.2384776527,-0.3207209224,0.2600917665

OEt 4-fluorophenyl carbonate

E (total electronic) = -748.6331811
E (total electronic) + ZPVE = -748.472909
Internal Thermal Energy = -748.460428
Enthalpy = -748.459483
Gibbs Free Energy = -748.514640

C,0,3.7153962974,-0.2000638119,0.3876675812
C,0,5.0094300493,0.2473923441,-0.2845392867
O,0,6.0940233967,-0.2046361936,0.4026784708
O,0,2.5884147167,0.3039751773,-0.376407216
C,0,1.3952866528,-0.0023134248,0.0747392045
O,0,1.1326516465,-0.6563580624,1.0485992822
O,0,0.480709635,0.5503500941,-0.749387742
C,0,-0.8585502279,0.3244714444,-0.4421638661
C,0,-1.5641851939,1.3120561196,0.2196313739
C,0,-2.9146970721,1.1245915969,0.4778375516
C,0,-3.5065065045,-0.0513201474,0.0628107407
C,0,-2.8114725422,-1.04464522,-0.5991765242
C,0,-1.4629038226,-0.8492001441,-0.8557861992
H,0,3.651206367,-1.2876579061,0.4214959653
H,0,3.6484241563,0.1932989569,1.4021124319
H,0,4.9492223323,1.3551213018,-0.3649286478
H,0,4.9523237645,-0.1131322175,-1.3352853919
H,0,-1.0603376806,2.2177250572,0.5259044411
H,0,-3.501236556,1.873092653,0.99031953
H,0,-3.3202116463,-1.9468123432,-0.9061287426

H,0,-0.88210519,-1.5997644027,-1.3731116649
F,0,-4.8172341682,-0.2373036618,0.3110551979

Transition states

TS-OEt methyl carbonate

E (total electronic) = -457.6168867
E (total electronic) + ZPVE = -457.503395
Internal Thermal Energy = -457.494454
Enthalpy = -457.493510
Gibbs Free Energy = -457.539528

O,0,0.0147802155,-0.7216886699,-0.0000019142
C,0,-1.0134514832,0.0228336324,0.0000007145
O,0,-1.0600463112,1.2502988838,0.0000078721
O,0,-2.1709989715,-0.7062275645,-0.0000056849
C,0,-3.3787586429,0.0439733293,-0.0000031926
C,0,1.6532888667,0.2559855474,0.0000015758
C,0,2.7689995886,-0.6745488217,-0.0000063965
O,0,3.5154835586,0.5005715447,-0.0000040004
H,0,-4.1855614785,-0.6831667846,-0.0000099472
H,0,-3.4457457096,0.6726453046,-0.8863572715
H,0,-3.4457496586,0.6726331134,0.8863592506
H,0,1.4251769595,0.7627968743,0.9211349775
H,0,1.4251735785,0.7628085705,-0.921124551
H,0,2.8649519049,-1.2976941132,-0.8958288746
H,0,2.8649553331,-1.2977054665,0.8958078198

TS-OEt ethyl carbonate

E (total electronic) = -496.9284102
E (total electronic) + ZPVE = -496.786552
Internal Thermal Energy = -496.776326
Enthalpy = -496.775382
Gibbs Free Energy = -496.824340

O,0,0.4970726996,-0.6347144121,0.030107108
C,0,-0.472985186,0.1848186506,0.0187069047
O,0,-0.4249186526,1.412760475,0.0135152612
O,0,-1.6810330992,-0.4551169724,0.0110840452
C,0,-2.8418482451,0.3771788054,-0.0014478079
C,0,2.2078448163,0.2114078121,-0.0090521554
C,0,3.2469115853,-0.8035833001,0.0130829121
O,0,4.0817211918,0.3096431719,-0.0345561861
C,0,-4.0526381138,-0.5254211262,-0.0266894098
H,0,-2.8116730981,1.0249044912,-0.8777154489
H,0,-2.838990167,1.0129974391,0.8842241586
H,0,2.028953159,0.7638272254,0.8965054246
H,0,2.0102576456,0.7035437501,-0.9449957079
H,0,3.2830696711,-1.4627298936,-0.8611189962
H,0,3.3047015261,-1.4013716355,0.9292383742
H,0,-4.9610867959,0.0753455323,-0.0357439573
H,0,-4.0459427889,-1.1537257213,-0.9164982696
H,0,-4.0730323082,-1.1682566518,0.8524412705

TS-OEt isopropyl carbonate

E (total electronic) = -536.2404701
E (total electronic) + ZPVE = -536.070674
Internal Thermal Energy = -536.059213
Enthalpy = -536.058269
Gibbs Free Energy = -536.109558

O,0,0.4545032058,-1.1045730492,-0.583771697
C,0,0.5066932337,0.1428977347,-0.3488780802
O,0,1.0758875905,0.709216533,0.581349843
O,0,-0.1842703424,0.8627132965,-1.2848416329
C,0,-0.1548564291,2.2949705143,-1.1816494892
C,0,1.4016078749,-2.1636952054,0.6949360878

C,0,1.2683187951,-3.5665960576,0.3433240129
O,0,2.0546364363,-3.7367092064,1.4797687443
C,0,1.1442888087,2.829400279,-1.7552665029
C,0,-1.3662867193,2.8016200864,-1.9364242896
H,0,-0.2296388292,2.5604209874,-0.1278228158
H,0,0.8211744611,-1.7980026578,1.5235088413
H,0,2.3421276911,-1.6833644947,0.4896881184
H,0,1.7318954115,-3.8635881814,-0.6036445549
H,0,0.2536426335,-3.9750230936,0.4023816958
H,0,1.1728841933,3.9158348181,-1.6718036276
H,0,1.9975105023,2.4168784968,-1.2202436767
H,0,1.2220809444,2.5622897386,-2.8102668052
H,0,-1.3073009525,2.5080696463,-2.9852215453
H,0,-2.2840015755,2.3973521052,-1.5118319464
H,0,-1.4080959344,3.8890457099,-1.8852736798

TS-OEt tert-butyl carbonate

E (total electronic) = -575.5482257
E (total electronic) + ZPVE = -575.350986
Internal Thermal Energy = -575.338104
Enthalpy = -575.337160
Gibbs Free Energy = -575.391804

O,0,0.9396362605,0.6297140462,-0.0020171083
C,0,-0.0743303128,-0.1388388166,-0.0007939535
O,0,-0.075197674,-1.3672956713,0.0005148544
O,0,-1.2365791068,0.5803348783,-0.0010958609
C,0,-2.535790109,-0.0609561747,0.000104526
C,0,-3.5006249216,1.1172155067,-0.0007639415
C,0,-2.732924951,-0.8888193658,1.2635866379
C,0,-2.7339317248,-0.8915052963,-1.2614558745
H,0,-3.3464584649,1.7321752705,-0.8872854823
H,0,-3.345752281,1.7340595095,0.8843243038
H,0,-4.5287248902,0.756701314,0.0000293272
H,0,-2.0778629204,-1.754790495,1.2714763066
H,0,-2.5303207685,-0.2776321932,2.1439636903
H,0,-3.7685280788,-1.2265051129,1.3135690525
H,0,-3.7695730117,-1.2292993895,-1.309891803
H,0,-2.532034261,-0.2821915531,-2.1432926947
H,0,-2.0788723962,-1.7574895333,-1.2680273711
C,0,2.6082160066,-0.3109331843,-0.0016649851
C,0,3.696736989,0.6500921978,-0.0030907583
O,0,4.4681090069,-0.5096961211,-0.002166162
H,0,2.3884945887,-0.8216375969,-0.9223873306
H,0,2.3891979515,-0.8197007031,0.9202963717
H,0,3.7792074315,1.2754575328,0.8923014942
H,0,3.7785236379,1.2735739514,-0.8998582389

TS-OEt phenyl carbonate

E (total electronic) = -649.3494658
E (total electronic) + ZPVE = -649.183569
Internal Thermal Energy = -649.171622
Enthalpy = -649.170677
Gibbs Free Energy = -649.225586

C,0,-3.3356180298,0.1988081332,0.278234935
C,0,-4.5284228497,-0.2934430988,-0.3927226893
O,0,-5.1865579005,0.501572673,0.5391048538
O,0,-1.7980887194,-0.5433824921,-0.5405775758
C,0,-0.7140060089,-0.1327875424,-0.0370240258
O,0,-0.5360704709,0.6384856222,0.8927990045
O,0,0.377571107,-0.699993848,-0.6885884716
C,0,1.6436714863,-0.2965654724,-0.316989616
C,0,2.4898709892,-1.2293924064,0.2596066985
C,0,3.7947704176,-0.8670034274,0.5713735428
C,0,4.2440554713,0.4203035354,0.3118755326
C,0,3.3839820063,1.3474161868,-0.2666133851
C,0,2.0820222417,0.9921195002,-0.5857284192
H,0,-3.0404140651,1.2151478961,0.0822273335
H,0,-3.1082912805,-0.2088688015,1.2480526082

H,0,-4.7037373342,-1.3716943051,-0.305812684
H,0,-4.6367505598,0.0124040294,-1.4394763182
H,0,2.1218301002,-2.22756778,0.4535333795
H,0,4.4585650896,-1.5942094594,1.018639577
H,0,3.7292904914,2.3512187988,-0.473452248
H,0,1.4020356585,1.7012419821,-1.0373389954
H,0,5.2591679198,0.7007452531,0.5560169228

TS-OEt 4-nitrophenyl carbonate

E (total electronic) = -853.868863
E (total electronic) + ZPVE = -853.700130
Internal Thermal Energy = -853.685748
Enthalpy = -853.684804
Gibbs Free Energy = -853.745361

C,0,4.4645098775,-0.3444561111,0.2663613044
C,0,5.6955954284,0.2077488665,-0.2795829613
O,0,6.3081479995,-0.7710204013,0.4935424226
O,0,2.9864946122,0.6010921893,-0.4167988166
C,0,1.8804940946,0.165323326,0.0015785641
O,0,1.6357178208,-0.7576771898,0.7567773966
O,0,0.8286229066,0.9396571876,-0.5149444663
C,0,-0.4625425129,0.5545796113,-0.3066659876
C,0,-0.9015520239,-0.7369007424,-0.5883997053
C,0,-2.2370976103,-1.0498701275,-0.4313210336
C,0,-3.1106622721,-0.063237941,0.0008483997
C,0,-2.6910666425,1.2273917993,0.276452701
C,0,-1.3524063803,1.5338183055,0.1211011507
N,0,-4.5248924643,-0.3962286858,0.167246211
O,0,-4.8773936723,-1.534590451,-0.0684582175
O,0,-5.281122536,0.4810649198,0.5335620864
H,0,4.1372377452,-1.2953084801,-0.1181528547
H,0,4.2358554926,-0.1188658238,1.2940119219
H,0,5.9087661136,1.2437014881,0.0084066044
H,0,5.8128354348,0.0994524805,-1.3640870267
H,0,-0.1988992339,-1.4819025241,-0.9276828436
H,0,-2.6047558702,-2.0413879717,-0.6447386315
H,0,-3.399759131,1.9698863801,0.6081997934
H,0,-0.9824637763,2.5278200959,0.3259785887

TS-OEt 4-cyanophenyl carbonate

E (total electronic) = -741.6041272
E (total electronic) + ZPVE = -741.439492
Internal Thermal Energy = -741.425782
Enthalpy = -741.424838
Gibbs Free Energy = -741.483751

C,0,-4.0337095589,-0.342333534,-0.2479503509
C,0,-5.2594376281,0.2394170684,0.2785999993
O,0,-5.8775284246,-0.7701886547,-0.4496038373
O,0,-2.5458670565,0.6245095313,0.3884598692
C,0,-1.4431795299,0.1562416392,-0.0051092078
O,0,-1.2106112265,-0.8037763153,-0.71804799
O,0,-0.3833161433,0.9338883104,0.4823472648
C,0,0.9033986323,0.5214898056,0.2756638651
C,0,1.7927479339,1.4489408313,-0.2512318561
C,0,3.1243353726,1.1113830461,-0.4094315291
C,0,3.5599860774,-0.1600524789,-0.0406631572
C,0,2.6629435594,-1.0875415461,0.4922890009
C,0,1.3345449002,-0.7463465054,0.6529654566
C,0,4.937631569,-0.5169406031,-0.2054289472
N,0,6.042277089,-0.803561094,-0.3374297052
H,0,-3.7084244672,-1.2765605866,0.1765714428
H,0,-3.8070914183,-0.1613404155,-1.2847326907
H,0,-5.4700006933,1.2624177393,-0.0538881467
H,0,-5.3734868401,0.1786234411,1.3670647229
H,0,1.4300462694,2.4278553429,-0.5298236728
H,0,3.8240928276,1.8255976599,-0.8188324443
H,0,3.0116686293,-2.0683899592,0.7820233693
H,0,0.6302900665,-1.4519120724,1.0668064844

TS-OEt 4-methoxyphenyl carbonate

E (total electronic) = -763.8760138

E (total electronic) + ZPVE = -763.677059

Internal Thermal Energy = -763.662670

Enthalpy = -763.661726

Gibbs Free Energy = -763.721728

C,0,-4.1623505591,0.0942239714,0.4684046072
C,0,-5.4171243702,-0.1763793105,-0.2146287187
O,0,-5.9748768351,0.279121295,0.9753143911
O,0,-2.7129913077,-0.3398536185,-0.6740185277
C,0,-1.5820314409,-0.0918396581,-0.1658268418
O,0,-1.3144489057,0.3731130704,0.9321631597
O,0,-0.5593429982,-0.4301982858,-1.0443217595
C,0,0.74062131,-0.1782605725,-0.6443475128
C,0,1.2575465266,1.1095774072,-0.7132094095
C,0,2.5758728541,1.3394501311,-0.3732112352
C,0,3.392307585,0.283040523,0.0353859414
C,0,2.87343397,-1.0047344247,0.1002861217
C,0,1.5411032747,-1.2266838036,-0.2406203006
O,0,4.6758305564,0.6068548985,0.3454114938
C,0,5.5316750306,-0.4413259647,0.7630733287
H,0,-3.8658755164,1.1233270553,0.5741094516
H,0,-3.8568517213,-0.5949395258,1.236561316
H,0,-5.6034975941,-1.2292423515,-0.454362616
H,0,-5.6126831615,0.4415077562,-1.0982213575
H,0,0.6194600225,1.9226934323,-1.0319352829
H,0,2.9967837617,2.3343986752,-0.4198477924
H,0,3.4837943097,-1.8388672301,0.410519063
H,0,1.1254233143,-2.2240794142,-0.1947886291
H,0,6.4966228627,0.0141673276,0.9609457679
H,0,5.6376207334,-1.1953867827,-0.018891823
H,0,5.1573192984,-0.9131476005,1.6732751645

TS-OEt 4-chlorophenyl carbonate

E (total electronic) = -1108.9603665

E (total electronic) + ZPVE = -1108.804097

Internal Thermal Energy = -1108.791001

Enthalpy = -1108.790057

Gibbs Free Energy = -1108.847451

C,0,0.0468024829,-3.6573217213,-0.7593207441
C,0,0.0652154817,-4.5595896302,-1.9000422963
O,0,-0.040804925,-5.5447585734,-0.9247192062
O,0,0.1720231874,-1.8705014852,-1.3646205446
C,0,0.1326451881,-1.0205024059,-0.4316146125
O,0,0.0332819364,-1.1919717773,0.7724254821
O,0,0.2360857461,0.2738576656,-0.9429763758
C,0,0.1387726341,1.3321366467,-0.0688923713
C,0,1.2272426691,2.1786263087,0.0618024604
C,0,1.1385190325,3.2992131581,0.8762966405
C,0,-0.0431882444,3.5478816676,1.5521649913
C,0,-1.1375868889,2.7054494989,1.4272887616
C,0,-1.0444843963,1.5923206095,0.6080421756
Cl,0,-0.1606598871,4.9522445795,2.5802835272
H,0,-0.896642369,-3.5036436889,-0.2644441719
H,0,0.939426622,-3.5978008431,-0.16057402
H,0,0.9955220288,-4.5623298818,-2.4793797182
H,0,-0.7893499987,-4.470352259,-2.5803914995
H,0,2.1380245786,1.9594070396,-0.4775538991
H,0,1.9789254727,3.9692572847,0.9846223094
H,0,-2.05169032,2.9205749057,1.9614499638
H,0,-1.884568031,0.9222099013,0.4934741473

TS-OEt 4-fluorophenyl carbonate

E (total electronic) = -748.6013095

E (total electronic) + ZPVE = -748.443563

Internal Thermal Energy = -748.430880

Enthalpy = -748.429936

Gibbs Free Energy = -748.486059

C,0,-3.516735538,-0.260055552,-0.3940059305
C,0,-4.7473204832,0.1523426527,0.2624000888
O,0,-5.3499685211,-0.5024152174,-0.8062576944
H,0,-3.2380880701,-1.2968700036,-0.318602987
H,0,-3.2280502218,0.2707938798,-1.284660429
H,0,-4.9120782982,1.2346803391,0.3106704774
H,0,-4.9220315669,-0.2892861976,1.2500281364
O,0,-2.0294531633,0.3461645584,0.6069512598
C,0,-0.9192059565,0.0384287631,0.0887122811
O,0,-0.6878543251,-0.5861982174,-0.9348880507
O,0,0.1365601008,0.5249766812,0.8563601101
C,0,1.4187342142,0.2479697392,0.426865347
C,0,2.1453653064,1.2429872794,-0.2059830288
C,0,3.4589541862,1.0035115164,-0.5865869266
C,0,4.0040692204,-0.2358749531,-0.321643354
C,0,3.2963074006,-1.2410663445,0.3080643324
C,0,1.9863927782,-0.9900432728,0.6872140275
F,0,5.2803355428,-0.4755546945,-0.6891935106
H,0,1.6810315726,2.2005753068,-0.3954795119
H,0,4.0522008687,1.7600941681,-1.0796382236
H,0,3.7671026697,-2.1952662805,0.4962003813
H,0,1.3997212838,-1.7508441509,1.1829462051

M06-2X/6-31+G(d)

IEFPCM, Solvent = Water

Substrates

OEt methyl carbonate

E (total electronic) = -457.4721497

E (total electronic) + ZPVE = -457.355430

Internal Thermal Energy = -457.346670

Enthalpy = -457.345726

Gibbs Free Energy = -457.390277

O,0,2.1769833121,-0.1144108888,0.6685899624
C,0,0.9418778825,0.3583544371,0.6637776765
O,0,-0.0781504507,-0.2991211581,0.6613445341
O,0,0.9904473133,1.6921260642,0.6619751808
C,0,-0.2817046831,2.351064417,0.656763702
C,0,2.3170250256,-1.5571794121,0.6711796096
C,0,3.8070312746,-1.9063391085,0.6766563006
O,0,3.9951461278,-3.2580045592,0.679271913
H,0,-0.0561261035,3.4154694054,0.65594816
H,0,-0.8497038392,2.0808831188,1.5487142468
H,0,-0.843746874,2.0782515913,-0.2381544475
H,0,1.8255197209,-1.9573892434,-0.2213591277
H,0,1.8195810512,-1.954765322,1.5615984718
H,0,4.244654258,-1.3849577795,1.562407403
H,0,4.2505499843,-1.3875625625,-0.207690586

OEt ethyl carbonate

E (total electronic) = -496.7701776

E (total electronic) + ZPVE = -496.625003

Internal Thermal Energy = -496.614955

Enthalpy = -496.614011

Gibbs Free Energy = -496.661723

O,0,0.1646901745,-0.493292766,-0.0000068753
C,0,-1.003737324,0.128829222,-0.0000012098
O,0,-1.1725986846,1.3310171478,0.0000072716

O,0,-1.978576109,-0.7812037031,-0.0000065473
C,0,-3.3220606684,-0.2578440294,-0.0000019879
C,0,1.3434370134,0.3496461707,-0.0000030224
C,0,2.5888773357,-0.5396940059,-0.0000139732
O,0,3.7266744498,0.2142706987,-0.0000120277
H,0,-3.4515336182,0.3668915976,-0.887856889
H,0,-3.4515329811,0.3668778306,0.8878626953
H,0,1.3191071596,0.9851941616,0.8911987532
H,0,1.3191024068,0.9852090898,-0.8911939818
H,0,2.490180708,-1.2139716936,-0.8850556447
H,0,2.4901867201,-1.2139852637,0.8850180267
C,0,-4.262448369,-1.4419604222,-0.0000108207
H,0,-4.1088271728,-2.0592496194,0.8893057198
H,0,-5.2962406931,-1.08567492,-0.0000079548
H,0,-4.1088274278,-2.0592360656,-0.889336812

OEt isopropyl carbonate

E (total electronic) = -536.0689847
E (total electronic) + ZPVE = -535.895539
Internal Thermal Energy = -535.884265
Enthalpy = -535.883321
Gibbs Free Energy = -535.933575

O,0,0.3510357812,-0.9091885713,0.0599274275
C,0,0.3556299567,0.381187546,0.3607339567
O,0,0.4556580385,0.848511959,1.4769742074
O,0,0.2255687243,1.0842023506,-0.7646566957
C,0,0.2437966073,2.5306032563,-0.6404529959
C,0,0.485922654,-1.8292178936,1.1708281038
C,0,0.4633187381,-3.2626356549,0.6354055571
O,0,0.5969867702,-4.164723944,1.6513624186
C,0,-0.4397156625,3.058361069,-1.8869324718
C,0,1.6794004796,3.0089493323,-0.5037647735
H,0,-0.3315650573,2.7897897755,0.2526751466
H,0,-0.3416331094,-1.6614364575,1.8677614946
H,0,1.430434693,-1.6212618638,1.6839067851
H,0,1.2709931187,-3.3210985987,-0.1339443716
H,0,-0.487947483,-3.3654483496,0.0590479338
H,0,-1.4610568729,2.6757236553,-1.9628467348
H,0,-0.4783006913,4.1507507217,-1.8496564781
H,0,0.116730731,2.7614690561,-2.7818385949
H,0,2.152508435,2.5828394701,0.3846833259
H,0,2.2568919106,2.7229918882,-1.3890964796
H,0,1.698156238,4.0994012537,-0.4150317611

OEt tert-butyl carbonate

E (total electronic) = -575.3644884
E (total electronic) + ZPVE = -575.163334
Internal Thermal Energy = -575.150706
Enthalpy = -575.149762
Gibbs Free Energy = -575.203018

O,0,0.1760524922,-0.4205422395,-0.031130193
C,0,-0.963619114,0.2620592298,-0.0247839161
O,0,-1.0526691102,1.4726679704,-0.0213709988
O,0,-1.9694823126,-0.6103835889,-0.0223298583
C,0,-3.3608567656,-0.1502430429,-0.0016870098
C,0,1.3943097235,0.3607918903,-0.0280680765
C,0,2.5923458778,-0.5897235962,0.0300158406
O,0,3.7678663349,0.1039278419,0.0439504523
H,0,1.3848304841,1.0245589955,0.8424204796
H,0,1.4237022699,0.9697066947,-0.9379265638
H,0,2.4839811178,-1.2825232411,-0.8396213588
H,0,2.4341263406,-1.2336202923,0.9290693191
C,0,-3.6326531744,0.6349837493,1.2774246621
H,0,-3.0994373091,1.5871466767,1.2851464792
H,0,-4.7062156559,0.8351713791,1.3504800966
H,0,-3.3338468814,0.0474962572,2.1517380057
C,0,-3.6653974193,0.6575445592,-1.2591717803
H,0,-3.387273866,0.086764145,-2.1511773667
H,0,-4.7408957712,0.8562914366,-1.3018692498
H,0,-3.1344180308,1.6108978105,-1.262772602

C,0,-4.1430425456,-1.4582439727,-0.0032856957
H,0,-3.8908162489,-2.0566097121,0.877462302
H,0,-5.2159273567,-1.2464495853,0.0134013173
H,0,-3.9151234591,-2.0398530346,-0.901708595

OEt phenyl carbonate

E (total electronic) = -649.1406123
E (total electronic) + ZPVE = -648.971488
Internal Thermal Energy = -648.959696
Enthalpy = -648.958752
Gibbs Free Energy = -649.013105

C,0,0.2162860283,-2.6304844955,-1.3972575669
C,0,0.0295436763,-3.2308502649,-2.7925753994
O,0,0.2905596419,-4.5698711929,-2.786658712
O,0,-0.0731846682,-1.2085549194,-1.4601147239
C,0,0.0413364168,-0.5363850911,-0.3330588714
O,0,0.3612025196,-0.9753830066,0.7471072164
O,0,-0.2636347256,0.7554485919,-0.5833782925
C,0,-0.1996039417,1.63700519,0.4982175212
C,0,0.9883676788,2.312589486,0.7448418382
C,0,1.0280860511,3.2404327945,1.7853976999
C,0,-0.109489833,3.4795387472,2.5576692779
C,0,-1.2930075972,2.7902198905,2.289753199
C,0,-1.3445550092,1.8600821008,1.2517676907
H,0,-0.4668873297,-3.0919674839,-0.6774066448
H,0,1.2460030827,-2.7597175502,-1.0496092134
H,0,0.6889710284,-2.6417324785,-3.4749805237
H,0,-1.0107828434,-2.9714341029,-3.1056327744
H,0,1.8596178511,2.1124651214,0.1287420978
H,0,1.9493631352,3.777213975,1.9895823777
H,0,-0.0745558865,4.2041176125,3.3652339151
H,0,-2.1803434003,2.9761918329,2.886935317
H,0,-2.2547798753,1.3144122432,1.0227685717

OEt 4-nitrophenyl carbonate

E (total electronic) = -853.5790017
E (total electronic) + ZPVE = -853.407023
Internal Thermal Energy = -853.392798
Enthalpy = -853.391854
Gibbs Free Energy = -853.451461

C,0,-0.0544206409,-3.4354129139,1.0020997583
C,0,-0.1042036797,-4.791160242,0.2949196058
O,0,-0.1632204823,-5.8062011813,1.2035830349
O,0,0.0139322418,-2.3867339237,-0.004044235
C,0,0.0576385021,-1.1524515932,0.4420116112
O,0,0.0394349451,-0.7836827584,1.5908766679
O,0,0.1449939328,-0.3291438642,-0.6356766468
C,0,0.1331987678,1.0366664701,-0.4279905779
C,0,1.168445289,1.7651921432,-1.0061376832
C,0,1.1675098883,3.1502465002,-0.8978468656
C,0,0.1244315947,3.7589377532,-0.2085694282
C,0,-0.9168813889,3.0379220407,0.3689702541
C,0,-0.9136518806,1.6545101381,0.2543712323
N,0,0.1191599252,5.2192625394,-0.0882544096
O,0,1.0344333764,5.8412818053,-0.6035749492
O,0,-0.8000639405,5.7422945857,0.5213895414
H,0,-0.9518173485,-3.2751214559,1.6073180417
H,0,0.8308023833,-3.3583244734,1.6408547644
H,0,0.7905997442,-4.8271353459,-0.37239287
H,0,-0.9776923075,-4.7483121004,-0.3996185898
H,0,1.9597745216,1.2442198538,-1.5335956829
H,0,1.9587594762,3.7467382813,-1.3352248295
H,0,-1.7142536862,3.5522903878,0.8913750596
H,0,-1.7118002335,1.0622543539,0.686642196

OEt 4-cyanophenyl carbonate

E (total electronic) = -741.3619276
E (total electronic) + ZPVE = -741.194134

Internal Thermal Energy = -741.180592
Enthalpy = -741.179648
Gibbs Free Energy = -741.237235

C,0,0.1180037527,-3.6784403163,-0.8632791878
C,0,0.1887204434,-4.5364469464,-2.1279783563
O,0,0.1580135245,-5.8629498825,-1.8129201769
O,0,0.1633088106,-2.27652665,-1.24759234
C,0,0.101509239,-1.4008656454,-0.2698070426
O,0,0.0026291491,-1.6255851902,0.9121827406
O,0,0.1822075936,-0.1625347341,-0.8195568574
C,0,0.0750626021,0.9343763208,0.0190352532
C,0,1.1218153747,1.8491489397,-0.0010609189
C,0,1.0255563891,3.005012829,0.7648022387
C,0,-0.1183136727,3.2239021588,1.541259985
C,0,-1.167258496,2.2944229973,1.5492999284
C,0,-1.0723341365,1.1424201232,0.7802329591
C,0,-0.2210157697,4.4185349558,2.3372361202
N,0,-0.3037172573,5.3798999551,2.9780146627
H,0,-0.8141859031,-3.8578898265,-0.3190220526
H,0,0.966586147,-3.8828294753,-0.2030910912
H,0,1.1119190205,-4.2172024008,-2.6693881302
H,0,-0.6548758137,-4.2019159423,-2.7788713496
H,0,1.9950649761,1.6508328444,-0.6130115784
H,0,1.8309846937,3.7315006298,0.7630331886
H,0,-2.0512145065,2.4778388924,2.1505978771
H,0,-1.8757241603,0.4141903634,0.7689931282

OEt 4-methoxyphenyl carbonate

E (total electronic) = -763.622738
E (total electronic) + ZPVE = -763.420267
Internal Thermal Energy = -763.406069
Enthalpy = -763.405125
Gibbs Free Energy = -763.463823

C,0,-0.2502513658,-3.9687829038,-0.9151651578
C,0,-0.2864651765,-4.8887874295,-2.137220065
O,0,-0.3355650764,-6.1986114234,-1.7577492143
O,0,-0.2027403746,-2.5901577408,-1.3686389416
C,0,-0.1541201442,-1.6664337554,-0.4297939053
O,0,-0.1445657909,-1.8465315361,0.7657882806
O,0,-0.1133421312,-0.4591270015,-1.0330833841
C,0,-0.0809096182,0.662484659,-0.2006909914
C,0,-1.2488113971,1.1021510854,0.4177412891
C,0,-1.2134796983,2.2535174536,1.1897493716
C,0,-0.0156140679,2.9674059955,1.3398141914
C,0,1.1479651564,2.5197349,0.7100368477
C,0,1.1082034728,1.3559435389,-0.0635224383
O,0,-0.0852939745,4.0830338091,2.1136146346
C,0,1.1039577427,4.8366407585,2.2941566547
H,0,-1.1458495993,-4.1008070041,-0.2998655284
H,0,0.6367201586,-4.1647383069,-0.3046402952
H,0,0.6084408249,-4.6257638785,-2.7514913616
H,0,-1.1604088723,-4.5588557809,-2.7494962243
H,0,-2.1716980704,0.5439642452,0.2927893303
H,0,-2.1070001682,2.6203552987,1.6849557208
H,0,2.084218003,3.0560722619,0.8078172954
H,0,2.0028172489,0.9939073594,-0.560546407
H,0,0.8335704391,5.6734137941,2.9366317238
H,0,1.4770471158,5.2143089554,1.336031478
H,0,1.8787033638,4.2345976466,2.7811180964

OEt 4-chlorophenyl carbonate

E (total electronic) = -1108.7096736
E (total electronic) + ZPVE = -1108.550172
Internal Thermal Energy = -1108.537245
Enthalpy = -1108.536301
Gibbs Free Energy = -1108.592932

C,0,3.7255626254,-0.2304250442,0.3701205228
C,0,5.0194685352,0.2765843807,-0.2697813392

O,0,6.108108216,-0.1869290559,0.4091335491
O,0,2.595993635,0.2988956783,-0.3755480795
C,0,1.4002845399,-0.0253434154,0.0679241508
O,0,1.1379408296,-0.7235816985,1.0186273673
O,0,0.4829562785,0.5688278293,-0.7305424184
C,0,-0.8565310031,0.3335841884,-0.4308872588
C,0,-1.5785089386,1.33582473,0.2023024785
C,0,-2.9365410388,1.1436429875,0.4494170729
C,0,-3.5333433158,-0.0504983633,0.056865168
C,0,-2.8073850245,-1.0544662856,-0.5794239824
C,0,-1.4516245973,-0.8575840999,-0.8275080729
H,0,3.6764673527,-1.3235358176,0.3438071929
H,0,3.6443146777,0.1087473016,1.4073662166
H,0,4.9381814589,1.3901903019,-0.2952313641
H,0,4.9826285726,-0.0376498535,-1.3408615989
H,0,-1.0831037452,2.2558909492,0.494848645
H,0,-3.5214133581,1.9135621326,0.9411166979
H,0,-3.2940792384,-1.9762586373,-0.8794932158
H,0,-0.8615207282,-1.6206482853,-1.324978997
Cl,0,-5.2360243828,-0.2948534928,0.3648788653

OEt 4-fluorophenyl carbonate

E (total electronic) = -748.3525885
E (total electronic) + ZPVE = -748.191635
Internal Thermal Energy = -748.179135
Enthalpy = -748.178191
Gibbs Free Energy = -748.233217

C,0,0.3883920915,-2.1470382635,-2.2511766388
C,0,0.2994584928,-2.4408204705,-3.7500058271
O,0,0.5208976735,-3.7640751622,-3.9983392907
O,0,0.1427433221,-0.7311158414,-2.0367538977
C,0,0.180930375,-0.3138305077,-0.7888397918
O,0,0.3962991759,-0.9794299336,0.1967248811
O,0,-0.064481031,1.0163805517,-0.7846965497
C,0,-0.0773445325,1.6460589861,0.4594709385
C,0,1.0573624065,2.3341619417,0.869150118
C,0,1.0361292379,3.0211854196,2.0817698276
C,0,-0.125991419,2.9879394063,2.8369130553
C,0,-1.2659751975,2.3058822149,2.4374813653
C,0,-1.2381430507,1.6237975534,1.223336577
F,0,-0.1513601011,3.6533425224,4.0140196579
H,0,-0.3629583953,-2.7169505817,-1.6958848678
H,0,1.3826992989,-2.3887673864,-1.8629065738
H,0,1.0288357423,-1.7557455834,-4.2459734767
H,0,-0.7039241948,-2.0771408333,-4.0793160475
H,0,1.9442017214,2.3330201165,0.2438696666
H,0,1.9000190461,3.5724399257,2.4368277096
H,0,-2.1514908449,2.3136491829,3.0636306253
H,0,-2.1084228171,1.0798267425,0.8704455392

Transition states

TS-OEt methyl carbonate

E (total electronic) = -457.4352118
E (total electronic) + ZPVE = -457.321011
Internal Thermal Energy = -457.312069
Enthalpy = -457.311124
Gibbs Free Energy = -457.357050

O,0,0.0182540543,-0.7189457006,-0.0000022948
C,0,-1.0158659543,0.026684029,0.0000005369
O,0,-1.0634733436,1.2604437652,0.0000077889
O,0,-2.1739951595,-0.7061428512,-0.0000057162
C,0,-3.3854178916,0.0426748965,-0.0000031066
C,0,1.6583673852,0.2597485972,0.0000015538
C,0,2.7719867134,-0.6808717118,-0.00000637
O,0,3.5197543541,0.4966607262,-0.000001081
H,0,-4.189819546,-0.6929861636,-0.000009695
H,0,-3.4536212115,0.6721820948,-0.890765556

H,0,-3.4536248504,0.6721700341,0.8907676002
H,0,1.4317724628,0.7708738032,0.9245999165
H,0,1.4317694256,0.7708857469,-0.9245894607
H,0,2.8682040915,-1.3049251442,-0.9004112361
H,0,2.8682072201,-1.3049367419,0.9003901247

TS-OEt ethyl carbonate

E (total electronic) = -496.7328566
E (total electronic) + ZPVE = -496.590132
Internal Thermal Energy = -496.579910
Enthalpy = -496.578965
Gibbs Free Energy = -496.627863

O,0,-0.9493479814,-0.6112412265,0.0381136597
C,0,0.0250222397,0.2116033827,0.0320554288
O,0,-0.024536933,1.4458446314,0.0331471154
O,0,1.2350344524,-0.4299929334,0.0222071087
C,0,2.3978763563,0.4034852536,0.0149597119
C,0,3.6087192398,-0.5059428751,-0.0216673597
H,0,2.3968172596,1.0322720332,0.9110975682
H,0,2.3655016342,1.0610279858,-0.8594023217
H,0,4.5237494035,0.0936740766,-0.0268006857
H,0,3.6295581069,-1.1603604105,0.8547391786
H,0,3.5986121145,-1.1281449482,-0.9214406677
C,0,-2.6630383846,0.2331314332,-0.0055185737
C,0,-3.6978386865,-0.7930602985,0.0215953016
O,0,-4.5357224771,0.3208835248,-0.0331136569
H,0,-2.4673904377,0.7244705908,-0.9476924041
H,0,-2.4875314635,0.7950971607,0.9004156091
H,0,-3.7558737748,-1.3866624937,0.9455739376
H,0,-3.7323106684,-1.4581668868,-0.85356395

TS-OEt isopropyl carbonate

E (total electronic) = -536.0312029
E (total electronic) + ZPVE = -535.860351
Internal Thermal Energy = -535.848883
Enthalpy = -535.847938
Gibbs Free Energy = -535.899302

O,0,0.4558755884,-1.1079541441,-0.5820010044
C,0,0.5070372683,0.1449243591,-0.346389942
O,0,1.0784691946,0.7136717218,0.5893751225
O,0,-0.1851480422,0.8652016729,-1.2848575009
C,0,-0.1549047093,2.2996652558,-1.1807479101
C,0,1.4042498792,-2.1684076026,0.6972415567
C,0,1.2641637223,-3.5740251599,0.3387707954
O,0,2.0532664003,-3.7438691599,1.4766146367
C,0,1.1486026304,2.8335075666,-1.7563384815
C,0,-1.3710035862,2.8043375024,-1.9379415799
H,0,-0.2306323771,2.5650852752,-0.1220301822
H,0,0.824944237,-1.8013823984,1.5320891289
H,0,2.3503383699,-1.6883398884,0.4923023988
H,0,1.7298035387,-3.8724891404,-0.6117061819
H,0,0.2451342853,-3.9826648363,0.4013359638
H,0,1.1792501686,3.9250213165,-1.6762462641
H,0,2.006028016,2.4221001586,-1.2171233581
H,0,1.2302296765,2.5620867948,-2.8148294636
H,0,-1.3129801457,2.5109942482,-2.99177055
H,0,-2.2916352477,2.3953323894,-1.5117045002
H,0,-1.4182878675,3.8963620686,-1.8860256843

TS-OEt tert-butyl carbonate

E (total electronic) = -575.3255439
E (total electronic) + ZPVE = -575.126929
Internal Thermal Energy = -575.114088
Enthalpy = -575.113143
Gibbs Free Energy = -575.167639

O,0,1.1210816017,0.7333791652,0.0000004188
C,0,0.0974349982,-0.0313209522,0.000001946
O,0,0.0891034717,-1.2660174566,0.0000030234
O,0,-1.0620587073,0.697742932,0.0000023225
C,0,-2.3654280013,0.0602877298,0.0000032935
C,0,-3.3254526823,1.2476545666,0.0000031522
C,0,-2.5649564818,-0.7700828873,1.2664679787
C,0,-2.5649576432,-0.7700841433,-1.2664603852
H,0,-3.1676626376,1.8666248711,-0.8891086758
H,0,-3.167661839,1.8666257281,0.8891142429
H,0,-4.3612455816,0.8945064051,0.000003791
H,0,-1.9125184494,-1.6442627346,1.2733141341
H,0,-2.355631778,-0.1597564557,2.1518830225
H,0,-3.6063215382,-1.1049323462,1.3212602903
H,0,-3.6063226674,-1.1049339312,-1.3212512684
H,0,-2.3556340433,-0.159758506,-2.1518762378
H,0,-1.9125193909,-1.6442638334,-1.2733064027
C,0,2.7851485541,-0.2185430011,0.000000073
C,0,3.8778884332,0.7451651946,-0.0000016718
O,0,4.642638741,-0.4222244444,-0.0000011301
H,0,2.5640600327,-0.7312536621,-0.9247961949
H,0,2.5640614272,-0.7312518913,0.924797657
H,0,3.9645217222,1.3699881372,0.9006444661
H,0,3.9645203589,1.3699864153,-0.9006491346

TS-OEt phenyl carbonate

E (total electronic) = -649.1065762
E (total electronic) + ZPVE = -648.940037
Internal Thermal Energy = -648.928037
Enthalpy = -648.927093
Gibbs Free Energy = -648.982710

C,0,0.217271346,-2.1557429684,-2.6697410169
C,0,0.325245999,-2.0719904325,-4.1225064438
O,0,0.2866835563,-3.4620359055,-4.035431501
O,0,0.2001388291,-0.4031655477,-1.9437066173
C,0,0.1508854249,-0.3831651393,-0.6751962675
O,0,0.1005856478,-1.3228201015,0.1137627767
O,0,0.1689156448,0.9264494834,-0.2002091834
C,0,0.0832727252,1.1159000734,1.1683437299
C,0,1.2268203678,1.4969226677,1.8626189266
C,0,1.1395435025,1.7624090038,3.2299411151
C,0,-0.0825027272,1.6435180457,3.8919523267
C,0,-1.22247122,1.2607943709,3.1814219503
C,0,-1.1445490878,0.9979688205,1.8150253486
H,0,-0.7456300171,-2.4185412368,-2.2550401188
H,0,1.0974645876,-2.4586553977,-2.1203699258
H,0,1.2654212933,-1.6448279453,-4.5018012663
H,0,-0.5288816547,-1.6033708018,-4.6335369506
H,0,2.1682897391,1.5843035702,1.3285853767
H,0,2.0290023371,2.0627144159,3.7758849655
H,0,-0.148293042,1.8504701739,4.9557114873
H,0,-2.1768822177,1.1692608243,3.6914616551
H,0,-2.021142034,0.7008670268,1.2469416329

TS-OEt 4-nitrophenyl carbonate

E (total electronic) = -853.5474616
E (total electronic) + ZPVE = -853.378062
Internal Thermal Energy = -853.363616
Enthalpy = -853.362672
Gibbs Free Energy = -853.423542

C,0,4.4765149594,-0.3442650722,0.2715172335
C,0,5.7064221443,0.2175532039,-0.2800153462
O,0,6.3202447594,-0.7580954043,0.5008735886
O,0,2.994567174,0.5956171926,-0.4207584649
C,0,1.8821448349,0.1583427263,-0.0034316945
O,0,1.6361576087,-0.7700692563,0.7554241287
O,0,0.8313871275,0.9334517311,-0.5243711027
C,0,-0.4627327524,0.5493729926,-0.3109318032

C,0,-0.9074747374,-0.7454724933,-0.5967928402
C,0,-2.249598036,-1.0562023068,-0.4366412239
C,0,-3.1224720744,-0.0624181144,0.001475344
C,0,-2.6965582964,1.2323452941,0.2811280693
C,0,-1.3509848957,1.5353497882,0.122923633
N,0,-4.5359272593,-0.3909469198,0.1700321175
O,0,-4.895197327,-1.5349216873,-0.0661280392
O,0,-5.2943936333,0.4931820929,0.5396104588
H,0,4.1542551896,-1.3032509775,-0.1098099214
H,0,4.2450911295,-0.1157754488,1.302679454
H,0,5.9163040325,1.2588712185,0.0072258844
H,0,5.8274159741,0.1023906472,-1.3676971226
H,0,-0.2059650311,-1.4964531073,-0.9396615705
H,0,-2.6206276335,-2.0508544676,-0.6528963846
H,0,-3.4033255762,1.980897483,0.618343329
H,0,-0.9755842815,2.5314410854,0.3311368735

TS-OEt 4-cyanophenyl carbonate

E (total electronic) = -741.3298378
E (total electronic) + ZPVE = -741.164590
Internal Thermal Energy = -741.150824
Enthalpy = -741.149880
Gibbs Free Energy = -741.209041

C,0,-0.0694302661,-3.8501598838,-1.5186496232
C,0,-0.0862539384,-4.5054790468,-2.8232803069
O,0,-0.2071792186,-5.6659024013,-2.0629117414
O,0,0.0982603223,-1.9839251409,-1.757762184
C,0,0.0950111784,-1.3352389155,-0.6695292829
O,0,-0.0074940722,-1.7374066695,0.4829923402
O,0,0.2586282395,0.0354136775,-0.9197398843
C,0,0.1603412494,0.9206267455,0.1224738343
C,0,1.2052134314,-1.82788175648,0.2918886274
C,0,1.1201986922,2.79950415,1.2815510616
C,0,-0.0141842877,2.8534673859,2.100286913
C,0,-1.0635208259,1.9401248751,1.9228708489
C,0,-0.9777429931,0.9743157648,0.9305040249
C,0,-0.1064787695,3.8547928827,3.1281171195
N,0,-0.1808323497,4.6615415655,3.9566795083
H,0,-1.0070479979,-3.781352568,-0.9849717213
H,0,0.8333773176,-3.9373358502,-0.9302680605
H,0,0.8418210895,-4.4135754008,-3.4071858813
H,0,-0.9499706995,-4.2614022088,-3.4598334864
H,0,2.0736386476,1.7635967509,-0.3552392004
H,0,1.9276810836,3.51039243,1.4224169295
H,0,-1.9415798769,1.9937138496,2.5581257844
H,0,-1.7818889561,0.2630873036,0.7797513805

TS-OEt 4-methoxyphenyl carbonate

E (total electronic) = -763.588363
E (total electronic) + ZPVE = -763.388499
Internal Thermal Energy = -763.374050
Enthalpy = -763.373106
Gibbs Free Energy = -763.433291

C,0,-4.1788756512,0.1091436128,0.4736918705
C,0,-5.4295625682,-0.1929491973,-0.2136504338
O,0,-5.9934961541,0.2904306495,0.9655342671
H,0,-3.8904555775,1.1476864411,0.5544959666
H,0,-3.8703141298,-0.5584611855,1.2658151999
H,0,-5.6079810586,-1.2576973859,-0.4248307376
H,0,-5.6287583459,0.4038765837,-1.1160114317
O,0,-2.7239686627,-0.3484886136,-0.6572429395
C,0,-1.5873764165,-0.0850404062,-0.1554190877
O,0,-1.319279644,0.4170576928,0.9332423919
O,0,-0.5651338982,-0.4538838868,-1.0255743297
C,0,0.7377558154,-0.1914545763,-0.6329389986
C,0,1.261200046,1.096552113,-0.7505262415
C,0,2.5873463079,1.3330892722,-0.4196364483
C,0,3.4020768815,0.2829690574,0.026580299

C,0,2.8768337892,-1.0056674893,0.1383771599
C,0,1.5372616944,-1.2344371085,-0.1932317606
O,0,4.6897766379,0.6153109375,0.3231869152
C,0,5.5474633073,-0.4192903581,0.7767930594
H,0,0.6243148888,1.9043599518,-1.0987691878
H,0,3.014963883,2.3276288263,-0.5029053476
H,0,3.4862352997,-1.83531142,0.4770862924
H,0,1.1155566116,-2.2318074481,-0.1114009194
H,0,6.5148638791,0.0486218835,0.9547121533
H,0,5.6525751411,-1.202708864,0.0181492906
H,0,5.1745619238,-0.857506082,1.7091019981

TS-OEt 4-chlorophenyl carbonate

E (total electronic) = -1108.6764646
E (total electronic) + ZPVE = -1108.519545
Internal Thermal Energy = -1108.506414
Enthalpy = -1108.505470
Gibbs Free Energy = -1108.563066

C,0,0.0546605109,-3.6670863885,-0.7585937461
C,0,0.0792350997,-4.5662817915,-1.9077485036
O,0,-0.0047233739,-5.5529556984,-0.9280021315
O,0,0.1479530524,-1.87658776,-1.3682159698
C,0,0.1160489073,-1.0199813638,-0.4331528297
O,0,0.0336016569,-1.191581975,0.7787399339
O,0,0.2036231552,0.2747577682,-0.9509546974
C,0,0.1204650933,1.3340184653,-0.0715839043
C,0,1.2261258816,2.1669160908,0.0629368907
C,0,1.1512091297,3.2921270488,0.8830186692
C,0,-0.03455784,3.5576275439,1.5589885842
C,0,-1.1462057411,2.7280585364,1.4289967861
C,0,-1.066644238,1.6102397865,0.6039422423
Cl,0,-0.1348787451,4.966507209,2.5926411456
H,0,-0.8910925946,-3.5297933617,-0.2533528281
H,0,0.9538878493,-3.5953129149,-0.1627759616
H,0,1.0099855318,-4.5560187518,-2.4943199897
H,0,-0.7860549002,-4.4913189865,-2.5831135815
H,0,2.1387877436,1.9340446403,-0.4764085897
H,0,2.0056742112,3.9513616958,0.9944044175
H,0,-2.0633358054,2.9549348169,1.9625439545
H,0,-1.9202525843,0.9507323901,0.4853311089

TS-OEt 4-fluorophenyl carbonate

E (total electronic) = -649.1065762
E (total electronic) + ZPVE = -648.940037
Internal Thermal Energy = -648.928037
Enthalpy = -648.927093
Gibbs Free Energy = -648.982710

C,0,0.217271346,-2.1557429684,-2.6697410169
C,0,0.325245999,-2.0719904325,-4.1225064438
O,0,0.2866835563,-3.4620359055,-4.035431501
O,0,0.2001388291,-0.4031655477,-1.9437066173
C,0,0.1508854249,-0.3831651393,-0.6751962675
O,0,0.1005856478,-1.3228201015,0.1137627767
O,0,0.1689156448,0.9264494834,-0.2002091834
C,0,0.0832727252,1.1159000734,1.1683437299
C,0,1.2268203678,1.4969226677,1.8626189266
C,0,1.1395435025,1.7624090038,3.2299411151
C,0,-0.0825027272,1.6435180457,3.8919523267
C,0,-1.22247122,1.2607943709,3.1814219503
C,0,-1.1445490878,0.9979688205,1.8150253486
H,0,-0.7456300171,-2.4185412368,-2.2550401188
H,0,1.0974645876,-2.4586553977,-2.1203699258
H,0,1.2654212933,-1.6448279453,-4.5018012663
H,0,-0.5288816547,-1.6033708018,-4.6335369506
H,0,2.1682897391,1.5843035702,1.3285853767
H,0,2.0290023371,2.0627144159,3.7758849655
H,0,-0.148293042,1.8504701739,4.9557114873
H,0,-2.1768822177,1.1692608243,3.6914616551

H,0,-2.021142034,0.7008670268,1.2469416329

M06-2X/6-311+G(2d,p) IEFPCM, Solvent = Water

Substrates

OEt methyl carbonate

E (total electronic) = -457.6131311

E (total electronic) + ZPVE = -457.497112

Internal Thermal Energy = -457.488388

Enthalpy = -457.487444

Gibbs Free Energy = -457.531666

O,0,2.1827968563,-0.1071374291,0.6686018593
C,0,0.9498934269,0.3620114378,0.663802491
O,0,-0.0637664933,-0.2921502187,0.6613828914
O,0,0.9965784448,1.6938076685,0.6619950309
C,0,-0.279504087,2.3421654057,0.6567830204
C,0,2.3156350645,-1.5501598585,0.6711655933
C,0,3.7999392983,-1.9062160296,0.6766315088
O,0,3.9814355425,-3.2571767806,0.6792218094
H,0,-0.0659733978,3.4062027228,0.6559272366
H,0,-0.8443486441,2.067832117,1.5456183396
H,0,-0.8384092176,2.0652081359,-0.2349883017
H,0,1.8239819392,-1.946798066,-0.2186774354
H,0,1.8180630339,-1.944184649,1.5588772014
H,0,4.2385971012,-1.3871974643,1.5584794608
H,0,4.2444651319,-1.3897879921,-0.2037977062

OEt ethyl carbonate

E (total electronic) = -496.9222036

E (total electronic) + ZPVE = -496.777830

Internal Thermal Energy = -496.767829

Enthalpy = -496.766884

Gibbs Free Energy = -496.814278

O,0,0.1638863408,-0.5036198357,-0.0000073132
C,0,-1.0015235499,0.1171860394,-0.0000015217
O,0,-1.1705909808,1.3121576679,0.0000066081
O,0,-1.9743630293,-0.7919187021,-0.0000066835
C,0,-3.3134623831,-0.2610572916,-0.0000018294
C,0,1.3369121469,0.3464059924,-0.0000032286
C,0,2.5848803421,-0.5324845893,-0.0000137357
O,0,3.7166932107,0.2275952724,-0.0000113647
H,0,-3.4387946814,0.3632864689,-0.8847533207
H,0,-3.4387938249,0.3632723305,0.8847597571
H,0,1.3090727337,0.9797050349,0.8884515531
H,0,1.3090684315,0.9797196867,-0.8884474051
H,0,2.4894768482,-1.2060964401,-0.8811330927
H,0,2.4894822469,-1.2061099612,0.8810958889
C,0,-4.2616197708,-1.4346442458,-0.0000107425
H,0,-4.1128108398,-2.0507249409,0.8867716149
H,0,-5.2888288641,-1.0701381763,-0.0000074929
H,0,-4.1128114566,-2.0507108802,-0.8868029714

OEt isopropyl carbonate

E (total electronic) = -536.23196

E (total electronic) + ZPVE = -536.059535

Internal Thermal Energy = -536.048291

Enthalpy = -536.047347

Gibbs Free Energy = -536.097383

O,0,0.3485961739,-0.908943119,0.05098563
C,0,0.3540793219,0.3782248338,0.351581681

O,0,0.4582236616,0.8434376751,1.4606093384
O,0,0.2189481331,1.0796239846,-0.7717049096
C,0,0.2415861113,2.5239760307,-0.6412715164
C,0,0.4870313268,-1.8219883838,1.1665287946
C,0,0.4660427623,-3.2548132487,0.6407116144
O,0,0.6037952157,-4.1506103924,1.6595969367
C,0,-0.4362560791,3.0608238179,-1.8830902382
C,0,1.6745848033,2.9983099494,-0.500526451
H,0,-0.332365248,2.7808654518,0.2492649277
H,0,-0.3370049451,-1.6523993151,1.8618219765
H,0,1.4291801722,-1.6104495222,1.6751000288
H,0,1.2681334497,-3.3144961513,-0.1288795375
H,0,-0.4824645227,-3.3611809768,0.0677877913
H,0,-1.4560906677,2.684773276,-1.9617002133
H,0,-0.4680062115,4.1496798747,-1.8390775425
H,0,0.1194340204,2.7662425843,-2.7750543838
H,0,2.1436459454,2.5638790032,0.3815271545
H,0,2.2487858414,2.7202944807,-1.3863251011
H,0,1.6929347348,4.0845201475,-0.4028009805

OEt tert-butyl carbonate

E (total electronic) = -575.5380954

E (total electronic) + ZPVE = -575.338288

Internal Thermal Energy = -575.325632

Enthalpy = -575.324688

Gibbs Free Energy = -575.378205

O,0,0.1729259767,-0.4286971138,-0.0239063245
C,0,-0.9631728729,0.253913178,-0.0202465061
O,0,-1.0505244749,1.4575864226,-0.0188195567
O,0,-1.9678485723,-0.6162902303,-0.017938634
C,0,-3.3562662913,-0.1502244993,-0.0012625174
C,0,1.3866268922,0.3587236706,-0.0205079152
C,0,2.5872707044,-0.5828978579,0.0225331999
O,0,3.7580020075,0.1158709502,0.0365645049
H,0,1.3783662251,1.0125668448,0.8531930545
H,0,1.40833369,0.9737540306,-0.9221782347
H,0,2.4768768118,-1.2667818835,-0.8490365141
H,0,2.4366466358,-1.2346521403,0.9124541756
C,0,-3.6300155243,0.6367104602,1.2727636498
H,0,-3.0958303928,1.5840946607,1.2793729076
H,0,-4.7003947527,0.8373251613,1.3395118717
H,0,-3.3364261861,0.0508404027,2.1455243847
C,0,-3.6571583705,0.6530028166,-1.2588712734
H,0,-3.3801563514,0.0795098179,-2.1451466309
H,0,-4.7291625696,0.8517303336,-1.3011321919
H,0,-3.1253084124,1.6016349238,-1.2637199214
C,0,-4.1435558128,-1.4520140378,-0.0012801978
H,0,-3.8959483562,-2.046205452,0.8792388776
H,0,-5.2115529737,-1.2337620343,0.0124552173
H,0,-3.9161874096,-2.0339220941,-0.8953597356

OEt phenyl carbonate

E (total electronic) = -649.3292165

E (total electronic) + ZPVE = -649.160825

Internal Thermal Energy = -649.149078

Enthalpy = -649.148134

Gibbs Free Energy = -649.201977

C,0,0.2144332379,-2.6154399051,-1.3923757331
C,0,0.0324563367,-3.22935897,-2.7778358796
O,0,0.2965893789,-4.5660617226,-2.7555475853
O,0,-0.0775206764,-1.1949227839,-1.467892531
C,0,0.0363340645,-0.5234217277,-0.3445156193
O,0,0.3540156909,-0.9567237801,0.7306347454
O,0,-0.2684220728,0.766620348,-0.5953974086
C,0,-0.2021963383,1.640842636,0.489737584
C,0,0.9822484057,2.3096619721,0.7403465954
C,0,1.0255515051,3.2258853028,1.7838876688
C,0,-0.1059403532,3.4601324032,2.5566774636
C,0,-1.2862763014,2.7774819509,2.2862259486
C,0,-1.3401568417,1.8592066349,1.2449830902

H,0,-0.4669790518,-3.0703200698,-0.6718079457
H,0,1.2405959682,-2.7390949898,-1.0428676179
H,0,0.6885511595,-2.64704096,-3.4630807993
H,0,-1.0037719985,-2.975313357,-3.095336263
H,0,1.8497925197,2.1118072922,0.1237776477
H,0,1.945496611,3.7573910377,1.9908152652
H,0,-0.0685263307,4.1758158807,3.3677045824
H,0,-2.1695034101,2.959243331,2.884965522
H,0,-2.248259503,1.3169464764,1.0142452697

OEt 4-nitrophenyl carbonate

E (total electronic) = -853.8302387
E (total electronic) + ZPVE = -853.658967
Internal Thermal Energy = -853.644820
Enthalpy = -853.643876
Gibbs Free Energy = -853.703104

C,0,-0.0522917024,-3.4210749867,0.9992572185
C,0,-0.1064124821,-4.7790386926,0.3056856311
O,0,-0.1605975111,-5.7856576295,1.221526413
O,0,0.0101197251,-2.3808433632,-0.0155592811
C,0,0.0597718959,-1.1497041172,0.4275302163
O,0,0.0524122332,-0.7800663001,-1.5687182541
O,0,0.1386211608,-0.3285803064,-0.6510092458
C,0,0.1300107439,1.0346432847,-0.4369905121
C,0,1.1637728238,1.7626464768,-1.0052932377
C,0,1.1640713615,3.1418785612,-0.8898381185
C,0,0.1245662838,3.746791771,-0.2033550389
C,0,-0.9148229492,3.0262735771,0.3650355068
C,0,-0.9128738672,1.6488664276,0.2439849538
N,0,0.1205187038,5.2071423716,-0.0762974791
O,0,1.0351498061,5.8267855843,-0.5832739426
O,0,-0.7971904341,5.725129196,0.5295192752
H,0,-0.9432722209,-3.2558325057,1.6065085062
H,0,0.8341100946,-3.3394293277,1.6299298409
H,0,0.7807844547,-4.8193088042,-0.3652441939
H,0,-0.9797845351,-4.7405257767,-0.3832008122
H,0,1.9532945694,1.2446678799,-1.5320952407
H,0,1.954241126,3.7393883026,-1.3198983886
H,0,-1.7098873388,3.5389658056,0.8860801943
H,0,-1.7092029416,1.0550195719,0.669764481

OEt 4-cyanophenyl carbonate

E (total electronic) = -741.5748923
E (total electronic) + ZPVE = -741.407779
Internal Thermal Energy = -741.394310
Enthalpy = -741.393366
Gibbs Free Energy = -741.450570

C,0,0.119122021,-3.6645444463,-0.8591498433
C,0,0.186538933,-4.5304314057,-2.1136359375
O,0,0.1623824844,-5.8529009795,-1.7884245312
O,0,0.1589204058,-2.265878287,-1.2548021881
C,0,0.1021777328,-1.3918836906,-0.2803897267
O,0,0.0124580447,-1.6118703049,0.895881873
O,0,0.1764088784,-0.1550978503,-0.831933479
C,0,0.0721219594,0.9362891356,0.0109667073
C,0,1.116850274,1.8453560562,-0.0009211128
C,0,1.0227461136,2.992775774,0.7680593511
C,0,-0.1173983709,3.2097419137,1.5405737822
C,0,-1.1646330873,2.2862347387,1.5415985991
C,0,-1.0708075312,1.1428052172,0.7697601622
C,0,-0.2181139545,4.3979425181,2.3414444601
N,0,-0.2987100737,5.3479178444,2.9816390998
H,0,-0.8072899576,-3.8412140907,-0.3109562836
H,0,0.9687267764,-3.8607790619,-0.2034768012
H,0,1.1019083134,-4.2115169054,-2.660746364
H,0,-0.6576065667,-4.2037697966,-2.7613613089
H,0,1.9880189523,1.6487993103,-0.6109326805
H,0,1.8274544366,3.7153314454,0.7722917175
H,0,-2.0463209339,2.4685187347,2.140900978
H,0,-1.8722128496,0.4170681304,0.7527225264

OEt 4-methoxyphenyl carbonate

E (total electronic) = -763.8462894
E (total electronic) + ZPVE = -763.644816
Internal Thermal Energy = -763.630670
Enthalpy = -763.629726
Gibbs Free Energy = -763.688180

C,0,-0.2487251595,-3.9535535592,-0.9108296
C,0,-0.2795680814,-4.8796096566,-2.1234517532
O,0,-0.3250436281,-6.1857171141,-1.7365647072
O,0,-0.2044477057,-2.5784141197,-1.3736273458
C,0,-0.1575835381,-1.6565745508,-0.4377865372
O,0,-0.1464872226,-1.8329547367,0.7511395304
O,0,-0.1204082861,-0.4513182009,-1.0413852553
C,0,-0.0860761756,0.6660067514,-0.2059076402
C,0,-1.2477479626,1.1032301699,0.4139386181
C,0,-1.2114652316,2.2471092471,1.1871564115
C,0,-0.0177553892,2.9580064959,1.3386039929
C,0,1.1401066254,2.51228666331,0.7086362687
C,0,1.0982824763,1.3553738805,-0.0663595409
O,0,-0.0856714768,4.0696413204,2.1147793932
C,0,1.1069137201,4.8170990106,2.292161127
H,0,-1.142358982,-4.0835999568,-0.2982787612
H,0,0.6349657413,-4.1422288348,-0.299350106
H,0,0.6118029893,-4.6167646692,-2.7361092014
H,0,-1.1494127338,-4.5559570439,-2.7380441608
H,0,-2.1677407601,0.5464904607,0.2881272344
H,0,-2.1018053935,2.6115074296,1.683147715
H,0,2.0741285247,3.0456636149,0.8076160026
H,0,1.9894146307,0.9948503721,-0.5639569672
H,0,0.8457836546,5.6525650286,2.9352110721
H,0,1.4776328861,5.1932214389,1.3362353809
H,0,1.8787944783,4.2125755892,2.7732398295

OEt 4-chlorophenyl carbonate

E (total electronic) = -1108.9314549
E (total electronic) + ZPVE = -1108.772598
Internal Thermal Energy = -1108.759699
Enthalpy = -1108.758754
Gibbs Free Energy = -1108.815330

C,0,3.7123349488,-0.2232499965,0.372337123
C,0,5.0092046404,0.2677318006,-0.2643843235
O,0,6.0907452899,-0.1988989007,0.4204964032
O,0,2.5899660709,0.3063191016,-0.3832719866
C,0,1.3971080853,-0.0147985153,0.0592927338
O,0,1.1330054454,-0.7011048095,1.0091758702
O,0,0.4818584224,0.5706646817,-0.7453033318
C,0,-0.8542417037,0.3341925035,-0.4392417272
C,0,-1.5717117076,1.3279205593,0.2005074066
C,0,-2.9227009101,1.133361667,0.4546782717
C,0,-3.5172289916,-0.0547391749,0.0622613168
C,0,-2.7973805076,-1.0509212804,-0.5797676727
C,0,-1.4486481011,-0.8514726555,-0.8343535512
H,0,3.6564240249,-1.312795007,0.3556238178
H,0,3.6286619016,0.1248911995,1.4028587381
H,0,4.9358002327,1.3778405396,-0.2994986497
H,0,4.9723237766,-0.0513579951,-1.3301207349
H,0,-1.0770860534,2.244730354,0.4931806126
H,0,-3.5048755865,1.8969593438,0.9520655079
H,0,-3.2842247404,-1.9690640899,-0.8788223535
H,0,-0.8608599683,-1.6091279392,-1.3361091633
Cl,0,-5.2166432181,-0.3031049564,0.3805472928

OEt 4-fluorophenyl carbonate

E (total electronic) = -748.5726885
E (total electronic) + ZPVE = -748.412423
Internal Thermal Energy = -748.399966
Enthalpy = -748.399021

Gibbs Free Energy = -748.453911

C,0,0.3871572883,-2.1368755709,-2.2436821183
C,0,0.3002656033,-2.4397706064,-3.736732854
O,0,0.5238925437,-3.7624811273,-3.9769659064
O,0,0.1401030284,-0.7201983831,-2.0390322659
C,0,0.1781026202,-0.3036015882,-0.7946458115
O,0,0.3924664927,-0.963089994,0.186541582
O,0,-0.0676404025,1.0247560334,-0.7912188436
C,0,-0.0786602648,1.6484159775,0.4542528501
C,0,1.0519612343,2.3304857472,0.8658989462
C,0,1.0324852886,3.0089874934,2.0772646664
C,0,-0.1236744295,2.9748022302,2.831582101
C,0,-1.259126719,2.2972417852,2.4301165728
C,0,-1.2330527493,1.6235280571,1.2174253185
F,0,-0.1471724273,3.6320390613,4.0074624876
H,0,-0.3619152073,-2.7020907786,-1.6871696045
H,0,1.3783289799,-2.3743800986,-1.8542707601
H,0,1.0251917424,-1.7572462031,-4.2342809065
H,0,-0.6994718146,-2.0792126939,-4.0677912552
H,0,1.9358154112,2.3308813926,0.2417260284
H,0,1.8948004638,3.5559372846,2.4337420868
H,0,-2.1412832506,2.3025672026,3.0559061307
H,0,-2.1006964319,1.082074779,0.8636185553

Transition states

TS-OEt methyl carbonate

E (total electronic) = -457.577206
E (total electronic) + ZPVE = -457.463721
Internal Thermal Energy = -457.454807
Enthalpy = -457.453863
Gibbs Free Energy = -457.499382

O,0,0.011246018,-0.7363217149,-0.0000021079
C,0,-1.0140251283,0.0131181405,0.0000006349
O,0,-1.0561508046,1.2403171197,0.0000078619
O,0,-2.1750213807,-0.7129633741,-0.0000057507
C,0,-3.3764797775,0.0491269831,-0.0000031336
C,0,1.6499373586,0.2547759837,0.0000015068
C,0,2.7709146948,-0.670889198,-0.0000063356
O,0,3.5123857441,0.5094804785,-0.000003259
H,0,-4.1894937366,-0.6727811614,-0.0000098758
H,0,-3.4373536893,0.6782437947,-0.887566881
H,0,-3.4373576322,0.6782315418,0.887569046
H,0,1.4164637254,0.7594348053,0.9224385309
H,0,1.4164604473,0.7594463994,-0.9224283389
H,0,2.8704842816,-1.292846574,-0.897281149
H,0,2.8704876293,-1.2928578444,0.8972602953

TS-OEt ethyl carbonate

E (total electronic) = -496.8858306
E (total electronic) + ZPVE = -496.744079
Internal Thermal Energy = -496.733838
Enthalpy = -496.732894
Gibbs Free Energy = -496.781896

O,0,-0.4990759327,-0.6483769031,-0.0218783951
C,0,0.4688793805,0.1744982131,-0.0147389102
O,0,0.4179020807,1.4019400114,-0.0132046379
O,0,1.679232549,-0.4640642664,-0.0075607981
C,0,2.8337326487,0.3784619479,0.0004088176
C,0,-2.2104056838,0.2127796568,0.0086579537
C,0,-3.2554883333,-0.7973820141,-0.0090517777
O,0,-4.0851552776,0.3223022861,0.0286060955
C,0,4.0519808332,-0.5162409266,0.0233006228
H,0,2.8005110708,1.0271925933,0.8771386144
H,0,2.8228718492,1.0129868111,-0.8874034539
H,0,-2.0231917116,0.7570917376,-0.9015968236

H,0,-2.0092242071,0.7093596326,0.9429340601
H,0,-3.2981875795,-1.4494620684,0.871183239
H,0,-3.3148518511,-1.4006116644,-0.9225330914
H,0,4.9570246148,0.0920190732,0.0289565513
H,0,4.0525592213,-1.143943771,0.9150918052
H,0,4.0745985985,-1.1604459191,-0.8563293516

TS-OEt isopropyl carbonate

E (total electronic) = -536.1951089
E (total electronic) + ZPVE = -536.025371
Internal Thermal Energy = -536.013916
Enthalpy = -536.012972
Gibbs Free Energy = -536.064194

O,0,0.4460281831,-1.1090229978,-0.5970430686
C,0,0.5002472204,0.1381880192,-0.3583276673
O,0,1.0726774912,0.7015422675,0.5712195096
O,0,-0.1943106251,0.8606326401,-1.2918315417
C,0,-0.156946824,2.2926769914,-1.1802366517
C,0,1.4032998494,-2.1611033145,0.6905434437
C,0,1.270473305,-3.5670326418,0.3472490843
O,0,2.0620991574,-3.7294080645,1.4833216165
C,0,1.1469921253,2.8238423708,-1.7490262952
C,0,-1.3658698114,2.8088493256,-1.935247125
H,0,-0.2331643845,2.5531957176,-0.1239667698
H,0,0.822821432,-1.7889838408,1.517854137
H,0,2.3421058514,-1.6784142395,0.4765083307
H,0,1.7327720333,-3.8690530082,-0.5997276604
H,0,0.2558875015,-3.9767661536,0.4138752246
H,0,1.1815576544,3.9109346199,-1.6588722195
H,0,1.9975039302,2.4031312755,-1.2135724489
H,0,1.2261333463,2.5623905789,-2.8066164435
H,0,-1.3072448073,2.5202084984,-2.986737261
H,0,-2.2867874556,2.4059095569,-1.5130107464
H,0,-1.4034741732,3.8974403988,-1.8783384477

TS-OEt tert-butyl carbonate

E (total electronic) = -575.5000782
E (total electronic) + ZPVE = -575.302839
Internal Thermal Energy = -575.289986
Enthalpy = -575.289042
Gibbs Free Energy = -575.343476

O,0,1.1135466024,0.7485728454,0.0000000885
C,0,0.0973407526,-0.0180131923,0.0000017165
O,0,0.093005597,-1.24608676,0.0000028123
O,0,-1.0633715329,0.7065532161,0.0000021522
C,0,-2.3612856707,0.0611097252,0.0000032705
C,0,-3.3281497893,1.2396478951,0.0000031481
C,0,-2.5583248743,-0.7683397886,1.2640736102
C,0,-2.5583262579,-0.7683411993,-1.2640659276
H,0,-3.1738715196,1.8565762943,-0.8867339126
H,0,-3.1738705518,1.8565772736,0.8867393601
H,0,-4.3574070723,0.8787041299,0.0000039135
H,0,-1.9036450169,-1.6362032788,1.2710808488
H,0,-2.3536078511,-0.1574874905,2.1457349911
H,0,-3.5954953808,-1.1052663998,1.3155741839
H,0,-3.595496737,-1.1052681448,-1.3155648446
H,0,-2.3536104976,-0.1574898006,-2.1457282253
H,0,-1.9036461781,-1.6362045279,-1.2710730482
C,0,2.7765355742,-0.2164579451,-0.0000000773
C,0,3.8766755076,0.7327059596,-0.0000014169
O,0,4.635245241,-0.4376250134,-0.000000908
H,0,2.5482928804,-0.7226081276,-0.9226281237
H,0,2.5482938945,-0.7226067028,0.9226290025
H,0,3.9666308717,1.355413668,0.8975406316
H,0,3.9666299086,1.3554122639,-0.8975445349

TS-OEt phenyl carbonate

E (total electronic) = -649.2962257
E (total electronic) + ZPVE = -649.130442
Internal Thermal Energy = -649.118499
Enthalpy = -649.117555
Gibbs Free Energy = -649.172389

C,0,-4.1468420111,-0.3177438124,-0.3274187437
C,0,-5.4073446771,0.2096850695,0.1733460049
O,0,-5.9596700862,-0.7043843789,-0.7201070306
O,0,-2.7013320436,0.5573178103,0.5439427642
C,0,-1.5729464095,0.1632608027,0.1314304506
O,0,-1.308363874,-0.6751947067,-0.7159409691
O,0,-0.5450428079,0.8392906673,0.7846762227
C,0,0.7516651269,0.4905446727,0.4572146266
C,0,1.4918137017,1.3470961128,-0.3417779523
C,0,2.8192850511,1.042775573,-0.621278893
C,0,3.3957249604,-0.1116421212,-0.1060434455
C,0,2.6410310448,-0.9627948446,0.6950247554
C,0,1.3159804681,-0.6634821837,0.9811363664
H,0,-3.8483906433,-1.2968233594,0.0091163456
H,0,-3.834347482,-0.0096530187,-1.3115029907
H,0,-5.5954118613,1.266342497,-0.0520426218
H,0,-5.6080468586,0.0167838088,1.2341191471
H,0,1.0242626288,2.2417625692,-0.733342071
H,0,3.4019977705,1.7106166513,-1.243196633
H,0,3.0860360823,-1.8626256194,1.1008534874
H,0,0.7136946212,-1.3139814148,1.6029536878
H,0,4.4293416388,-0.3470260748,-0.3248057479

TS-OEt 4-nitrophenyl carbonate

E (total electronic) = -853.7997661
E (total electronic) + ZPVE = -853.631159
Internal Thermal Energy = -853.616770
Enthalpy = -853.615826
Gibbs Free Energy = -853.676274

C,0,4.4574722041,-0.3464493152,0.2667301694
C,0,5.6958321804,0.1989644834,-0.2718353254
O,0,6.2979202686,-0.7899519864,0.4998047665
O,0,2.9859757541,0.6182591272,-0.4233316285
C,0,1.8795872654,0.1802329321,-0.0070760115
O,0,1.6344825419,-0.741547112,0.748825368
O,0,0.8273784122,0.9521294155,-0.5312989759
C,0,-0.4616504154,0.5608955008,-0.3151917168
C,0,-0.8974848172,-0.7330462221,-0.5945351969
C,0,-2.232051037,-1.0508254908,-0.4316413442
C,0,-3.1079847217,-0.0664333164,0.0042131969
C,0,-2.691202105,1.2265375303,0.2776259878
C,0,-1.3533039276,1.5376039982,0.1163574616
N,0,-4.519389276,-0.4040678434,0.1764351941
O,0,-4.8688871529,-1.5465513439,-0.0550336583
O,0,-5.2790026431,0.473041353,0.5434255136
H,0,4.1213377601,-1.2924782643,-0.1254998169
H,0,4.2234329726,-0.1217833409,1.2946768018
H,0,5.9167626837,1.2319718847,0.0239085579
H,0,5.8170451874,0.0937156093,-1.3570349862
H,0,-0.1923511607,-1.4768600873,-0.9356565487
H,0,-2.5973042041,-2.0451503201,-0.6433706125
H,0,-3.4016596883,1.9677956351,0.6130013688
H,0,-0.9852920303,2.5340873733,0.3197360358

TS-OEt 4-cyanophenyl carbonate

E (total electronic) = -741.5439419
E (total electronic) + ZPVE = -741.379410
Internal Thermal Energy = -741.365723
Enthalpy = -741.364779
Gibbs Free Energy = -741.423171

C,0,-0.0832093578,-3.8341614097,-1.5139402199

C,0,-0.0888898051,-4.5045366081,-2.806665276
O,0,-0.2440320412,-5.6571680269,-2.0424935289
O,0,0.1192576247,-1.9696110303,-1.7653630813
C,0,0.1056538951,-1.3285350407,-0.6790504773
O,0,-0.0124071559,-1.7293033314,0.4648350658
O,0,0.2794556038,0.0426549677,-0.9238119323
C,0,0.1725105192,0.921214566,0.119267402
C,0,1.2021955104,1.8387462724,0.2865767867
C,0,1.1104298916,2.8030661434,1.274920402
C,0,-0.0158106961,2.8406905616,2.0964719591
C,0,-1.0503426222,1.9180495833,1.9220398769
C,0,-0.9573540661,0.959068857,0.9315073119
C,0,-0.1153807732,3.835937053,3.1254922081
N,0,-0.1951941865,4.6326259957,3.9495307176
H,0,-1.0260094967,-3.74004708,-1.0003032059
H,0,0.8059229017,-3.9268588668,-0.9118120774
H,0,0.8479847973,-4.43319357,-3.3727129047
H,0,-0.9332086129,-4.2505562184,-3.4592638595
H,0,2.065423706,1.7875423607,-0.3634533319
H,0,1.9070091708,3.5217971177,1.4136097953
H,0,-1.923281873,1.9595451785,2.5598782214
H,0,-1.7501559339,0.2397135252,0.7830271482

TS-OEt 4-methoxyphenyl carbonate

E (total electronic) = -763.8128867
E (total electronic) + ZPVE = -763.614112
Internal Thermal Energy = -763.599688
Enthalpy = -763.598744
Gibbs Free Energy = -763.658847

C,0,-4.4506016831,-0.0373645351,0.1824232985
C,0,-5.7015018672,-0.330980591,-0.4997772994
O,0,-6.2626351391,0.0220293634,0.725003142
H,0,-4.2027429662,0.9986786353,0.3439363028
H,0,-4.0939615228,-0.7560479817,0.9016507168
H,0,-5.8376190871,-1.3768078645,-0.8003043511
H,0,-5.9437630855,0.3299967308,-1.34060956
O,0,-2.9985111444,-0.327315446,-1.0137023263
C,0,-1.8714834917,-0.1172187173,-0.4791800263
O,0,-1.6114571045,0.2401628119,0.6597199821
O,0,-0.8429587693,-0.3539722062,-1.3861386557
C,0,0.4517806566,-0.1517482276,-0.9401318528
C,0,1.0024055882,1.1241251585,-0.9542062038
C,0,2.3164619634,1.3094970477,-0.5684718364
C,0,3.092992523,0.2198946194,-0.1674612975
C,0,2.53995873,-1.0564493047,-0.1568909343
C,0,1.2132229625,-1.2331899928,-0.5453574977
O,0,4.3746114891,0.5032275393,0.190833086
C,0,5.1895152016,-0.580215508,0.6050614795
H,0,0.3936311817,1.9634045258,-1.2668618804
H,0,2.7645683127,2.29506462,-0.5724443893
H,0,3.1193385812,-1.9164242192,0.1465076492
H,0,0.7702165324,-2.2212921595,-0.5420383208
H,0,6.1589012499,-0.1538811863,0.8471870753
H,0,5.3030151116,-1.3136048732,-0.1964464382
H,0,4.7732557771,-1.067024239,1.4898411378

TS-OEt 4-chlorophenyl carbonate

E (total electronic) = -1108.8992734
E (total electronic) + ZPVE = -1108.743086
Internal Thermal Energy = -1108.729973
Enthalpy = -1108.729029
Gibbs Free Energy = -1108.786737

C,0,0.05705102,-3.6507733315,-0.7552004458
C,0,0.0606393926,-4.5624965493,-1.889626661
O,0,-0.0336058468,-5.540989827,-0.9039227763
O,0,0.1741480297,-1.8631253035,-1.3818639573
C,0,0.1368500997,-1.0127889881,-0.4484649799
O,0,0.0521236689,-1.1836276633,0.7563569687

O,0,0.2211693153,0.2831158819,-0.9639911833
C,0,0.1297011635,1.3345932019,-0.0796088018
C,0,1.2246385242,2.1716095565,0.0625631004
C,0,1.1411220625,3.2865666448,0.8870644905
C,0,-0.0421394862,3.5378592363,1.5598651492
C,0,-1.1433030615,2.7054208142,1.4237019305
C,0,-1.0550191613,1.5977730053,0.594930634
Cl,0,-0.1535771576,4.9382798761,2.6026505593
H,0,-0.8810048908,-3.4894761578,-0.249905336
H,0,0.9588989412,-3.5835183562,-0.1689680151
H,0,0.984924886,-4.57112702,-2.4800243262
H,0,-0.8039170668,-4.4787990717,-2.5593068697
H,0,2.1370245772,1.9495848504,-0.475512192
H,0,1.987513788,3.9495936796,1.0047712574
H,0,-2.0592066482,2.9227978801,1.9565251028
H,0,-1.9005201492,0.9339346413,0.4712873515

TS-OEt 4-fluorophenyl carbonate

E (total electronic) = -748.5401035
E (total electronic) + ZPVE = -748.382501
Internal Thermal Energy = -748.369784
Enthalpy = -748.368840
Gibbs Free Energy = -748.425176

C,0,-3.5091380847,-0.2506388178,-0.3999327672
C,0,-4.7467751744,0.1471896192,0.2541491564
O,0,-5.3393228101,-0.4966539533,-0.8290142495
H,0,-3.2231987049,-1.2874727262,-0.3350779981
H,0,-3.214086226,0.2958363912,-1.2804969383
H,0,-4.9176842596,1.2287885256,0.3146983926
H,0,-4.9265305565,-0.3104721726,1.2344530912
O,0,-2.0275634649,0.3518554641,0.6247332338
C,0,-0.917272001,0.0451916296,0.1046529611
O,0,-0.6861341728,-0.5686420065,-0.9250101856
O,0,0.1390310116,0.5190759761,0.8823024577
C,0,1.4180305067,0.2430988952,0.4401875251
C,0,2.1352939777,1.2365633435,-0.2070882058
C,0,3.4461556914,0.9976514468,-0.6004007311
C,0,3.9974446316,-0.2390290354,-0.3322588862
C,0,3.2993265182,-1.2422938615,0.3122661607
C,0,1.9918401309,-0.9920562995,0.70379839
F,0,5.2707398852,-0.4778188535,-0.7119822936
H,0,1.6653412165,2.1925306301,-0.3984573321
H,0,4.0332074762,1.7529507001,-1.1056184835
H,0,3.775717733,-2.1949132872,0.5019957111
H,0,1.4115656759,-1.751691608,1.2115739911

Anions

Methyl carbonate

E (total electronic) = -303.843913
E (total electronic) + ZPVE = -303.789133
Internal Thermal Energy = -303.784207
Enthalpy = -303.783263
Gibbs Free Energy = -303.817177

O,0,-1.6660098184,-0.6251763497,-0.000000429
C,0,-0.6214428614,0.0488802315,0.0000005687
O,0,-0.4740927388,1.2823272653,0.0000045724
O,0,0.5359883788,-0.7320660228,-0.0000026077
C,0,1.7649156323,-0.0267095819,-0.000000838
H,0,2.5512601169,-0.7798053938,-0.0000042718
H,0,1.8603188144,0.6020360346,0.8860548849
H,0,1.8603174763,0.602042817,-0.8860518795

Ethyl carbonate

E (total electronic) = -343.1522899
E (total electronic) + ZPVE = -343.069147
Internal Thermal Energy = -343.062931

Enthalpy = -343.061987
Gibbs Free Energy = -343.099470

O,0,-1.6805620534,-0.6026918958,-0.0000141345
C,0,-0.628739427,0.0608490395,0.0000147544
O,0,-0.4717000365,1.2934589373,-0.0000049646
O,0,0.5197507168,-0.7315545117,0.0000063662
C,0,1.7670095999,-0.0486586101,0.0000011167
H,0,1.8364012156,0.5931706564,0.8810310461
H,0,1.8363925843,0.5931763612,-0.881025394
C,0,2.8642619021,-1.0913645046,-0.0000077245
H,0,3.8416243822,-0.6070438872,-0.0000107415
H,0,2.7937383629,-1.7249645008,0.8852504741
H,0,2.793729933,-1.7249586842,-0.8852694083

Isopropyl carbonate

E (total electronic) = -382.4613476
E (total electronic) + ZPVE = -382.350251
Internal Thermal Energy = -382.342801
Enthalpy = -382.341856
Gibbs Free Energy = -382.382067

O,0,-2.7822346933,-0.6347685264,-0.5442163923
C,0,-1.7443189625,0.0253867426,-0.7311441075
O,0,-1.6171399497,1.1888278294,-1.1474658392
O,0,-0.583419924,-0.6893141896,-0.4252322955
C,0,0.6677380065,-0.0054688558,-0.5140353559
C,0,0.8893007784,0.8502874169,0.7225889491
C,0,1.7353653242,-1.0738990462,-0.6623602798
H,0,0.6528943542,0.6319920432,-1.3993377267
H,0,0.9101841443,0.2183906451,1.6138670615
H,0,1.8410822571,1.3807580313,0.6544476651
H,0,0.0884340969,1.5820346506,0.8242294946
H,0,1.5597799557,-1.6744689948,-1.5556129429
H,0,2.7213522962,-0.6133378672,-0.7411327229
H,0,1.732744316,-1.734743879,0.2073604923

tert-Butyl carbonate

E (total electronic) = -421.7657441
E (total electronic) + ZPVE = -421.627222
Internal Thermal Energy = -421.618388
Enthalpy = -421.617444
Gibbs Free Energy = -421.660563

O,0,-2.5008880202,-0.86949267,0.0000089279
C,0,-1.5369144236,-0.080433652,-0.0000031663
O,0,-1.5464966044,1.1609909001,-0.0000143983
O,0,-0.3094886301,-0.7460680155,-0.000000216
C,0,0.9468027279,-0.0409157942,0.0000005085
C,0,1.1126630188,0.8004852579,-1.2624952381
C,0,1.1126612908,0.8004815888,1.2624987953
C,0,1.9783791179,-1.1654930897,0.000001043
H,0,0.4114657327,1.6311061039,-1.2709564446
H,0,2.13141882,1.1913421203,-1.3092097803
H,0,0.944253992,0.1809155316,-2.1461746322
H,0,0.9442403596,0.1809114229,2.1461757138
H,0,2.1314205667,1.1913281649,1.3092209689
H,0,0.4114717225,1.6311088893,1.2709577476
H,0,1.8565633691,-1.7905387065,-0.8864171434
H,0,2.9882797195,-0.752527962,-0.0000018952
H,0,1.8565662407,-1.79053709,0.8864189457

Phenyl carbonate

E (total electronic) = -495.565359
E (total electronic) + ZPVE = -495.458265
Internal Thermal Energy = -495.450325
Enthalpy = -495.449380
Gibbs Free Energy = -495.493816

O,0,-0.4455274523,-2.8892782707,-2.1802457522
C,0,-0.166109683,-2.1373805202,-1.2417323479
O,0,0.1939768851,-2.3710610171,-0.0850752714
O,0,-0.2810754978,-0.7578019404,-1.6117434142
C,0,-0.0678692669,0.192405664,-0.6462999636
C,0,1.0676514799,0.9872344591,-0.7246889656
C,0,1.2638610804,2.0056952469,0.2017160698
C,0,0.3307279718,2.2275361073,1.2066400721
C,0,-0.8055974651,1.4267391799,1.278438175
C,0,-1.0086452309,0.4119808127,0.3538509723
H,0,1.7854684644,0.8012419419,-1.5140293912
H,0,2.1497456093,2.6252930404,0.1363233065
H,0,0.4844543214,3.0199724189,1.9278921515
H,0,-1.5388084791,1.5955148284,2.057535819
H,0,-1.8882307373,-0.2182159512,0.3977525397

4-Nitrophenyl carbonate

E (total electronic) = -700.0711185

E (total electronic) + ZPVE = -699.961276

Internal Thermal Energy = -699.950862

Enthalpy = -699.949918

Gibbs Free Energy = -699.999699

O,0,-0.5647732015,-3.3356439089,-2.4721305312
C,0,-0.2731783507,-2.7464266698,-1.4350556145
O,0,-0.1581948625,-3.1105773204,-0.2678758577
O,0,0.0229773501,-1.3421563115,-1.7000481936
C,0,0.1434902376,-0.4594063853,-0.6879978016
C,0,1.1616134867,0.4913480129,-0.7930441498
C,0,1.2987902827,1.4771780718,0.1644329062
C,0,0.4089304878,1.4994608598,1.2285956638
C,0,-0.6144977905,0.5680052601,1.3500720267
C,0,-0.748409118,-0.4135953801,0.3887328961
N,0,0.5483289015,2.5333534976,2.2446900079
O,0,-0.2346042418,2.5351387837,3.1783878853
O,0,1.4420397826,3.3517429843,2.1168402892
H,0,1.8370102922,0.4407058455,-1.6365334785
H,0,2.0829264986,2.2172125821,0.0968667547
H,0,-1.2965501065,0.6226671992,2.1862168936
H,0,-1.5372256483,-1.1472451209,0.4604443035

4-Cyanophenyl carbonate

E (total electronic) = -587.8148232

E (total electronic) + ZPVE = -587.708969

Internal Thermal Energy = -587.699318

Enthalpy = -587.698374

Gibbs Free Energy = -587.745525

O,0,-0.6358445485,-4.0984499722,-1.4117970885
C,0,-0.3382661437,-3.2185731771,-0.6063356453
O,0,-0.1567799564,-3.2282082486,0.6094952204
O,0,-0.1424130731,-1.9431223492,-1.2742742273
C,0,-0.0024151417,-0.808322162,-0.5497314429
C,0,1.011499554,0.0715169728,-0.9256129955
C,0,1.1565551929,1.2853838412,-0.2794910147
C,0,0.2839168378,1.6245647551,0.7552024904
C,0,-0.7357194756,0.7453220067,1.1309956225
C,0,-0.8798217238,-0.4648390376,0.4811208682
C,0,0.4306454686,2.8797828209,1.4320821906
N,0,0.5483539855,3.8860711586,1.975146988
H,0,1.6775599996,-0.2117402728,-1.7299473897
H,0,1.9434483519,1.9690884592,-0.5696696986
H,0,-1.4139623252,1.0184847678,1.9288380353
H,0,-1.6648930026,-1.1511855629,0.7636080871

4-Methoxyphenyl carbonate

E (total electronic) = -610.08166

E (total electronic) + ZPVE = -609.941523

Internal Thermal Energy = -609.931150

Enthalpy = -609.930206

Gibbs Free Energy = -609.979054

O,0,-0.2191751761,-3.7779552631,-2.7964856586
C,0,-0.0204920596,-2.9550739493,-1.8964928909
O,0,0.4564539295,-3.0841007869,-0.7648058558
O,0,-0.4225442825,-1.6375069338,-2.2775711555
C,0,-0.2750989351,-0.6323011493,-1.3511654634
C,0,-1.2263188975,-0.4493853619,-0.3513673903
C,0,-1.1036866963,0.598993152,0.5409248073
C,0,-0.0276499197,1.4839905355,0.443992639
C,0,0.9209199818,1.3078666819,-0.5571250521
C,0,0.7888433027,0.2446965824,-1.4498329885
O,0,0.0062436097,2.4851510897,1.3681231348
C,0,1.0935377659,3.3910901265,1.3033114184
H,0,-2.0577247436,-1.1399009449,-0.280002841
H,0,-1.8349958743,0.7526018847,1.3246866705
H,0,1.7612066491,1.9797861935,-0.6578084659
H,0,1.5231491502,0.0973546849,-2.2322210166
H,0,0.9475355795,4.0982754261,2.1150715231
H,0,1.1025424626,3.9260021462,0.3508028471
H,0,2.0450471539,2.871604886,1.4386877384

4-Chlorophenyl carbonate

E (total electronic) = -955.169009

E (total electronic) + ZPVE = -955.071456

Internal Thermal Energy = -955.062372

Enthalpy = -955.061428

Gibbs Free Energy = -955.107791

C,0,2.8115506683,-0.4576431269,0.015063077
O,0,2.3482983774,-1.1503749162,0.9223611821
O,0,1.8682932661,0.3131177121,-0.7531319006
C,0,0.5318337158,0.1316237301,-0.5444848944
C,0,-0.2438353782,1.2452381816,-0.2484829544
C,0,-1.621173297,1.125379977,-0.1112608069
C,0,-2.206143396,-0.1188587443,-0.2670909773
C,0,-1.4458232117,-1.2407583148,-0.5629137169
C,0,-0.0731169256,-1.1121360841,-0.704638807
O,0,3.9670993764,-0.2714593652,-0.3718111091
Cl,0,-3.9414452357,-0.2815975431,-0.0915717825
H,0,0.2383550729,2.2072111478,-0.1309146488
H,0,-2.2296634962,1.9903369024,0.1167470278
H,0,-1.9233286961,-2.2039268787,-0.685082289
H,0,0.5369731593,-1.975056678,-0.9346704

4-Fluorophenyl carbonate

E (total electronic) = -594.8094626

E (total electronic) + ZPVE = -594.710564

Internal Thermal Energy = -594.701878

Enthalpy = -594.700933

Gibbs Free Energy = -594.745961

O,0,-0.1768670211,-3.2480422935,-1.9036915585
C,0,0.0033438511,-2.37488023,-1.0507901145
O,0,0.2513204148,-2.444201271,0.1551234179
O,0,-0.08847373,-1.0570139502,-1.6127893579
C,0,0.0138762776,0.0182016862,-0.7704929845
C,0,1.0912319972,0.881277142,-0.9164654332
C,0,1.1853393457,2.0243349589,-0.1301946444
C,0,0.19095652,2.2696297353,0.7932277495
C,0,-0.8919905939,1.4266493589,0.9593081512
C,0,-0.9783005904,0.2928903853,0.1652697766
F,0,0.2747995124,3.3778450399,1.5638066692
H,0,1.8527685961,0.6543887633,-1.6514773547
H,0,2.0140164203,2.7131225405,-0.2283132877
H,0,-1.6498696021,1.6621974905,1.6949086401
H,0,-1.8121813976,-0.3890283561,0.2688423308

Epoxide

Ethylene oxide

E (total electronic) = -153.7746802
E (total electronic) + ZPVE = -153.716557
Internal Thermal Energy = -153.713422
Enthalpy = -153.712478
Gibbs Free Energy = -153.740625

C,0,-0.7913602504,-0.0089250795,0.0901878759
C,0,0.6288545153,0.1353913882,-0.2345635341
O,0,-0.1976915777,1.2790651123,-0.0411304436
H,0,-1.0782755612,-0.2776509058,1.09962858
H,0,-1.4894329594,-0.2711726981,-0.6955764819
H,0,0.9566452425,-0.0226323364,-1.2549012037
H,0,1.3678055909,-0.0290974809,0.5402932074

M06-2X/6-311+G(3df,2p) IEFPCM, Solvent = Water

Substrates

OEt methyl carbonate

E (total electronic) = -457.6345118
E (total electronic) + ZPVE = -457.518506
Internal Thermal Energy = -457.509791
Enthalpy = -457.508847
Gibbs Free Energy = -457.553097

O,0,2.1742425694,-0.1135971552,0.6685767164
C,0,0.9443496016,0.35740357,0.6637844945
O,0,-0.0691065536,-0.2944089361,0.6613679398
O,0,0.9927144349,1.6868208066,0.6619882607
C,0,-0.2752903296,2.3441781217,0.6567960855
C,0,2.3147855145,-1.5523314231,0.6711638412
C,0,3.8014931922,-1.9052946307,0.6766372537
O,0,3.9888417422,-3.2502360309,0.6792421007
H,0,-0.0568582965,3.4062550426,0.6559607206
H,0,-0.8433821151,2.0748469661,1.5443416823
H,0,-0.8374581088,2.0722301041,-0.2337185946
H,0,1.825188467,-1.9529163599,-0.2175634897
H,0,1.81927346,-1.9503015533,1.5577852198
H,0,4.237361647,-1.381818258,1.5577562771
H,0,4.2432287745,-1.3844112641,-0.2030955083

OEt ethyl carbonate

E (total electronic) = -496.9444579
E (total electronic) + ZPVE = -496.800201
Internal Thermal Energy = -496.790189
Enthalpy = -496.789245
Gibbs Free Energy = -496.836710

O,0,0.1610081258,-0.4921518017,-0.000008532
C,0,-1.0029076586,0.126710435,-0.000009725
O,0,-1.1722445268,1.3201325537,0.000009886
O,0,-1.9741614253,-0.7807764947,-0.0000080384
C,0,-3.3137945616,-0.2603631825,-0.0000025577
C,0,1.3368951891,0.347875186,-0.0000036896
C,0,2.5830581338,-0.5364198404,-0.0000136689
O,0,3.7153945088,0.2135522527,-0.000011143
H,0,-3.4446249186,0.3636585565,-0.8835467557
H,0,-3.4446230893,0.3636449165,0.8835515572
H,0,1.3140636261,0.9822529915,0.8873547506
H,0,1.3140601975,0.9822680662,-0.8873512097
H,0,2.4815652523,-1.2107825541,-0.8804005675
H,0,2.4815701259,-1.2107956363,0.8803637497
C,0,-4.2562914838,-1.4388532701,-0.0000105595
H,0,-4.1042955867,-2.0538831688,0.885761747

H,0,-5.2845021823,-1.0803753697,-0.0000072111
H,0,-4.1042968061,-2.0538702099,-0.885792065

OEt isopropyl carbonate

E (total electronic) = -536.2553548
E (total electronic) + ZPVE = -536.083075
Internal Thermal Energy = -536.071822
Enthalpy = -536.070878
Gibbs Free Energy = -536.120980

O,0,0.3488692157,-0.9038479859,0.0610983331
C,0,0.3549998807,0.381400582,0.3600642003
O,0,0.4594669664,0.8465360143,1.4674418435
O,0,0.2203987072,1.0817336463,-0.7611995491
C,0,0.2417346525,2.5234220062,-0.6400872773
C,0,0.4867296448,-1.8221046686,1.1678247942
C,0,0.465013652,-3.2547143136,0.6367542437
O,0,0.6004686567,-4.1531899481,1.6466365766
C,0,-0.4358933717,3.0553211195,-1.8842713593
C,0,1.6744825035,3.0005275731,-0.5021941565
H,0,-0.3310757935,2.7863271095,0.2487809212
H,0,-0.3358197949,-1.657090602,1.8653643765
H,0,1.4281943403,-1.6150744038,1.678665698
H,0,1.2666574293,-3.3094803841,-0.1342756004
H,0,-0.4827220174,-3.3552596901,0.0606945831
H,0,-1.454472098,2.6786941204,-1.9624839863
H,0,-0.4683418679,4.1433119441,-1.8446756424
H,0,0.1201596119,2.757636933,-2.773764943
H,0,2.1441024856,2.5710185527,0.3807412005
H,0,2.2477705834,2.7184352109,-1.386123095
H,0,1.6920906131,4.0861671845,-0.4099061614

OEt tert-butyl carbonate

E (total electronic) = -575.5627856
E (total electronic) + ZPVE = -575.363120
Internal Thermal Energy = -575.350463
Enthalpy = -575.349519
Gibbs Free Energy = -575.403094

O,0,0.1713731414,-0.4167066488,-0.0219368704
C,0,-0.9637076582,0.2630607417,-0.0182867533
O,0,-1.0526225542,1.4651095555,-0.0169254725
O,0,-1.9662440179,-0.606038279,-0.0159332902
C,0,-3.3541211886,-0.1504639206,-0.0008848324
C,0,1.3874094409,0.360530703,-0.0196774769
C,0,2.5853293428,-0.5873548255,0.0208273512
O,0,3.7564847283,0.100330639,0.0325536219
H,0,1.3860727397,1.0146026459,0.8534482941
H,0,1.4130476788,0.97691428,-0.9198698456
H,0,2.4662727552,-1.2714715251,-0.8499567793
H,0,2.4299484332,-1.2395177866,0.910171926
C,0,-3.6338031106,0.6368761797,1.2716992645
H,0,-3.1011178977,1.5839660486,1.278574219
H,0,-4.7036370369,0.8358754646,1.3348762173
H,0,-3.3420161062,0.0527329352,2.1450331857
C,0,-3.6583029463,0.6521245556,-1.2582208918
H,0,-3.3811822132,0.0796645763,-2.1439605545
H,0,-4.7296094645,0.8490894897,-1.2993905707
H,0,-3.1280025006,1.6004989796,-1.2629336908
C,0,-4.1368351089,-1.4547387609,-0.001233785
H,0,-3.8880551375,-2.0471627099,0.8789222136
H,0,-5.2046538811,-1.2404736865,0.0113147762
H,0,-3.9064878179,-2.0356323213,-0.8940045662

OEt phenyl carbonate

E (total electronic) = -649.3562685
E (total electronic) + ZPVE = -649.187991
Internal Thermal Energy = -649.176234
Enthalpy = -649.175290
Gibbs Free Energy = -649.229450

C,0,0.2155082684,-2.6201658064,-1.3916263152
C,0,0.0304923031,-3.224740465,-2.7827567081
O,0,0.2904106136,-4.5570524318,-2.7759051057
O,0,-0.0732943821,-1.2019895238,-1.4547560562
C,0,0.0403517914,-0.5317140965,-0.3334157653
O,0,0.3576488574,-0.9645886713,0.7403880909
O,0,-0.2636764039,0.7563645645,-0.5827509345
C,0,-0.2004621905,1.636674594,0.4939731996
C,0,0.9828462105,2.3078069981,0.7424491951
C,0,1.0230615044,3.2292677572,1.7805299398
C,0,-0.1085386127,3.4668639637,2.550731937
C,0,-1.2867263116,2.781248234,2.2824287016
C,0,-1.3391456339,1.8574202268,1.246999822
H,0,-0.4643418432,-3.0808706497,-0.6739119324
H,0,1.2412879151,-2.750028215,-1.0445370372
H,0,0.6853506383,-2.634515008,-3.4631218891
H,0,-1.0055590173,-2.9625017937,-3.0956957216
H,0,1.8507153366,2.108125129,0.1286772376
H,0,1.9413861921,3.7626005186,1.9852255213
H,0,-0.0729253548,4.1864724565,3.3569855107
H,0,-2.1701336725,2.9651067736,2.8786265053
H,0,-2.2457442083,1.3135524452,1.0188058046

OEt 4-nitrophenyl carbonate

E (total electronic) = -853.8665288

E (total electronic) + ZPVE = -853.695377

Internal Thermal Energy = -853.681194

Enthalpy = -853.680250

Gibbs Free Energy = -853.739639

C,0,-0.0597649017,-3.4255439611,0.9999168458
C,0,-0.1105604116,-4.7796462787,0.294972764
O,0,-0.1766080438,-5.791367101,1.1966608899
O,0,0.019994248,-2.3776386099,-0.0006716927
C,0,0.0639885349,-1.149794441,0.4455075587
O,0,0.0370650376,-0.7837166173,1.5859862882
O,0,0.1648982972,-0.3265948635,-0.6267576676
C,0,0.1453560367,1.0348374382,-0.4241486166
C,0,1.1694343123,1.766824268,-1.0048482955
C,0,1.1615325217,3.1459532488,-0.8983464324
C,0,0.1230009331,3.7473824455,-0.2087972589
C,0,-0.9072352135,3.024625752,0.3710046139
C,0,-0.8967990267,1.6467950049,0.2594579128
N,0,0.1097808568,5.2098678061,-0.0915008334
O,0,1.0153328185,5.8296899169,-0.6056161715
O,0,-0.8058752864,5.7238612606,0.5133716295
H,0,-0.9567543734,-3.2637754055,1.5984123609
H,0,0.8175785616,-3.3547314596,1.6437785819
H,0,0.7828091604,-4.8140567505,-0.3687268626
H,0,-0.975832897,-4.7302513532,-0.4040111456
H,0,1.9579284452,1.2512124733,-1.5336091449
H,0,1.943252839,3.7461480756,-1.3373697084
H,0,-1.7013081582,3.5358216686,0.89286786
H,0,-1.6861077353,1.052054483,0.6939515244

OEt 4-cyanophenyl carbonate

E (total electronic) = -741.6058552

E (total electronic) + ZPVE = -741.438798

Internal Thermal Energy = -741.425330

Enthalpy = -741.424385

Gibbs Free Energy = -741.481446

C,0,0.1013150184,-3.6714656017,-0.8630789881
C,0,0.1736829437,-4.5244495681,-2.1282367404
O,0,0.0764475728,-5.8445620425,-1.8282110459
O,0,0.1968728883,-2.2721013905,-1.2333951121
C,0,0.1219250672,-1.4057722605,-0.2563831762
O,0,-0.0150961337,-1.6328515147,0.9123496719
O,0,0.2418160466,-0.1684141588,-0.7932709384
C,0,0.1102501453,0.9279956442,0.0328341512

C,0,1.1284240006,1.8663864631,-0.0036816815
C,0,1.0104741115,3.0212297989,0.7489349109
C,0,-0.1262982794,3.2188613619,1.5306738204
C,0,-1.1465673524,2.267164013,1.5555332555
C,0,-1.0303784719,1.1155646834,0.8001338372
C,0,-0.2511696345,4.4135665771,2.3142311993
N,0,-0.351272613,5.3697002138,2.9414912692
H,0,-0.8448296065,-3.8270076206,-0.3439461883
H,0,0.9234544747,-3.9060695491,-0.1858858197
H,0,1.1211335214,-4.2387747866,-2.6385835414
H,0,-0.6300511237,-4.1460484331,-2.7994275643
H,0,1.997347214,1.6855580859,-0.6200134481
H,0,1.7939111907,3.7652441614,0.7335217913
H,0,-2.0262651537,2.4344737452,2.1604473228
H,0,-1.8123838259,0.3706661781,0.8030720148

OEt 4-methoxyphenyl carbonate

E (total electronic) = -763.8793685

E (total electronic) + ZPVE = -763.677992

Internal Thermal Energy = -763.663850

Enthalpy = -763.662906

Gibbs Free Energy = -763.721355

C,0,-0.251104497,-3.9559279016,-0.9116158053
C,0,-0.2848779813,-4.8777919718,-2.1293563198
O,0,-0.3341276331,-6.1812513529,-1.7523659652
O,0,-0.2008987671,-2.5807988916,-1.3629179
C,0,-0.1537804988,-1.6608428903,-0.4284203183
O,0,-0.147124677,-1.8377174763,0.7590048606
O,0,-0.1102623258,-0.4569182184,-1.0289296886
C,0,-0.0792132624,0.6631318669,-0.2014510547
C,0,-1.2416717014,1.0991929427,0.417055969
C,0,-1.2080758724,2.2446802796,1.1868769951
C,0,-0.0167840613,2.9590144836,1.3377205887
C,0,1.1416282164,2.5136855698,0.7091587927
C,0,1.1033100637,1.3553084003,-0.0625359176
O,0,-0.0852855015,4.0700390997,2.1087353723
C,0,1.1003269752,4.8220048569,2.2874616956
H,0,-1.144639009,-4.0879644228,-0.3001002239
H,0,0.6302508255,-4.1537736064,-0.3003880892
H,0,0.6067342271,-4.6115188918,-2.7409369098
H,0,-1.152871807,-4.5454379479,-2.7426646796
H,0,-2.1597087444,0.5407342349,0.2927392797
H,0,-2.0988427895,2.6078691832,1.6810346619
H,0,2.073178701,3.0495998015,0.8078367209
H,0,1.9950423418,0.9960071385,-0.5579057661
H,0,0.8370282708,5.6576653981,2.9278514016
H,0,1.4727675696,5.1973652497,1.3325663424
H,0,1.874529938,4.2225800693,2.7698869574

OEt 4-chlorophenyl carbonate

E (total electronic) = -1108.9618893

E (total electronic) + ZPVE = -1108.803177

Internal Thermal Energy = -1108.790286

Enthalpy = -1108.789342

Gibbs Free Energy = -1108.845987

C,0,3.7148445378,-0.2282729241,0.3705058694
C,0,5.0090313266,0.2727216983,-0.2677702085
O,0,6.0925456813,-0.1877580868,0.4077499276
O,0,2.5879135258,0.2985671536,-0.3734739326
C,0,1.3972012873,-0.0232376243,0.0676642612
O,0,1.1340212827,-0.7143477134,1.0124664965
O,0,0.4822150486,0.5670285139,-0.7296986896
C,0,-0.8537687886,0.3343260532,-0.4331546389
C,0,-1.5738546513,1.329669949,0.2005060873
C,0,-2.9254099524,1.1366770943,0.448313807
C,0,-3.5216539583,-0.0514135764,0.0572847025
C,0,-2.7969888676,-1.0487290359,-0.5782454691
C,0,-1.447636576,-0.851663685,-0.8269456149
H,0,3.6658011604,-1.13176647276,0.3485845101
H,0,3.636008374,0.1114527456,1.4037450887

H,0,4.926223109,1.3826938175,-0.2991459913
H,0,4.9679187247,-0.0404780445,-1.3355109424
H,0,-1.0805711815,2.2461613916,0.4930208131
H,0,-3.5084304951,1.9018697415,0.9403933394
H,0,-3.2823480808,-1.9667810859,-0.8769448145
H,0,-0.8590243304,-1.6110268402,-1.3231318843
Cl,0,-5.2122058256,-0.2958183842,0.3659388835

OEt 4-fluorophenyl carbonate

E (total electronic) = -748.603527

E (total electronic) + ZPVE = -748.443392

Internal Thermal Energy = -748.430924

Enthalpy = -748.429980

Gibbs Free Energy = -748.485031

C,0,0.3882034753,-2.1388483931,-2.2443220429
C,0,0.2974844239,-2.4371092714,-3.7397243361
O,0,0.5178523137,-3.7537256049,-3.9870776664
O,0,0.1436963988,-0.7266811159,-2.0301520633
C,0,0.18239166,-0.3102717869,-0.7881001633
O,0,0.3971325358,-0.9689620022,0.1917734235
O,0,-0.0627855447,1.0157571007,-0.7832995818
C,0,-0.0768369496,1.6457875462,0.4558782281
C,0,1.0521636818,2.3295093146,0.8680625255
C,0,1.0305064422,3.0118647281,2.0764733799
C,0,-0.1261498493,2.9799509634,2.8298144505
C,0,-1.259913566,2.3002006573,2.4280142287
C,0,-1.2313896521,1.6227891149,1.2181436522
F,0,-0.1517480946,3.6388817218,3.9995324678
H,0,-0.3584976551,-2.7078536655,-1.6893456049
H,0,1.3793927932,-2.3811993031,-1.8591633122
H,0,1.0208408198,-1.7506378572,-4.2350343615
H,0,-0.7023776008,-2.0710871537,-4.065749721
H,0,1.9365261922,2.3284108355,0.246175732
H,0,1.8918467386,3.5596966975,2.4311274393
H,0,-2.1428339944,2.306237324,3.0511125876
H,0,-2.0976275688,1.0800601497,0.8656077379

Transition states

TS-OEt methyl carbonate

E (total electronic) = -457.5982785

E (total electronic) + ZPVE = -457.484714

Internal Thermal Energy = -457.475816

Enthalpy = -457.474872

Gibbs Free Energy = -457.520519

O,0,0.0139493012,-0.7226109878,-0.0000014443
C,0,-1.0117291301,0.0229262141,0.0000009406
O,0,-1.0569726956,1.2482149166,0.0000079011
O,0,-2.168963291,-0.7048322849,-0.0000055292
C,0,-3.3746516688,0.0443432529,-0.0000033177
C,0,1.6484314858,0.2538080506,0.0000017156
C,0,2.7680763893,-0.6734544797,-0.0000065256
O,0,3.5075642053,0.5022873422,-0.0000006548
H,0,-4.1827575756,-0.6817233861,-0.0000100331
H,0,-3.4423618518,0.6734605677,-0.8863960467
H,0,-3.4423660069,0.6734486964,0.8863975359
H,0,1.4203557464,0.7610964588,0.921214272
H,0,1.4203519534,0.7611082082,-0.921203427
H,0,2.8667835164,-1.2972728956,-0.8959548479
H,0,2.8667873718,-1.2972842935,0.8959334386

TS-OEt ethyl carbonate

E (total electronic) = -496.9078249

E (total electronic) + ZPVE = -496.766046

Internal Thermal Energy = -496.755821

Enthalpy = -496.754877

Gibbs Free Energy = -496.803917

O,0,-0.9440349595,-0.6158563746,-0.0108435135
C,0,0.0225564439,0.2055099403,-0.0189545866
O,0,-0.0277669065,1.4310272073,-0.033426476
O,0,1.2309655508,-0.4318826538,-0.0085774618
C,0,2.3884039284,0.4005614481,-0.0165699781
C,0,3.6024046084,-0.5001050829,0.0142123893
H,0,2.3641862744,1.0623630891,0.8500665875
H,0,2.3796606194,1.0236411084,-0.9119409448
H,0,4.5100456393,0.102386874,0.0081494376
H,0,3.6029404266,-1.1151321276,0.9136154642
H,0,3.618276311,-1.1562401106,-0.8554850009
C,0,-2.651510358,0.2278942064,0.0197426247
C,0,-3.6934125171,-0.7857421754,0.0238511998
O,0,-4.5227800688,0.3281925954,0.0519822317
H,0,-2.4779223828,0.7620419681,-0.8980817061
H,0,-2.450205488,0.7402197482,0.9443305841
H,0,-3.7272351384,-1.4273554466,0.9120087474
H,0,-3.757271983,-1.403606214,-0.8793745987

TS-OEt isopropyl carbonate

E (total electronic) = -536.2182507

E (total electronic) + ZPVE = -536.048527

Internal Thermal Energy = -536.037089

Enthalpy = -536.036145

Gibbs Free Energy = -536.087311

O,0,0.4496761082,-1.1035119911,-0.5839850837
C,0,0.5041525705,0.1420662189,-0.3476034082
O,0,1.0747522498,0.7061664505,0.58013274
O,0,-0.1874045481,0.8625731409,-1.2814164016
C,0,-0.155044909,2.2917414527,-1.1787518152
C,0,1.3994582081,-2.159497135,0.6890377804
C,0,1.2679932562,-3.5645165813,0.3414198156
O,0,2.0565687035,-3.7282697292,1.4732743508
C,0,1.1468828343,2.8246073093,-1.7515238247
C,0,-1.3651634782,2.8025714569,-1.9356617137
H,0,-0.2304781846,2.5594495732,-0.1247377009
H,0,0.8219943572,-1.7938630596,1.5200860068
H,0,2.3395108215,-1.6787505568,0.4810567649
H,0,1.7288771077,-3.8639944406,-0.6069401195
H,0,0.2539560247,-3.9759328496,0.4043426914
H,0,1.1784189161,3.9112194331,-1.6673424329
H,0,1.9986896648,2.4096294767,-1.2156357227
H,0,1.2254962568,2.5575831285,-2.8067903947
H,0,-1.3056561132,2.5099783542,-2.9849942134
H,0,-2.2845852831,2.3996159028,-1.5127373423
H,0,-1.4052935636,3.8902900238,-1.8832129765

TS-OEt tert-butyl carbonate

E (total electronic) = -575.5245467

E (total electronic) + ZPVE = -575.327337

Internal Thermal Energy = -575.314500

Enthalpy = -575.313556

Gibbs Free Energy = -575.367999

O,0,1.1142993851,0.7351301474,0.0000007793
C,0,0.0984085285,-0.0284317043,0.0000021268
O,0,0.0913489623,-1.2546505379,0.0000030915
O,0,-1.0595048112,0.6961314927,0.0000024374
C,0,-2.3582728558,0.0612205367,0.0000032949
C,0,-3.3209626499,1.2428430086,0.0000031473
C,0,-2.5599573531,-0.7684880056,1.2632503295
C,0,-2.5599583584,-0.768489155,-1.2632428237
H,0,-3.1646042866,1.8586849956,-0.8859224647
H,0,-3.1646035958,1.8586857803,0.8859280929
H,0,-4.3505359706,0.8857573059,0.0000037098
H,0,-1.9073754599,-1.6366714105,1.2702350569
H,0,-2.3553163164,-0.1591524124,2.1448328213

H,0,-3.596883439,-1.1030633356,1.3127866798
H,0,-3.5968844098,-1.1030647741,-1.3127779208
H,0,-2.3553182808,-0.1591542889,-2.1448260411
H,0,-1.9073762692,-1.6366724191,-1.2702273958
C,0,2.7731657969,-0.2141130168,0.0000002184
C,0,3.8714729104,0.737165554,-0.00000185
O,0,4.6290266351,-0.4278617799,-0.0000013251
H,0,2.5508874213,-0.7231033093,-0.9213994092
H,0,2.5508891787,-0.7231013359,0.921401363
H,0,3.960072431,1.3618377416,0.8961927142
H,0,3.9600707069,1.3618358222,-0.8961979217

TS-OEt phenyl carbonate

E (total electronic) = -649.3230608
E (total electronic) + ZPVE = -649.157280
Internal Thermal Energy = -649.145355
Enthalpy = -649.144411
Gibbs Free Energy = -649.198973

C,0,0.2599273146,-3.3178539667,-0.8580738055
C,0,0.2077510045,-4.1216497155,-2.0702364239
O,0,0.2910931753,-5.1815588954,-1.1791594656
O,0,0.181074235,-1.4840641606,-1.3066925044
C,0,0.19159261,-0.7240755164,-0.2988135397
O,0,0.2597533802,-1.0094699227,0.8840935383
O,0,0.1248713642,0.6098994259,-0.6893783339
C,0,0.0387363602,1.5757068561,0.2886101936
C,0,1.0694613383,2.4954630451,0.3967052601
C,0,0.97047264,3.5261412024,1.323968605
C,0,-0.1486190168,3.6303049551,2.1386440945
C,0,-1.1754604833,2.6995679309,2.020053042
C,0,-1.0877485658,1.6708117444,1.0939621113
H,0,-0.6266254571,-3.2837699755,-0.248147224
H,0,1.2109286234,-3.2330218688,-0.3606288561
H,0,1.0601772252,-4.0025457778,-2.7497600261
H,0,-0.7264489836,-4.050976736,-2.6402298707
H,0,1.9333517019,2.3986262151,-0.2471140982
H,0,1.7725289732,4.2473171953,1.4079198033
H,0,-0.2232584761,4.4323225633,2.8601796062
H,0,-2.0516387926,2.7765879203,2.650114836
H,0,-1.8791351707,0.9409334814,0.9901140577

TS-OEt 4-nitrophenyl carbonate

E (total electronic) = -853.835803
E (total electronic) + ZPVE = -853.667175
Internal Thermal Energy = -853.652787
Enthalpy = -853.651843
Gibbs Free Energy = -853.712447

C,0,4.4591668631,-0.3454417574,0.2608406409
C,0,5.6938535807,0.2078695099,-0.2785102173
O,0,6.2998152014,-0.7760511825,0.4873542862
O,0,2.9846678642,0.603168107,-0.4148208243
C,0,1.8813363621,0.1653791307,0.003705607
O,0,1.6380066618,-0.7590419524,0.7539923952
O,0,0.8289863403,0.9417386602,-0.5078488055
C,0,-0.4598068165,0.556218465,-0.3030167717
C,0,-0.8979135682,-0.7368436525,-0.5817948911
C,0,-2.2337842931,-1.0507159243,-0.426751636
C,0,-3.1087850922,-0.0632683398,0.0010030819
C,0,-2.6914890477,1.2288847809,0.2737725354
C,0,-1.3525412988,1.5357343141,0.1199391018
N,0,-4.5235565483,-0.3970460173,0.1650046621
O,0,-4.8733988281,-1.5352097683,-0.0674319018
O,0,-5.2800047231,0.4801286791,0.5258603198
H,0,4.13214955,-1.2939281676,-0.1305029122
H,0,4.2303325896,-0.1278985526,1.2904886917
H,0,5.9095080442,1.2419965532,0.0169899676
H,0,5.8138621678,0.1078788767,-1.3642777141

H,0,-0.1938535941,-1.4827936351,-0.9172405142
H,0,-2.6008979875,-2.043268256,-0.638272166
H,0,-3.4022290977,1.9714888191,0.6021199085
H,0,-0.9837609301,2.5311115102,0.3226317565

TS-OEt 4-cyanophenyl carbonate

E (total electronic) = -741.5746707
E (total electronic) + ZPVE = -741.410155
Internal Thermal Energy = -741.396467
Enthalpy = -741.395523
Gibbs Free Energy = -741.454247

C,0,-0.0899659237,-3.8333074777,-1.5190762433
C,0,-0.0932669198,-4.4958350885,-2.8160338677
O,0,-0.2635135658,-5.6472107788,-2.06250565
O,0,0.1298143755,-1.9791887958,-1.7478028879
C,0,0.1123178656,-1.3416878406,-0.661817364
O,0,-0.019433111,-1.7428308982,0.4784321562
O,0,0.3019295873,0.0264369961,-0.9004570713
C,0,0.185391658,0.9122308899,0.1305142666
C,0,1.2055140729,1.8421901175,0.2884256137
C,0,1.1055572127,2.8132512695,1.2680493194
C,0,-0.0189526382,2.8470651579,2.0913087589
C,0,-1.0435633142,1.9128620827,1.9269028705
C,0,-0.9432813625,0.9465589458,0.94428264
C,0,-0.1267207513,3.8485332545,3.1103173147
N,0,-0.213348798,4.6510547046,3.927263345
H,0,-1.034648551,-3.7393327921,-1.0109301794
H,0,0.7923158412,-3.9434547913,-0.911513587
H,0,0.8468534528,-4.428537504,-3.377058505
H,0,-0.929368098,-4.2291085999,-3.4740074174
H,0,2.0673978405,1.7946195801,-0.3621190248
H,0,1.894126217,3.5407934428,1.3989182068
H,0,-1.9152369162,1.951695081,2.5642270997
H,0,-1.7293511738,0.2198840443,0.8037772064

TS-OEt 4-methoxyphenyl carbonate

E (total electronic) = -763.8457457
E (total electronic) + ZPVE = -763.646932
Internal Thermal Energy = -763.632558
Enthalpy = -763.631614
Gibbs Free Energy = -763.691538

C,0,-4.4563135792,-0.0062391775,0.1636771731
C,0,-5.7103058386,-0.2692207044,-0.5262222545
O,0,-6.2688227225,0.1690517443,0.6660218677
H,0,-4.1643627079,1.0224161139,0.2872590574
H,0,-4.1528582392,-0.705583899,0.9237381745
H,0,-5.8954659542,-1.3195557671,-0.780972163
H,0,-5.9053243758,0.3597605622,-1.4030169369
O,0,-3.0008366956,-0.4126698095,-0.9738209092
C,0,-1.8784622815,-0.1769872285,-0.4446614287
O,0,-1.6257674694,0.2473418586,0.6706145725
O,0,-0.8449013183,-0.474852633,-1.3239593955
C,0,0.4468161029,-0.2325758042,-0.8995585753
C,0,0.9581055594,1.0597586056,-0.9121426062
C,0,2.2705007849,1.2826908918,-0.5448876282
C,0,3.08723347,0.2155443282,-0.1640784905
C,0,2.5738079232,-1.0765472446,-0.1554271847
C,0,1.2473069531,-1.2916674116,-0.5234823492
O,0,4.3621346563,0.533612281,0.1758024513
C,0,5.219286943,-0.5212503624,0.5662187768
H,0,0.3202112537,1.8817566693,-1.209040371
H,0,2.6871437295,2.2810039068,-0.5479944531
H,0,3.1843578289,-1.9191072703,0.1320935864
H,0,0.8359443599,-2.2923213772,-0.5207000679
H,0,6.1783159662,-0.0669913435,0.7944442064
H,0,5.3423793902,-1.2456171517,-0.2413045847
H,0,4.836516261,-1.029205777,1.4535405326

TS-OEt 4-chlorophenyl carbonate

E (total electronic) = -1108.929499
E (total electronic) + ZPVE = -1108.773344
Internal Thermal Energy = -1108.760261
Enthalpy = -1108.759317
Gibbs Free Energy = -1108.816648

C,0,0.0416201369,-3.6513389132,-0.7603809808
C,0,0.0636087423,-4.5580679441,-1.8987582247
O,0,-0.0526933321,-5.5366060139,-0.9225654637
O,0,0.1781542376,-1.8690204698,-1.3638143336
C,0,0.1351075692,-1.022026452,-0.4303692377
O,0,0.0253519599,-1.1939841868,0.7703643717
O,0,0.2488535406,0.27201166,-0.9392487702
C,0,0.1459528786,1.3289319627,-0.0683796164
C,0,1.2293880555,2.1829749115,0.0591656648
C,0,1.1359125507,3.304157205,0.8725539876
C,0,-0.0453933737,3.5482489086,1.5520782514
C,0,-1.1346277437,2.6976793362,1.4296475433
C,0,-1.0371518303,1.583725702,0.6117922324
Cl,0,-0.1684652549,4.9485653243,2.5752346087
H,0,-0.9046272529,-3.4940309545,-0.2714070626
H,0,0.9304070376,-3.5958285413,-0.1550573012
H,0,0.9978051585,-4.5668593805,-2.4731836188
H,0,-0.7862190249,-4.4675576896,-2.5860582057
H,0,2.1406898439,1.9686956806,-0.4821476436
H,0,1.9735700935,3.9789456198,0.9773666946
H,0,-2.049614662,2.9072722832,1.9654640918
H,0,-1.8741173299,0.908518952,0.5010240126

TS-OEt 4-fluorophenyl carbonate

E (total electronic) = -748.5706941
E (total electronic) + ZPVE = -748.413053
Internal Thermal Energy = -748.400372
Enthalpy = -748.399428
Gibbs Free Energy = -748.455558

C,0,-3.5097379925,-0.253367084,-0.3951828567
C,0,-4.7448810294,0.1496571355,0.2606631309
O,0,-5.3390863027,-0.4980893002,-0.8127549085
H,0,-3.2291328084,-1.2905206499,-0.3281637793
H,0,-3.2217913189,0.2847475021,-1.2820651828
H,0,-4.9145874552,1.2315786959,0.3173076077
H,0,-4.9216798251,-0.2996885524,1.2452615188
O,0,-2.0275923046,0.3468863265,0.6093668515
C,0,-0.9190724601,0.0398013612,0.0907298707
O,0,-0.6877718976,-0.5785397637,-0.9340172327
O,0,0.1360456191,0.5193860438,0.8624803785
C,0,1.4159095381,0.2451239405,0.431883873
C,0,2.139304816,1.2386348205,-0.2077388028
C,0,3.4522616034,1.000539483,-0.592216121
C,0,4.0013595047,-0.2369977902,-0.3246358515
C,0,3.2971986597,-1.2410796367,0.3115619743
C,0,1.9878283799,-0.9907923923,0.6943143398
F,0,5.2729271366,-0.4747443061,-0.694690334
H,0,1.6722687644,2.1949863907,-0.3995057095
H,0,4.0419320606,1.7572526999,-1.0902146383
H,0,3.7699331891,-2.1943265984,0.5019889053
H,0,1.4043531227,-1.7513983257,1.1950999662

M06-2X/AUG-cc-pVDZ SMD, Solvent = Water

Substrates

OEt methyl carbonate

E (total electronic) = -457.5489088
E (total electronic) + ZPVE = -457.432751
Internal Thermal Energy = -457.424106
Enthalpy = -457.423162
Gibbs Free Energy = -457.466881

O,0,2.1903101853,-0.10337562,0.6686122404
C,0,0.9509380917,0.3661695858,0.6637894619
O,0,-0.0646445671,-0.3015477609,0.6613923911
O,0,0.9941737871,1.6984975736,0.6619744421
C,0,-0.2893505821,2.3474231035,0.6567455588
C,0,2.3170058739,-1.5488193298,0.6711658164
C,0,3.8000078066,-1.8935625935,0.6766155949
O,0,3.9756811287,-3.2773082315,0.6792414596
H,0,-0.0721165627,3.4167252779,0.6558979379
H,0,-0.8505654984,2.0691817137,1.5540475161
H,0,-0.8445779269,2.0665405105,-0.2434537826
H,0,1.8259060381,-1.9435413118,-0.2266040957
H,0,1.8199302931,-1.9408967042,1.5668033241
H,0,4.2503872991,-1.3982255009,1.5644679583
H,0,4.2562986336,-1.4008417124,-0.2096728235

OEt ethyl carbonate

E (total electronic) = -496.8510073
E (total electronic) + ZPVE = -496.706660
Internal Thermal Energy = -496.696652
Enthalpy = -496.695707
Gibbs Free Energy = -496.743043

O,0,-0.1289809314,0.7767403729,-0.7172255018
C,0,-0.1910885002,-0.073400232,0.2995717296
O,0,-0.225997911,0.2291755885,1.4767944994
O,0,-0.2098296222,-1.3163183575,-0.1768020519
C,0,-0.2709188218,-2.3647640884,0.8216033629
C,0,-0.1149058034,2.1834023716,-0.3639363558
C,0,-0.0273126499,2.996561812,-1.6493398265
O,0,-0.0363049885,4.359865887,-1.3591449358
C,0,-0.3081803345,-3.6813211721,0.0856239725
H,0,-1.1705538087,-2.2094428469,1.4265097514
H,0,0.6138175483,-2.2784066637,1.4615216541
H,0,0.751898179,2.3730289964,0.2807312722
H,0,-1.0377689062,2.4142107714,0.1821816866
H,0,-0.8781616561,2.6852345474,-2.2943253469
H,0,0.8929743212,2.6727364248,-2.1830169122
H,0,0.5903569629,-3.8111496347,-0.528406872
H,0,-0.3490330639,-4.4947499166,0.8188559267
H,0,-1.1959380136,-3.7445448601,-0.5540970524

OEt isopropyl carbonate

E (total electronic) = -536.1533452
E (total electronic) + ZPVE = -535.981219
Internal Thermal Energy = -535.970040
Enthalpy = -535.969096
Gibbs Free Energy = -536.018736

O,0,0.3283888522,-0.9111328459,0.0580745277
C,0,0.3346657937,0.3824361561,0.3587991452
O,0,0.4383736619,0.8450124936,1.4786859793
O,0,0.1971986824,1.0823814945,-0.7646025574
C,0,0.2484187298,2.5355587986,-0.640004204
C,0,0.4475815566,-1.8232831841,1.1789818913
C,0,0.5070020484,-3.2409400846,0.6264771247
O,0,0.5943275765,-4.1671721675,1.6654721854
C,0,-0.4499030217,3.0773949828,-1.8677465898
C,0,1.6948914402,2.9751718602,-0.532075222
H,0,-0.3068519152,2.8022325596,0.2650152214
H,0,-0.426142575,-1.6909659376,1.8290640783
H,0,1.3607700896,-1.5795210949,1.7347787355
H,0,1.3742051599,-3.286964075,-0.0681499232
H,0,-0.396002516,-3.3853049687,-0.0065945227

H,0,-1.4879132127,2.7295342687,-1.9114491709
H,0,-0.4493005946,4.1725093053,-1.8260704461
H,0,0.0752389612,2.7613775843,-2.7778350521
H,0,2.183078618,2.5213782269,0.3373768298
H,0,2.2413947245,2.6947248062,-1.4411951664
H,0,1.7333919404,4.0653418214,-0.4219178643

OEt tert-butyl carbonate

E (total electronic) = -575.452584
E (total electronic) + ZPVE = -575.253140
Internal Thermal Energy = -575.240439
Enthalpy = -575.239495
Gibbs Free Energy = -575.292797

O,0,0.1784862019,-0.4414937211,-0.000251785
C,0,-0.9625282847,0.2480078927,0.0000957711
O,0,-1.0380218773,1.4607844558,-0.000402735
O,0,-1.9695057661,-0.6179844917,0.0010598178
C,0,-3.3678196591,-0.1457930616,0.0016647206
C,0,1.39063184,0.3521884102,-0.0013109878
C,0,2.5849131072,-0.5920816881,-0.0015795783
O,0,3.7734994721,0.1378579812,-0.0026014713
H,0,1.395560878,0.9854982924,0.8942471607
H,0,1.3945223911,0.9846927975,-0.8974434643
H,0,2.4832488118,-1.2553111032,-0.8883701497
H,0,2.4842824143,-1.254511697,0.8859261556
C,0,-3.6471424658,0.6481185769,1.2699153071
H,0,-3.1311147734,1.6117629044,1.2717129085
H,0,-4.7263483127,0.8313395246,1.3320220257
H,0,-3.3436513278,0.0712523817,2.1517817759
C,0,-3.648616847,0.6470083332,-1.2669551725
H,0,-3.346140468,0.069374848,-2.1486680126
H,0,-4.7278957264,0.8301650463,-1.3279736668
H,0,-3.1326017378,1.6106555618,-1.2701917507
C,0,-4.1503192751,-1.4501371287,0.0026905375
H,0,-3.9118029972,-2.0400478569,0.8956293239
H,0,-5.2232547302,-1.2287010135,0.0032175268
H,0,-3.9128412476,-2.0408289147,-0.8900085669

OEt phenyl carbonate

E (total electronic) = -649.243098
E (total electronic) + ZPVE = -649.074161
Internal Thermal Energy = -649.062653
Enthalpy = -649.061709
Gibbs Free Energy = -649.113299

C,0,0.0793883293,-2.6445018411,-1.3766668116
C,0,0.0841209792,-3.2081419825,-2.7914059001
O,0,0.2017830924,-4.5966519713,-2.7643573449
O,0,-0.0568276882,-1.200569151,-1.4752912284
C,0,0.0023329022,-0.5371152798,-0.3367525175
O,0,0.1480882361,-1.006957197,0.7697669144
O,0,-0.1228684801,0.7784363763,-0.6129594313
C,0,-0.1122866111,1.6523097457,0.4860736993
C,0,1.0133500165,2.4403930932,0.6808339325
C,0,1.0077333423,3.3618881275,1.7297697411
C,0,-0.1087447727,3.4756478041,2.5589623796
C,0,-1.2282947685,2.6689070266,2.3415198838
C,0,-1.2380943612,1.7470724418,1.2950146014
H,0,-0.7676336247,-3.0313761222,-0.797124006
H,0,1.0181986063,-2.8698367168,-0.857371341
H,0,0.9168837963,-2.7128009029,-3.3370801069
H,0,-0.8500029675,-2.8622474499,-3.2859088208
H,0,1.8710135489,2.3330684023,0.0191382702
H,0,1.8805197665,3.9914025286,1.8961402945
H,0,-0.1090207188,4.1960573839,3.3754452829
H,0,-2.1009776696,2.7583970225,2.9865600785
H,0,-2.1001489534,1.109955662,1.1030364303

OEt 4-nitrophenyl carbonate

E (total electronic) = -853.7162814

E (total electronic) + ZPVE = -853.544678
Internal Thermal Energy = -853.530663
Enthalpy = -853.529719
Gibbs Free Energy = -853.587842

C,0,0.1699192374,-3.1020170903,-1.7307061125
C,0,-0.0211981925,-3.5963125532,-3.1579738141
O,0,0.1264877362,-4.9808027297,-3.2171635002
O,0,-0.0313385845,-1.6607557991,-1.7308944017
C,0,0.0463213518,-1.0707517482,-0.5576269855
O,0,0.2710385224,-1.5901004461,0.5100639918
O,0,-0.1533036113,0.2582021488,-0.7529895397
C,0,-0.2336569115,1.0786948898,0.3674177316
C,0,0.5957752859,2.1950987746,0.3834825867
C,0,0.4934643362,3.0949190585,1.4376591247
C,0,-0.437370614,2.8360763829,2.438780262
C,0,-1.2734104354,1.7221212083,2.4257312054
C,0,-1.1713520525,0.8285767389,1.3677668828
N,0,-0.5496715262,3.7820765667,3.5507305161
O,0,0.1760295633,4.7624324046,3.5523324876
O,0,-1.364582916,3.5502001688,4.4279296569
H,0,-0.5681935725,-3.5505590948,-1.0554870192
H,0,1.1834182407,-3.3085294485,-1.3665127749
H,0,0.7108048656,-3.0544091647,-3.7957336511
H,0,-1.0257954608,-3.2534793959,-3.4892813916
H,0,1.3058926655,2.354054654,-0.4247159877
H,0,1.1248356272,3.9777045966,1.4803505137
H,0,-1.9948310511,1.5616571191,3.2220290263
H,0,-1.8166285039,-0.0447722409,1.3141841925

OEt 4-cyanophenyl carbonate

E (total electronic) = -741.4770365
E (total electronic) + ZPVE = -741.309595
Internal Thermal Energy = -741.296297
Enthalpy = -741.295352
Gibbs Free Energy = -741.351267

C,0,0.1570360172,-3.6706933285,-0.8507616365
C,0,0.1066622319,-4.5180493318,-2.114752404
O,0,0.0335367124,-5.871569749,-1.7910168553
O,0,0.1990050979,-2.2740226241,-1.2555965079
C,0,0.1799827683,-1.3918959702,-0.2786175945
O,0,0.1372619705,-1.616874877,0.908598893
O,0,0.2347908641,-0.1575060852,-0.8367042129
C,0,0.1093720221,0.9404230376,0.0143817175
C,0,1.1422266965,1.8699950958,0.0043627344
C,0,1.015286543,3.0214543422,0.7738033509
C,0,-0.1422232731,3.2114487391,1.5374361036
C,0,-1.1761042708,2.2649941821,1.5361831595
C,0,-1.0509893691,1.1180011956,0.7632205874
C,0,-0.2750654968,4.4019864209,2.3321044289
N,0,-0.3805634141,5.3631643562,2.97278307
H,0,-0.7389324005,-3.8235087043,-0.2377483357
H,0,1.0550621979,-3.8853885497,-0.2591328293
H,0,1.0052026873,-4.2644012703,-2.7185055806
H,0,-0.7665885649,-4.1668802596,-2.7069866256
H,0,2.0261762589,1.6917027993,-0.6039796912
H,0,1.8057663062,3.7686918144,0.7850016102
H,0,-2.0706169833,2.4344046013,2.1315901558
H,0,-1.8435426016,0.3734181653,0.7334454621

OEt 4-methoxyphenyl carbonate

E (total electronic) = -763.7410282
E (total electronic) + ZPVE = -763.539250
Internal Thermal Energy = -763.525269
Enthalpy = -763.524325
Gibbs Free Energy = -763.581564

C,0,-0.3171999988,-3.9710143292,-0.9243495834
C,0,-0.2667766147,-4.8649586911,-2.1562054203

O,0,-0.3982770405,-6.2044451453,-1.7946400994
O,0,-0.19191765,-2.5942197474,-1.3719075484
C,0,-0.1648402591,-1.6778963666,-0.4228271407
O,0,-0.2326335698,-1.8700071533,0.7709333324
O,0,-0.041735644,-0.470994951,-1.0139595766
C,0,-0.031767999,0.6510208405,-0.1692463657
C,0,-1.2024226128,1.0524681847,0.4696469835
C,0,-1.1851674239,2.2069419649,1.2395496838
C,0,-0.0059061727,2.9562242972,1.3600893178
C,0,1.1606453295,2.5441619181,0.7110576271
C,0,1.1406661167,1.3766474502,-0.0585710382
O,0,-0.093085356,4.0806811412,2.1326922956
C,0,1.0874156862,4.8690417811,2.2578802025
H,0,-1.2728376447,-4.0760089296,-0.3964803481
H,0,0.5108205048,-4.1909626625,-0.2401427292
H,0,0.6910921726,-4.6485692869,-2.6780478075
H,0,-1.0705094917,-4.520928744,-2.8435397173
H,0,-2.1130447737,0.4655977478,0.360589547
H,0,-2.0837246334,2.5471477005,1.7513634248
H,0,2.0841961287,3.1104773059,0.7887133969
H,0,2.0376293614,1.0398910503,-0.5750813058
H,0,0.8182007651,5.712639432,2.8973257486
H,0,1.4136571168,5.2360647831,1.276000273
H,0,1.893051703,4.2899174092,2.7274978473

OEt 4-chlorophenyl carbonate

E (total electronic) = -1108.8368282
E (total electronic) + ZPVE = -1108.677641
Internal Thermal Energy = -1108.664797
Enthalpy = -1108.663853
Gibbs Free Energy = -1108.719617

C,0,3.7128188295,-0.2564930534,0.3837101664
C,0,5.0045732529,0.2565738122,-0.2369381702
O,0,6.1077991793,-0.2546397867,0.4451969607
O,0,2.6016133655,0.3058386373,-0.3676263473
C,0,1.3986253286,-0.0080845996,0.0692289191
O,0,1.1294042757,-0.7079313581,1.0193770421
O,0,0.4918327126,0.5959499401,-0.7319133561
C,0,-0.8565968727,0.3534854477,-0.4378157073
C,0,-1.5959400271,1.3781776046,0.1356873399
C,0,-2.9558254793,1.1795730004,0.3730204931
C,0,-3.5254696159,-0.0426575681,0.0298117485
C,0,-2.7813579892,-1.0708459174,-0.5442222663
C,0,-1.4243018303,-0.8667186902,-0.783093148
H,0,3.6492319782,-1.3496267742,0.3224531717
H,0,3.6206533193,0.0634333284,1.4283301789
H,0,4.9598214632,1.3674518667,-0.2164160063
H,0,4.9894916613,-0.0286403433,-1.3115855054
H,0,-1.1156423889,2.3210501547,0.3898267998
H,0,-3.5598729016,1.9667109758,0.819186087
H,0,-3.2526251754,-2.015904001,-0.8053596955
H,0,-0.811847731,-1.6459200604,-1.2335542114
Cl,0,-5.2345540047,-0.2968097865,0.3248471066

OEt 4-fluorophenyl carbonate

E (total electronic) = -748.4668483
E (total electronic) + ZPVE = -748.306175
Internal Thermal Energy = -748.293813
Enthalpy = -748.292869
Gibbs Free Energy = -748.346657

C,0,0.0952599243,-2.6759305029,-1.5884012754
C,0,-0.0429671403,-3.1506380365,-3.0286260012
O,0,0.1985386439,-4.5205279049,-3.1160913228
O,0,-0.1792057985,-1.248186967,-1.5639541133
C,0,-0.0286801749,-0.6525971181,-0.3975296918
O,0,0.3084789512,-1.1692938623,0.6441229706
O,0,-0.3150675456,0.6582504954,-0.5581489626
C,0,-0.2216655627,1.4612191577,0.588153353
C,0,0.8565112845,2.3293283089,0.6914433572
C,0,0.9322946304,3.1852645582,1.7900637646

C,0,-0.0776730714,3.1261921663,2.7377844993
C,0,-1.1586757145,2.2608970653,2.6447915289
C,0,-1.2303393531,1.4110345036,1.5429062895
F,0,-0.0082223484,3.957000514,3.8067807181
H,0,-0.6287032478,-3.1756765515,-0.9333519588
H,0,1.1119059606,-2.8404333999,-1.2126571999
H,0,0.6616681035,-2.5462887648,-3.6408533456
H,0,-1.0623261224,-2.8677316076,-3.371388601
H,0,1.6236508961,2.3379836523,-0.0802878524
H,0,1.7572881322,3.8843873418,1.9106928804
H,0,-1.9257210394,2.2583428708,3.4165379827
H,0,-2.0597364078,0.7161720812,1.4228469806

Transition states

TS-OEt methyl carbonate

E (total electronic) = -457.5091147
E (total electronic) + ZPVE = -457.394823
Internal Thermal Energy = -457.386268
Enthalpy = -457.385324
Gibbs Free Energy = -457.428826

O,0,-0.0112767638,-0.7076679461,0.000006592
C,0,1.0227084827,0.0376405868,0.000009212
O,0,1.0662575905,1.2747470539,-0.0000084674
O,0,2.1813090237,-0.6947216472,0.0000055932
C,0,3.3950148131,0.0618657403,0.000000869
C,0,-1.6795728112,0.2691763704,-0.0000016776
C,0,-2.7550274624,-0.7115186772,0.0000047268
O,0,-3.5480301696,0.456100491,-0.0000049183
H,0,4.2029818661,-0.673799692,0.0000037532
H,0,3.4592508894,0.6884256072,0.8963829362
H,0,3.4592493945,0.6884168968,-0.8963873772
H,0,-1.4511288328,0.7720564068,-0.9330755338
H,0,-1.4511302223,0.7720707687,0.9330648023
H,0,-2.8399043706,-1.3295963148,0.9047381823
H,0,-2.8399025173,-1.3296099046,-0.9047196219

TS-OEt ethyl carbonate

E (total electronic) = -496.8109094
E (total electronic) + ZPVE = -496.668787
Internal Thermal Energy = 496.658666
Enthalpy = -496.657721
Gibbs Free Energy = -496.705832

O,0,-0.4977493995,-0.651467006,-0.0024740712
C,0,0.4719888519,0.1777214803,0.0047164063
O,0,0.408014814,1.4144886988,0.0094604318
O,0,1.685698936,-0.4536466169,0.0069709328
C,0,2.8477067877,0.3951048433,0.0150064664
C,0,-2.2312274902,0.2101105046,-0.0058797877
C,0,-3.2554925523,-0.8252059705,-0.0141316859
O,0,-4.1037408447,0.3031673444,-0.0129450304
C,0,4.0640408351,-0.5007992036,0.0162011215
H,0,2.8190044909,1.029773129,0.9085112902
H,0,2.8260639475,1.0369806413,-0.8735347547
H,0,-2.027903638,0.7287434275,-0.9358952025
H,0,-2.0353162729,0.7212069081,0.9298811536
H,0,-3.3146400487,-1.4499375606,0.8879478202
H,0,-3.307448996,-1.4426287898,-0.9216695784
H,0,4.9678902975,0.1197987016,0.0222955851
H,0,4.0766173144,-1.1407667039,0.9066177169
H,0,4.0836958173,-1.1335380576,-0.879239284

TS-OEt isopropyl carbonate

E (total electronic) = -536.1126856
E (total electronic) + ZPVE = -535.943080
Internal Thermal Energy = -535.931584

Enthalpy = -535.930640

Gibbs Free Energy = -535.981725

O,0,0.8561773242,-0.6985355917,0.1283531377
C,0,0.1466575773,-0.0055185289,-0.2506355911
O,0,0.1260095164,1.0900889368,-0.8274083797
O,0,1.3308000187,-0.6247045519,0.0442177359
C,0,2.5543271215,0.0905907383,-0.2499641971
C,0,-2.5563682426,0.183748679,-0.1497419478
C,0,-3.5854845623,-0.6478429862,0.4574107167
O,0,-4.4153016283,0.3901630588,-0.0175981035
C,0,2.80047297,1.1499676942,0.8090938255
C,0,3.6510282957,-0.9550456537,-0.2895366584
H,0,2.44354047,0.5554785807,-1.2356521934
H,0,-2.4568240761,0.1633909676,-1.229131566
H,0,-2.2432160267,1.0730796079,0.3852720043
H,0,-3.5415823505,-0.7419284872,1.5515270582
H,0,-3.7523614097,-1.6271052228,-0.0125189878
H,0,3.7201055176,1.6991777979,0.5727751877
H,0,1.9712990154,1.8642333548,0.8525860629
H,0,2.9191040646,0.6772803618,1.7927967724
H,0,3.7458321714,-1.4483852632,0.6864178663
H,0,3.4399870181,-1.7127509432,-1.0528934409
H,0,4.6063309138,-0.4740997492,-0.5302311618

TS-OEt tert-butyl carbonate

E (total electronic) = -575.4106496

E (total electronic) + ZPVE = -575.213598

Internal Thermal Energy = -575.200695

Enthalpy = -575.199751

Gibbs Free Energy = -575.254259

O,0,1.1347647171,0.7279568785,-0.0139245156
C,0,0.112307413,-0.0403016892,-0.0052429143
O,0,0.1158254015,-1.2773082114,0.0131198958
O,0,-1.0469128861,0.6825332761,-0.0193163244
C,0,-2.3578661498,0.036214457,-0.0100110596
C,0,-3.3121213573,1.2243409687,-0.0149981964
C,0,-2.5515216172,-0.7790108772,1.26356523
C,0,-2.5566402345,-0.7959970668,-1.2711806369
H,0,-3.1496611186,1.8418757185,-0.9068202628
H,0,-3.1581433995,1.8430013868,0.8776365374
H,0,-4.3478306642,0.8664201219,-0.0195950833
H,0,-1.9541165108,-1.6941052683,1.260502867
H,0,-2.283719593,-0.1758193942,2.1400326428
H,0,-3.610022445,-1.0543136088,1.3470914916
H,0,-3.6057359527,-1.1124024611,-1.3221703632
H,0,-2.3360720711,-0.1913753826,-2.1596374581
H,0,-1.9250807455,-1.6880338284,-1.2758637793
C,0,2.8284615118,-0.2201282296,0.0161704073
C,0,3.8862168674,0.7792274291,0.0020009901
O,0,4.6922224357,-0.3795756966,0.0320616299
H,0,2.6115193109,-0.7444642735,-0.9074219161
H,0,2.5992101154,-0.7048253577,0.9582869868
H,0,3.9579704634,1.4167026105,0.8941082285
H,0,3.9699866091,1.3782392986,-0.915352797

TS-OEt phenyl carbonate

E (total electronic) = -649.2061474

E (total electronic) + ZPVE = -649.039436

Internal Thermal Energy = -649.027755

Enthalpy = -649.026811

Gibbs Free Energy = -649.079198

C,0,-3.3479026709,0.192479249,0.3070486077
C,0,-4.5316007026,-0.2874704242,-0.3935691278
O,0,-5.1941622892,0.4134029159,0.6359654939
O,0,-1.8050978175,-0.4352727556,-0.6511342684
C,0,-0.7072461762,-0.1173986011,-0.1002558534
O,0,-0.5184890724,0.4853841838,0.9573462313

O,0,0.3756245432,-0.5504116442,-0.8600701491
C,0,1.648927789,-0.2296769832,-0.3875757142
C,0,2.4065314479,-1.2267915684,0.2161747476
C,0,3.7072486981,-0.9307742207,0.6287971052
C,0,4.2314805855,0.3485964258,0.438962554
C,0,3.4533991692,1.3378356078,-0.1677873613
C,0,2.154571631,1.0517913256,-0.5873266523
H,0,-3.0728234858,1.2340356641,0.1810104069
H,0,-3.0658020373,-0.3107341659,1.2253894153
H,0,-4.6814352332,-1.3764026129,-0.3833674767
H,0,-4.6860476605,0.11698836,-1.4039014974
H,0,1.9797508859,-2.2189935384,0.3545671145
H,0,4.3110372046,-1.7049765109,1.1002324847
H,0,3.8596286245,2.3370642728,-0.3188593827
H,0,1.531655348,1.8074496538,-1.0641445454
H,0,5.2464136187,0.5754574072,0.7618009476

TS-OEt 4-nitrophenyl carbonate

E (total electronic) = -853.6809747

E (total electronic) + ZPVE = -853.511586

Internal Thermal Energy = -853.497401

Enthalpy = -853.496457

Gibbs Free Energy = -853.555492

C,0,4.4419368831,-0.3571257486,0.3467668335
C,0,5.6687053568,0.1025061934,-0.2919257041
O,0,6.2625315606,-0.8347697751,0.5786462895
O,0,2.9811934371,0.6083987716,-0.4274508369
C,0,1.8523957941,0.2300912317,0.0032718557
O,0,1.5821045038,-0.6172300244,0.8505971721
O,0,0.8235629908,0.9539095373,-0.6143184767
C,0,-0.4815611404,0.5755451361,-0.3721497562
C,0,-0.9227549246,-0.7121762535,-0.6859016674
C,0,-2.2612215221,-1.0313366685,-0.5082549488
C,0,-3.122053789,-0.0473815629,-0.0242426468
C,0,-2.6954444808,1.240514771,0.2860739476
C,0,-1.3525843441,1.5514473473,0.1092801327
N,0,-4.5335761133,-0.3804160253,0.1560834702
O,0,-4.9030569586,-1.5109110606,-0.1179804405
O,0,-5.2870987374,0.4846238595,0.5729859171
H,0,4.0489454156,-1.3226512162,0.0471992714
H,0,4.2328629051,-0.0019966634,1.3501366226
H,0,5.9401533847,1.1503078509,-0.0998783991
H,0,5.7638596075,-0.1328808878,-1.3615232346
H,0,-0.2229098885,-1.4489686505,-1.0731300485
H,0,-2.6349580102,-2.0231232717,-0.7473330845
H,0,-3.396010756,1.982147406,0.6593996951
H,0,-0.9739398244,2.5456109236,0.3358685966

TS-OEt 4-cyanophenyl carbonate

E (total electronic) = -741.4413024

E (total electronic) + ZPVE = -741.275879

Internal Thermal Energy = -741.262428

Enthalpy = -741.261484

Gibbs Free Energy = -741.318101

C,0,-0.0815128329,-3.8783955797,-1.5187410536
C,0,-0.0448514638,-4.4873970919,-2.8419667874
O,0,-0.1115724381,-5.6821578594,-2.0953080479
O,0,-0.0131904537,-1.9778119468,-1.7577487471
C,0,0.0542905138,-1.3295361208,-0.6718519826
O,0,0.0457659404,-1.7420639371,0.4855959451
O,0,0.1809841043,0.0405172439,-0.9292680311
C,0,0.1203688923,0.9270383797,0.1305020272
C,0,1.1606467356,1.8462132211,0.2489291237
C,0,1.1039119627,2.8171097814,1.2421028575
C,0,0.0045639033,2.8484655129,2.1083926143
C,0,-1.0395516996,1.9211491789,1.9819379921
C,0,-0.9832910535,0.9567651781,0.9848709797
C,0,-0.0581136209,3.8487089308,3.1377146431

N,0,-0.1076143896,4.6570191779,3.9687597316
H,0,-1.0352201304,-3.8460901254,-1.0029486358
H,0,0.8269327878,-3.9047559774,-0.9266770072
H,0,0.8887539525,-4.3441263516,-3.4043580902
H,0,-0.9172855674,-4.2903321654,-3.4810295798
H,0,2.0007657307,1.7979584831,-0.4406799773
H,0,1.9045734916,3.5460018644,1.3487580751
H,0,-1.8899731108,1.9659876893,2.6591658586
H,0,-1.7888142544,0.236413514,0.8621350918

TS-OEt 4-methoxyphenyl carbonate

Not optimized.

TS-OEt 4-chlorophenyl carbonate

E (total electronic) = -1108.8003715
E (total electronic) + ZPVE = -1108.643457
Internal Thermal Energy = -1108.630444
Enthalpy = -1108.629500
Gibbs Free Energy = -1108.686662

C,0,-3.77277946,-0.2026379672,-0.3645941127
C,0,-4.9791522331,0.2307049184,0.3282495718
O,0,-5.6107237041,-0.4472998128,-0.7351835036
H,0,-3.4788465253,-1.2415747829,-0.2638781361
H,0,-3.4873339616,0.3321514433,-1.2641558541
H,0,-5.149905183,1.3162962745,0.3538377951
H,0,-5.1413242482,-0.2119392666,1.3213101123
O,0,-2.265355865,0.447770543,0.6274587313
C,0,-1.1494874989,0.0982662307,0.1372315673
O,0,-0.9184527501,-0.6314515641,-0.8270145644
O,0,-0.0943753908,0.676294056,0.8428700728
C,0,1.194998371,0.3423646217,0.4387444928
C,0,1.9402472328,1.2881050527,-0.2557701265
C,0,3.2581014152,0.9984268925,-0.6094906914
C,0,3.7900218272,-0.2383838104,-0.2597033085
C,0,3.0484316353,-1.1901430689,0.4361643054
C,0,1.7347595684,-0.8915590765,0.7903973074
H,0,1.4934019359,2.2465753887,-0.5134578435
H,0,3.8591000595,1.7265034016,-1.1501338472
H,0,3.4897379418,-2.1488870987,0.7001820336
H,0,1.1294159263,-1.6122560201,1.3376589584
Cl,0,5.4452932968,-0.611146025,-0.7052237201

TS-OEt 4-fluorophenyl carbonate

E (total electronic) = -748.4300855
E (total electronic) + ZPVE = -748.271759
Internal Thermal Energy = -748.259181
Enthalpy = -748.258237
Gibbs Free Energy = -748.313363

C,0,-3.7774900148,-0.247482032,-0.3410108504
C,0,-4.9760794896,0.2387387358,0.3292574719
O,0,-5.6181361844,-0.5121905128,-0.6776304542
H,0,-3.4845328044,-1.2772039507,-0.1680740443
H,0,-3.4958590172,0.2213876519,-1.2777970133
H,0,-5.1443355291,1.3237508711,0.277437545
H,0,-5.1316489675,-0.1305409304,1.3528302737
O,0,-2.2616821876,0.4675170699,0.5972847342
C,0,-1.1465279948,0.1063681189,0.1130070369
O,0,-0.919819516,-0.6631623492,-0.8211046372
O,0,-0.092124554,0.7260260352,0.7806619657
C,0,1.2019005374,0.3723873925,0.404089026
C,0,1.9814207806,1.320048195,-0.2494326951
C,0,3.3072132843,1.0193635863,-0.5649405286
C,0,3.7968090546,-0.2287961593,-0.2152019728
C,0,3.0324814608,-1.1882254479,0.433957881
C,0,1.7120135586,-0.8765390567,0.7502982411
F,0,5.0860565639,-0.5273675426,-0.5190115971
H,0,1.5548263779,2.2888358396,-0.5026678873

H,0,3.9488373741,1.7379550811,-1.0710869985
H,0,3.4667634041,-2.1530892794,0.6884019324
H,0,1.0769325832,-1.5969826363,1.2630976107

M06-2X/6-311+G(2d,p) **SMD, Solvent = Water**

Substrates

OEt methyl carbonate

E (total electronic) = -457.6278257
E (total electronic) + ZPVE = -457.511119
Internal Thermal Energy = -457.502522
Enthalpy = -457.501578
Gibbs Free Energy = -457.545166

O,0,2.1892943513,-0.1022385634,0.6686095466
C,0,0.9540182085,0.3668045837,0.6638056783
O,0,-0.0562764929,-0.298007113,0.6614194278
O,0,0.9947789064,1.6953624205,0.6619833798
C,0,-0.2872698172,2.3425437143,0.6567583041
C,0,2.3159278953,-1.5453974599,0.6711561059
C,0,3.7960279438,-1.8905936282,0.6765974586
O,0,3.9701973814,-3.2732280836,0.6792127803
H,0,-0.074114478,3.406902057,0.6559010265
H,0,-0.8463834977,2.0667274161,1.5486793904
H,0,-0.8404296877,2.0640960293,-0.2380528389
H,0,1.8270375134,-1.9399759268,-0.2207519041
H,0,1.8210993884,-1.9373529964,1.5609434618
H,0,4.2448004542,-1.3983147743,1.5587364375
H,0,4.2506759304,-1.4009086755,-0.203975255

OEt ethyl carbonate

E (total electronic) = -496.9372225
E (total electronic) + ZPVE = -496.792271
Internal Thermal Energy = -496.782297
Enthalpy = -496.781352
Gibbs Free Energy = -496.828647

O,0,0.0501529839,-0.9949518501,-0.3340631266
C,0,0.1248725774,0.1903343553,0.2486753853
O,0,0.243522317,0.385903475,1.436853818
O,0,0.0481717557,1.1359912162,-0.6797659956
C,0,0.1216189195,2.4959297716,-0.1912303327
C,0,0.106163786,-2.1386803172,0.5525208597
C,0,0.0194396489,-3.4010679198,-0.2910829139
O,0,0.0455329523,-4.5283434773,0.5260229176
C,0,-0.0063968908,3.4071985672,-1.3839613391
H,0,1.0762116591,2.6235607731,0.3186604855
H,0,-0.6865697693,2.6463057103,0.5239144453
H,0,-0.7309430423,-2.0797214832,1.2497590985
H,0,1.044455222,-2.1044421011,1.1079933321
H,0,0.8556791845,-3.3721497568,-1.0135178414
H,0,-0.9030653925,-3.3283941204,-0.8960751398
H,0,-0.9634992753,3.2584738587,-1.8846195294
H,0,0.0501002595,4.4429605885,-1.0482103168
H,0,0.7996271044,3.2310727099,-2.0967308067

OEt isopropyl carbonate

E (total electronic) = -536.2466854
E (total electronic) + ZPVE = -536.073795
Internal Thermal Energy = -536.062684
Enthalpy = -536.061740
Gibbs Free Energy = -536.111192

O,0,0.3337180748,-0.9089060431,0.0569374371
C,0,0.3394348345,0.3810277025,0.3563924719
O,0,0.4406134511,0.84020064,1.4714806021
O,0,0.2055484534,1.0813123257,-0.7628450291
C,0,0.2490678486,2.5326315449,-0.6373777935
C,0,0.4498654655,-1.8200657775,1.1761578969
C,0,0.5018310005,-3.2360275449,0.6262366987
O,0,0.5864354591,-4.1600003038,1.6657769255
C,0,-0.4483608379,3.0718654404,-1.8641808174
C,0,1.6915305105,2.9781968777,-0.5311413444
H,0,-0.3051785991,2.796033011,0.2628529528
H,0,-0.4165312935,-1.6848486565,1.825599054
H,0,1.3592658114,-1.5828673777,1.7296867768
H,0,1.3620373872,-3.2871367078,-0.0662551319
H,0,-0.3970940337,-3.3766613795,-0.0019207753
H,0,-1.4781882651,2.7175876848,-1.9143467509
H,0,-0.457197449,4.1614564786,-1.8229229749
H,0,0.0789677563,2.763625322,-2.769005474
H,0,2.183381112,2.5244374965,0.3295864956
H,0,2.2348616307,2.7053863339,-1.4379401765
H,0,1.7288056823,4.0625229332,-0.4176860434

OEt tert-butyl carbonate

E (total electronic) = -575.5525934
E (total electronic) + ZPVE = -575.352493
Internal Thermal Energy = -575.339825
Enthalpy = -575.338880
Gibbs Free Energy = -575.392147

O,0,0.1760747784,-0.4411742489,-0.0002547951
C,0,-0.9618971172,0.2459380415,0.000111495
O,0,-1.0368215037,1.4527998461,-0.0003334729
O,0,-1.9679455918,-0.6156190606,0.0010280351
C,0,-3.3643026297,-0.1453177267,0.0016380717
C,0,1.3867223339,0.3509701774,-0.0012607804
C,0,2.5793551798,-0.590900913,-0.0015532927
O,0,3.7660166566,0.1396732511,-0.0025184551
H,0,1.3930901002,0.9822977415,0.8886057838
H,0,1.3920841327,0.9815759679,-0.8916455981
H,0,2.478920948,-1.2509343581,-0.8826444592
H,0,2.4799168941,-1.2502213068,0.8801843617
C,0,-3.645716938,0.6468800715,1.2681377944
H,0,-3.1300997511,1.6049607263,1.2734585552
H,0,-4.7193437575,0.8321541141,1.3293792256
H,0,-3.3462193372,0.0723265173,2.1465406529
C,0,-3.6471503538,0.6459648048,-1.2651156451
H,0,-3.3485575307,0.0708155061,-2.1434369597
H,0,-4.720858603,0.8311053276,-1.3253252272
H,0,-3.1316211395,1.6040844379,-1.2716704618
C,0,-4.1475506287,-1.4472897773,0.0025497528
H,0,-3.911102634,-2.0352450079,0.8907361143
H,0,-5.215327307,-1.2271544569,0.0030875504
H,0,-3.9121265807,-2.0358733446,-0.8854925557

OEt phenyl carbonate

E (total electronic) = -649.344151
E (total electronic) + ZPVE = -649.174653
Internal Thermal Energy = -649.163225
Enthalpy = -649.162281
Gibbs Free Energy = -649.213657

C,0,-0.456707884,-2.8027625033,-1.3936762615
C,0,-0.4171141799,-3.4902835513,-2.7488965104
O,0,-0.2738825298,-4.8666017871,-2.5946536542
O,0,-0.6200925993,-1.3790192161,-1.6230863822
C,0,-0.5943256042,-0.6164080763,-0.5518438322
O,0,-0.4592317115,-0.9808820325,0.5887324213
O,0,-0.7408457508,0.6627294419,-0.9437825119
C,0,-0.7599122781,1.6310745285,0.0698529298
C,0,0.3470422323,2.4455916885,0.2106771545
C,0,0.313880679,3.4524114653,1.1688214974
C,0,-0.8120776236,3.6228263822,1.9648736158

C,0,-1.9131068359,2.788058276,1.8038977785
C,0,-1.8939323137,1.7814286512,0.8474578305
H,0,-1.299332165,-3.1543564973,-0.7964839128
H,0,0.4720169206,-2.9617908275,-0.8446626734
H,0,0.4097470913,-3.0317733876,-3.3218159743
H,0,-1.3431606493,-3.2109837932,-3.2843729714
H,0,1.2113993341,2.2911850463,-0.4224981338
H,0,1.1712743515,4.1020232146,1.2906550516
H,0,-0.8342685257,4.4080497269,2.709754457
H,0,-2.7917866705,2.9205220041,2.4222376887
H,0,-2.7390342876,1.1202062465,0.700719393

OEt 4-nitrophenyl carbonate

E (total electronic) = -853.842532
E (total electronic) + ZPVE = -853.670737
Internal Thermal Energy = -853.656725
Enthalpy = -853.655781
Gibbs Free Energy = -853.714033

C,0,-0.0244541333,-3.4136885399,1.0051839441
C,0,-0.1653903741,-4.7542596757,0.3033447822
O,0,-0.2765641729,-5.7815808583,1.236113827
O,0,0.0473920009,-2.3835849627,-0.0169730069
C,0,0.120835387,-1.1486807834,0.4186486491
O,0,0.1448312415,-0.7810165266,1.5633230342
O,0,0.1846170443,-0.3332573565,-0.6601656925
C,0,0.1602842632,1.0381293075,-0.4424686987
C,0,1.1913345003,1.777310416,-0.9969847836
C,0,1.168121388,3.1557824958,-0.878006479
C,0,0.1109922251,3.7408844021,-0.2008369013
C,0,-0.9255616718,3.0054877008,0.3538932462
C,0,-0.9015435336,1.629082145,0.2270340192
N,0,0.082122776,5.197499815,-0.0729396443
O,0,0.9835091985,5.8390697629,-0.5807493971
O,0,-0.842236475,5.7047079501,0.5351794799
H,0,-0.8892834804,-3.2094452132,1.6374301451
H,0,0.8867315211,-3.3701234503,1.6031921225
H,0,0.7084566318,-4.8695834842,-0.3636848973
H,0,-1.0444828341,-4.6804992293,-0.3628986698
H,0,1.9951005429,1.2735133749,-1.5165485656
H,0,1.9558551783,3.7619230803,-1.3008987051
H,0,-1.7380079865,3.4995750249,0.8668295625
H,0,-1.6975502372,1.0208916053,0.6344676293

OEt 4-cyanophenyl carbonate

E (total electronic) = -741.588231
E (total electronic) + ZPVE = -741.420426
Internal Thermal Energy = -741.407149
Enthalpy = -741.406205
Gibbs Free Energy = -741.462160

C,0,0.1557983626,-3.6591929421,-0.8479427083
C,0,0.1148258316,-4.5098882702,-2.1067068935
O,0,0.0382357985,-5.8605565163,-1.7784778107
O,0,0.1989192167,-2.265799806,-1.2557147033
C,0,0.1737508318,-1.3828497519,-0.2850103617
O,0,0.1272165063,-1.6041308322,0.8967682195
O,0,0.2247875788,-0.1523624994,-0.8418969603
C,0,0.102019028,0.9436857243,0.0082827835
C,0,1.1437727999,1.853687386,0.0225065695
C,0,1.0219380646,2.9969397352,0.7942639561
C,0,-0.1399425878,3.1995882125,1.5372421518
C,0,-1.1828596576,2.2718376658,1.5119415394
C,0,-1.0622553486,1.1336261124,0.7361042604
C,0,-0.2675091191,4.3835602649,2.3357936382
N,0,-0.3682202404,5.3335542885,2.9762533971
H,0,-0.7381699099,-3.8126687619,-0.242468778
H,0,1.0442435717,-3.8716042022,-0.2517433469
H,0,1.0123635643,-4.2604902536,-2.7017377266
H,0,-0.7478842796,-4.1625138574,-2.7044367323
H,0,2.0304410683,1.6653147068,-0.5679554296
H,0,1.8189647574,3.7278789701,0.8238185816

H₀, -2.0791911587, 2.4488911204, 2.0913629183
H₀, -1.8585026784, 0.4023875058, 0.6888624355

OEt 4-methoxyphenyl carbonate

E (total electronic) = -763.8612705
E (total electronic) + ZPVE = -763.658800
Internal Thermal Energy = -763.644848
Enthalpy = -763.643904
Gibbs Free Energy = -763.701288

C₀, -0.2313118862, -3.9353508225, -0.9003568703
C₀, -0.2275518372, -4.8617696378, -2.1041815792
O₀, -0.2181625449, -6.1920645653, -1.6890470977
O₀, -0.2410764508, -2.5673805408, -1.3847082187
C₀, -0.1992323863, -1.6320423617, -0.460073043
O₀, -0.1584113875, -1.8017074069, 0.7325256024
O₀, -0.2056268548, -0.4337227118, -1.0711327464
C₀, -0.1480696841, 0.6906010598, -0.2336265609
C₀, -1.3010890401, 1.1421748074, 0.3884630063
C₀, -1.2395064722, 2.2811239859, 1.1688132425
C₀, -0.0300108335, 2.9627298602, 1.3205303716
C₀, 1.1189430895, 2.5002981537, 0.6871230923
C₀, 1.0527887877, 1.3504470264, -0.0952431984
O₀, -0.0692876329, 4.0757183525, 2.1091432796
C₀, 1.1585300295, 4.7606510792, 2.3293369943
H₀, -1.120393308, -4.0905782372, -0.2876062079
H₀, 0.6623729594, -4.0816729848, -0.2923837268
H₀, 0.6526394961, -4.5959481835, -2.7179414603
H₀, -1.1109983577, -4.6080804376, -2.7181541569
H₀, -2.2302872472, 0.6005730837, 0.2618864861
H₀, -2.1216224501, 2.6580633763, 1.6707932767
H₀, 2.0628173061, 3.0157160065, 0.7897794336
H₀, 1.9350702511, 0.9731797871, -0.5966438693
H₀, 0.9247715538, 5.585894781, 2.9966502422
H₀, 1.5608913633, 5.1503537967, 1.3922748064
H₀, 1.8893415372, 4.1017277337, 2.8021199016

OEt 4-chlorophenyl carbonate

E (total electronic) = -1108.9462214
E (total electronic) + ZPVE = -1108.786500
Internal Thermal Energy = -1108.773753
Enthalpy = -1108.772809
Gibbs Free Energy = -1108.828244

C₀, 3.7080257684, -0.2529331534, 0.3507443049
C₀, 4.9926853626, 0.2787849516, -0.2619456253
O₀, 6.0993302536, -0.2430465868, 0.4035825375
O₀, 2.5920618294, 0.3191464508, -0.3814509005
C₀, 1.3959932961, -0.0076335929, 0.0533700414
O₀, 1.1373020933, -0.7239242037, 0.9864624473
O₀, 0.4828779777, 0.6038098018, -0.7276505523
C₀, -0.860403011, 0.3539677356, -0.4267565914
C₀, -1.590882579, 1.3561637934, 0.1815540347
C₀, -2.9414727807, 1.1497835502, 0.4294238027
C₀, -3.5138308624, -0.056942234, 0.0625402564
C₀, -2.777712316, -1.0619183157, -0.5464072214
C₀, -1.4298709624, -0.8511011992, -0.7959764485
H₀, 3.6512434831, -1.3391823115, 0.2676046075
H₀, 3.6210425623, 0.0392995806, 1.3978733356
H₀, 4.944040807, 1.3822366826, -0.2170409127
H₀, 4.9748229773, 0.0205682256, -1.3366527878
H₀, -1.1099567327, 2.2863392888, 0.4550411062
H₀, -3.5364332088, 1.9194281561, 0.9026021207
H₀, -3.2480594275, -1.9952316788, -0.8254829099
H₀, -0.8246884918, -1.6127486558, -1.2713032227
Cl₀, -5.2142846873, -0.3208898552, 0.3720201777

OEt 4-fluorophenyl carbonate

E (total electronic) = -748.5869382
E (total electronic) + ZPVE = -748.425737

Internal Thermal Energy = -748.413462
Enthalpy = -748.412517
Gibbs Free Energy = -748.466068

C₀, -0.0224577087, -3.0984805116, -0.1882882412
C₀, -0.1656582828, -4.1726599429, -1.2540758214
O₀, 0.0060600271, -5.4372520251, -0.6973537033
O₀, -0.2230246312, -1.8101220482, -0.8266071852
C₀, -0.0597821231, -0.7559305414, -0.0586388381
O₀, 0.2334458486, -0.7527529848, 1.1098201803
O₀, -0.2748702813, 0.3444913727, -0.8054108936
C₀, -0.1518456819, 1.576492196, -0.1509664983
C₀, 0.9674888772, 2.3437132614, -0.4115014505
C₀, 1.0775891647, 3.5967295528, 0.1770945375
C₀, 0.0595106158, 4.0222894633, 1.0059759578
C₀, -1.0622766926, 3.261520238, 1.2739557607
C₀, -1.1684454349, 2.0121926015, 0.6801762923
F₀, 0.16246425, 5.2392473329, 1.5795956279
H₀, -0.7741220365, -3.214677519, 0.5938492166
H₀, 0.9734288917, -3.1148454859, 0.2557825131
H₀, 0.571944717, -3.9460874462, -2.0457182844
H₀, -1.1583589143, -4.039019754, -1.7218931153
H₀, 1.7395399087, 1.9655837704, -1.0688191512
H₀, 1.9348618429, 4.2324110525, -0.0007791826
H₀, -1.8326980731, 3.6441291751, 1.9302789914
H₀, -2.0291122834, 1.3798682425, 0.8580052875

Transition states

TS-OEt methyl carbonate

E (total electronic) = -457.5879592
E (total electronic) + ZPVE = -457.473257
Internal Thermal Energy = -457.464706
Enthalpy = -457.463761
Gibbs Free Energy = -457.507271

O₀, 0.0140377407, -0.7100905759, -0.0000080634
C₀, -1.0201921426, 0.0268456992, -0.0000021574
O₀, -1.0700398749, 1.2577608015, 0.0000072478
O₀, -2.1726369978, -0.7090142498, -0.0000066577
C₀, -3.3890196178, 0.0393695854, -0.0000018931
C₀, 1.6789524706, 0.2809367339, 0.0000005999
C₀, 2.7584279271, -0.68798204, -0.0000054644
O₀, 3.5477598994, 0.4800726938, 0.0000042364
H₀, -4.1896361135, -0.6959725378, -0.0000047801
H₀, -3.4581483415, 0.6620868813, -0.8911231498
H₀, -3.4581468196, 0.6620781588, 0.8911255612
H₀, 1.4494440658, 0.7819269421, 0.9267294237
H₀, 1.4494458118, 0.7819410416, -0.9267210529
H₀, 2.8461259379, -1.3032151868, -0.8992101114
H₀, 2.8461238043, -1.3032285675, 0.8991902386

TS-OEt ethyl carbonate

E (total electronic) = -496.8970694
E (total electronic) + ZPVE = -496.754410
Internal Thermal Energy = -496.744330
Enthalpy = -496.743385
Gibbs Free Energy = -496.791305

O₀, -0.4976134418, -0.6502026338, -0.0062434138
C₀, 0.4745237091, 0.1689281608, 0.0071646974
O₀, 0.4193556691, 1.4000345297, 0.0249287053
O₀, 1.6814837841, -0.4683033774, -0.0001744417
C₀, 2.8473963661, 0.3711679683, 0.0138252775
C₀, -2.2259119369, 0.2308056345, 0.0038496321
C₀, -3.2586268109, -0.7891234321, -0.0125174373
O₀, -4.0989947109, 0.3428448378, 0.0025840825
C₀, 4.0563325665, -0.530964236, 0.0026538712
H₀, 2.8255604596, 0.9947285298, 0.9084276523

H,0,2.8283452164,1.0203904698,-0.8623969975
H,0,-2.0220748296,0.756585007,-0.9148539048
H,0,-2.0249335154,0.7297460425,0.9380207425
H,0,-3.3207869629,-1.4202530133,0.8776302185
H,0,-3.318013495,-1.3942023506,-0.9207596415
H,0,4.9619621248,0.0769017304,0.0128879133
H,0,4.0664582582,-1.1783447404,0.880549927
H,0,4.0692498194,-1.1526346971,-0.8935963629

TS-OEt isopropyl carbonate

E (total electronic) = -536.2059427
E (total electronic) + ZPVE = -536.035706
Internal Thermal Energy = -536.024248
Enthalpy = -536.023304
Gibbs Free Energy = -536.074375

O,0,0.3479848124,-1.1041822423,-0.5111837135
C,0,0.4289105608,0.1480425518,-0.3029097559
O,0,1.0168986232,0.714168204,0.6204982028
O,0,-0.2473061585,0.8634421741,-1.2488995747
C,0,-0.1747818075,2.3054047327,-1.1819315979
C,0,1.388051312,-2.1636684304,0.7372367903
C,0,1.3218795111,-3.5454733998,0.2997881835
O,0,2.1393316441,-3.7367498794,1.4320472294
C,0,1.1560991141,2.7803152738,-1.7310936162
C,0,-1.3463680773,2.8215369679,-1.9897865154
H,0,-0.2825978424,2.5993433221,-0.1377498021
H,0,0.785351426,-1.8699781292,1.5814440586
H,0,2.2935745229,-1.6143246985,0.5363608091
H,0,1.8019722637,-3.765226399,-0.6573416705
H,0,0.3381250342,-4.0185016944,0.3561982791
H,0,1.216708905,3.8678399104,-1.6627803355
H,0,1.9880215041,2.3527898959,-1.1715949696
H,0,1.2507969471,2.4945011273,-2.7810956405
H,0,-1.2583961787,2.508012974,-3.0321817093
H,0,-2.2900810316,2.4501443628,-1.5887083013
H,0,-1.3613740849,3.9117213759,-1.9582993506

TS-OEt tert-butyl carbonate

E (total electronic) = -575.5106001
E (total electronic) + ZPVE = -575.313008
Internal Thermal Energy = -575.300104
Enthalpy = -575.299160
Gibbs Free Energy = -575.353939

O,0,0.0128219601,-1.1015829646,-0.3541651496
C,0,0.002418544,0.0865400795,0.1066733266
O,0,0.0558201292,0.4181778217,1.2912112609
O,0,-0.0779444905,1.0040177842,-0.8982932276
C,0,-0.1081355907,2.4385782763,-0.6334748342
C,0,-0.2102879843,3.0331426144,-2.0311333871
C,0,1.1855668238,2.8926120796,0.0277696188
C,0,-1.3401965271,2.8147041341,0.1780903174
C,0,0.1187409295,-2.474199337,1.0207011148
C,0,0.1226013392,-3.7602188727,0.3502320024
O,0,0.1997405198,-4.2250738585,1.6793039758
H,0,-1.1214926042,2.6915334934,-2.5254178371
H,0,0.6496004244,2.7376769248,-2.634883897
H,0,-0.2348014539,4.1215205593,-1.9683458064
H,0,1.2680157089,2.5340734173,1.0514900755
H,0,2.0442585141,2.53801171,-0.5459837442
H,0,1.2107691374,3.9839167261,0.0411496212
H,0,-1.4483636547,3.9009534784,0.171332213
H,0,-2.233840211,2.3800032184,-0.2745330754
H,0,-1.2670126066,2.4824488447,1.2112330886
H,0,-0.7959590613,-2.1506230814,1.4903746582
H,0,1.0547065858,-2.0984291794,1.4010891119
H,0,0.9998524424,-3.9761996108,-0.2647692608
H,0,-0.7961858744,-4.0267872576,-0.1781781658

TS-OEt phenyl carbonate

E (total electronic) = -649.3070464
E (total electronic) + ZPVE = -649.139941
Internal Thermal Energy = -649.128306
Enthalpy = -649.127362
Gibbs Free Energy = -649.179674

C,0,-4.1621998049,-0.3464009626,-0.330623869
C,0,-5.3990796337,0.214751656,0.1826792025
O,0,-5.9774429507,-0.7373148422,-0.6801279887
O,0,-2.6999743747,0.5710694613,0.5233110273
C,0,-1.5657770114,0.1936816121,0.1119930361
O,0,-1.296665064,-0.6246560576,-0.7601719449
O,0,-0.5460027863,0.8470436626,0.7913892389
C,0,0.7610792127,0.4961345717,0.4608489732
C,0,1.5008727702,1.3580992048,-0.3297597226
C,0,2.8267617353,1.0463165209,-0.6091555368
C,0,3.3939731801,-0.1169439605,-0.102990701
C,0,2.6337571822,-0.9722442188,0.6883695064
C,0,1.3099813096,-0.6672936234,0.9761200788
H,0,-3.8527361662,-1.3097602228,0.0427238904
H,0,-3.8531936389,-0.0589490285,-1.3230308927
H,0,-5.5926536029,1.2567901115,-0.085682217
H,0,-5.5906215606,0.0494849618,1.2462687441
H,0,1.0397020724,2.2591324701,-0.7146321319
H,0,3.4149553272,1.7153692956,-1.2246588315
H,0,3.0719784147,-1.8793038388,1.0855906677
H,0,0.6997460649,-1.3181947278,1.5904037782
H,0,4.4266336648,-0.3566873454,-0.3225075472

TS-OEt 4-nitrophenyl carbonate

E (total electronic) = -853.8070705
E (total electronic) + ZPVE = -853.637459
Internal Thermal Energy = -853.623290
Enthalpy = -853.622346
Gibbs Free Energy = -853.681304

C,0,4.500387827,-0.3965139357,0.2684229191
C,0,5.7052127845,0.2620309988,-0.2048865225
O,0,6.3448830818,-0.7449593191,0.5440486384
O,0,3.001497048,0.553599398,-0.4620781228
C,0,1.8860622448,0.1481303229,-0.0362317062
O,0,1.6337532023,-0.7293323178,0.7763881263
O,0,0.8466528533,0.8825191516,-0.6168281633
C,0,-0.4533741797,0.5115065956,-0.3554738203
C,0,-0.9131470301,-0.761386408,-0.675886706
C,0,-2.2450943615,-1.0679000889,-0.4747029113
C,0,-3.0834547844,-0.0873780825,0.0373883991
C,0,-2.6376929709,1.1855882568,0.3550096793
C,0,-1.3016091291,1.4838262864,0.1562596611
N,0,-4.4929756423,-0.4075441949,0.2394426578
O,0,-4.8753878651,-1.531700979,-0.0324752387
O,0,-5.2296191908,0.4620502117,0.6702715825
H,0,4.2201128503,-1.3284432517,-0.1971416096
H,0,4.2058158631,-0.2271114567,1.2920552683
H,0,5.8609129556,1.2794676825,0.1640871259
H,0,5.8775089052,0.2142837904,-1.2835747158
H,0,-0.2322395508,-1.4953724596,-1.0848094967
H,0,-2.6311312884,-2.0473843678,-0.717822033
H,0,-3.3186773148,1.9252435634,0.7503763727
H,0,-0.9091855077,2.4647149035,0.3886546156

TS-OEt 4-cyanophenyl carbonate

E (total electronic) = -741.5523426
E (total electronic) + ZPVE = -741.386773
Internal Thermal Energy = -741.373278
Enthalpy = -741.372334
Gibbs Free Energy = -741.429570

C,0,-0.0883710957,-3.868905819,-1.5015766185
C,0,-0.0295745784,-4.4898585287,-2.813025204
O,0,-0.1314084416,-5.6783922525,-2.0636448898
O,0,0.0088216632,-1.9675370192,-1.7594373925
C,0,0.058048112,-1.3116578466,-0.6827720745
O,0,0.039910925,-1.7119282241,0.4727408133
O,0,0.1699758485,0.0551323747,-0.9471488857
C,0,0.1123947892,0.938488082,0.1129192473
C,0,1.1803540727,1.8071715242,0.2798090175
C,0,1.1278925337,2.7643304589,1.2784793824
C,0,0.0041714712,2.8337938379,2.100959762
C,0,-1.0681142202,1.956286434,1.925212378
C,0,-1.0143379148,1.0055001563,0.923392445
C,0,-0.0538826353,3.8219290943,3.1370103522
N,0,-0.0995275523,4.6157602796,3.9685707471
H,0,-1.047190803,-3.8206679429,-1.0096893295
H,0,0.7991635948,-3.9032897438,-0.8896134116
H,0,0.9135782706,-4.3646931121,-3.3518154155
H,0,-0.8780762941,-4.2857628603,-3.4716839202
H,0,2.0386639659,1.7288239423,-0.374342376
H,0,1.9496536032,3.4530820751,1.4234893878
H,0,-1.9355364425,2.0288831221,2.5680283252
H,0,-1.8360418719,0.3201929676,0.7624246599

TS-OEt 4-methoxyphenyl carbonate

Not optimized.

TS-OEt 4-chlorophenyl carbonate

Not optimized.

TS-OEt 4-fluorophenyl carbonate

E (total electronic) = -748.5499347

E (total electronic) + ZPVE = -748.391287

Internal Thermal Energy = -748.378790

Enthalpy = -748.377846

Gibbs Free Energy = -748.432855

C,0,0.218533704,-3.4971922052,-0.4728825434
C,0,0.2496370755,-4.4389387992,-1.5777867494
O,0,0.5009612298,-5.3660305447,-0.547021575
O,0,-0.134233903,-1.7513199021,-1.2018088426
C,0,-0.0713235942,-0.8244365394,-0.3446916146
O,0,0.165234447,-0.8988312034,0.8549737491
O,0,-0.3051189775,0.412164676,-0.9353918199
C,0,-0.2896992044,1.5326933283,-0.1116709444
C,0,0.7337848542,2.4502401417,-0.2747635047
C,0,0.7356949736,3.6160110418,0.4813370204
C,0,-0.2911307404,3.813725693,1.3808719383
C,0,-1.3191016625,2.9075667638,1.5579676341
C,0,-1.3170348153,1.7497173889,0.7939775853
F,0,-0.2941214316,4.9447209704,2.1206031158
H,0,-0.6602781963,-3.4838905465,0.1522120384
H,0,1.1602907284,-3.2012019955,-0.038948989
H,0,1.0692643116,-4.3067012351,-2.2891013132
H,0,-0.6976930684,-4.5815045206,-2.1046665928
H,0,1.5193830143,2.253933386,-0.9929951173
H,0,1.5168186955,4.357528282,0.3767025345
H,0,-2.102484958,3.1111786553,2.2762524642
H,0,-2.1049274822,1.0146541645,0.8990895261

Other
2-oxyethyl alkyl/aryl carbonates
(OEt alkyl/aryl carbonates)

M06-2X/6-311+G(2d,p)
IEFPCM, Solvent = Water

Substrates

ALIPHATIC CARBONATES

OEt hydrogen carbonate

E (total electronic) = -418.3250001
E (total electronic) + ZPVE = -418.237141
Internal Thermal Energy = -418.230016
Enthalpy = -418.229072
Gibbs Free Energy = -418.269248

O,0,-0.3347174813,-0.5200041417,-0.0000595993
C,0,-1.5060480875,0.0762025375,0.000026315
O,0,-1.7099532603,1.2648025628,0.0001960455
O,0,-2.469952619,-0.8522310802,-0.0001104866
C,0,0.8261399149,0.3504464147,0.0000672459
C,0,2.0857212429,-0.5116529495,-0.0000763996
O,0,3.2076964826,0.2619350009,0.0000345287
H,0,-3.3192571899,-0.3905330388,-0.0000408395
H,0,0.785709186,0.9814113774,0.8893142003
H,0,0.7856938351,0.9816901095,-0.8889808736
H,0,1.9985109063,-1.1860743753,-0.8814515985
H,0,1.9985250702,-1.1863434173,0.8810944618

OEt ethenyl carbonate (Point group: Cs)

E (total electronic) = -495.6917353
E (total electronic) + ZPVE = -495.571437
Internal Thermal Energy = -495.561925
Enthalpy = -495.560981
Gibbs Free Energy = -495.607485

O,0,-0.5140975499,-0.387802714,0.
C,0,0.5700231597,0.3517127334,0.
O,0,0.6286864063,1.5524790317,0.
O,0,1.6357064289,-0.4763473032,0.
C,0,-1.7773477863,0.3291898827,0.
C,0,-2.91532924,-0.6875625517,0.
O,0,-4.1248239392,-0.0609657626,0.
C,0,2.889729718,0.1000998054,0.
C,0,3.9624877887,-0.6675911481,0.
H,0,-1.8174333512,0.9598254637,-0.8894123117
H,0,-1.8174333512,0.9598254637,0.8894123117
H,0,-2.7419652735,-1.3452782,0.881206906
H,0,-2.7419652735,-1.3452782,-0.881206906
H,0,2.8936864764,1.1806051316,0.
H,0,4.9396122495,-0.2083209163,0.
H,0,3.8860434776,-1.7467917962,0.

OEt ethynyl carbonate

E (total electronic) = -494.4255007
E (total electronic) + ZPVE = -494.329364
Internal Thermal Energy = -494.320145
Enthalpy = -494.319200
Gibbs Free Energy = -494.365038

O,0,0.1229178885,-0.4304832482,0.0000020976
C,0,-0.9871398341,0.2467783372,0.0000019726
O,0,-1.1594500434,1.427103318,0.0000009212
O,0,-2.0207574099,-0.6757717411,0.0000036123
C,0,1.3490621882,0.3630398951,0.0000003271
C,0,2.54461119,-0.5842640947,-0.0000011412
O,0,3.7104415769,0.1191637131,-0.0000031422
H,0,1.3433707823,0.9919119582,0.8908397913
H,0,1.3433684039,0.9919116575,-0.8908393309
H,0,2.4122909671,-1.2504415734,-0.881558134
H,0,2.412293642,-1.2504410503,0.8815566534
C,0,-3.237979089,-0.190158624,0.0000042187
C,0,-4.3706221889,0.1826698208,0.0000049908
H,0,-5.3809884735,0.5181127519,0.0000066033

OEt propyl carbonate

E (total electronic) = -536.2266462
E (total electronic) + ZPVE = -536.053614
Internal Thermal Energy = -536.042318
Enthalpy = -536.041373
Gibbs Free Energy = -536.092342

O,0,-0.3257951809,-1.5172894683,-0.7263034332
C,0,0.0550351889,-0.5702263626,0.1117241186
O,0,0.6091870419,-0.7391903187,1.1705091667
O,0,-0.2719314839,0.6143823652,-0.3990795014
C,0,0.0720078965,1.7532213908,0.4129412527
C,0,-0.0411904308,-2.8781492207,-0.3194866608
C,0,-0.5667351437,-3.8337483368,-1.3872515999
O,0,-0.319208392,-5.1300485643,-1.0454482102
C,0,-0.3413933918,2.996596264,-0.3413316524
C,0,0.4243257758,3.1795279401,-1.6473631302
H,0,1.1480149141,1.7364992377,0.5960919505
H,0,-0.4465856744,1.6667496853,1.3680715879
H,0,-0.5269822523,-3.065341549,0.6396111826
H,0,1.0380362851,-2.987961308,-0.1985640115
H,0,-0.0959148859,-3.5177181896,-2.3452751169
H,0,-1.6467447379,-3.5945168098,-1.5121974661
H,0,-0.1671856931,3.8483606673,0.320184923
H,0,-1.4169447386,2.9555078077,-0.529999225
H,0,0.2456741885,2.3440329998,-2.3249362799
H,0,0.119024442,4.0959282516,-2.1526810889
H,0,1.4985052727,3.2387825183,-1.4592508054

OEt fluoromethyl carbonate

E (total electronic) = -556.8620918
E (total electronic) + ZPVE = -556.752802
Internal Thermal Energy = -556.743677
Enthalpy = -556.742732
Gibbs Free Energy = -556.788538

O,0,-0.0283483156,-0.0788964864,-0.6164194477
C,0,0.0501918818,0.6592032531,0.4626205239
O,0,0.1610645426,0.2839380944,1.5984630776
O,0,-0.0111973166,1.9597130472,0.0886840189
C,0,0.0440415586,2.8864671726,1.130576207
C,0,0.0224306001,-1.5176236285,-0.4143585679
C,0,-0.0828347413,-2.2017872594,-1.7745904006
O,0,-0.0373022403,-3.5567733453,-1.6438471818
F,0,-1.1970292246,2.9747724047,1.7144471282
H,0,0.7537786799,2.5812541451,1.8942822245
H,0,0.2797802517,3.8451295254,0.6800813709
H,0,-0.8066862144,-1.8037873408,0.2345276199
H,0,0.9653325216,-1.7636832454,0.0761208971
H,0,0.7358829026,-1.7765310986,-2.3974504909
H,0,-1.019009886,-1.8199622378,-2.2401839792

OEt chloromethyl carbonate

E (total electronic) = -917.2166604
E (total electronic) + ZPVE = -917.109220

Internal Thermal Energy = -917.099799
Enthalpy = -917.098855
Gibbs Free Energy = -917.145964

O,0,0.004941181,-0.6608978418,-0.2285072147
C,0,0.006327674,0.6269615502,0.0079708203
O,0,-0.015167979,1.1768791294,1.0753831041
O,0,0.0424346403,1.2738586684,-1.1824380057
C,0,0.0203070194,2.6656864878,-1.1128968261
C,0,-0.0189259985,-1.5211473034,0.9442270811
C,0,-0.0166257856,-2.9773163761,0.4888360498
O,0,-0.0335033505,-3.8170760854,1.5618623431
Cl,0,-1.6629202083,3.27245256,-0.8906867881
H,0,0.5983518331,3.0391420674,-0.2756058579
H,0,0.3643470137,3.0401106553,-2.0681240139
H,0,-0.917582035,-1.2919984472,1.5185184354
H,0,0.8610973217,-1.3002740872,1.5497093264
H,0,0.8737410168,-3.0947763224,-0.1686444705
H,0,-0.8885913433,-3.090678655,-0.1934049835

OEt bromomethyl carbonate

E (total electronic) = -3031.1837131
E (total electronic) + ZPVE = -3031.076896
Internal Thermal Energy = -3031.067303
Enthalpy = -3031.066359
Gibbs Free Energy = -3031.114794

O,0,0.0292441465,-0.5160938556,-0.526620853
C,0,-0.0299164468,0.4870397173,0.3116707594
O,0,-0.0596197304,0.443199404,1.51102147
O,0,-0.0489130411,1.6362112834,-0.409201298
C,0,-0.1377297772,2.8104987931,0.3267716492
C,0,0.0805951296,-1.8418544955,0.0703982501
C,0,0.1690941164,-2.8794908388,-1.0447773405
O,0,0.2258086814,-4.1387011859,-0.5278593519
Br,0,-2.004852034,3.1974799091,0.828015756
H,0,0.4111075309,2.7577371607,1.2589557272
H,0,0.1702225435,3.6250213433,-0.3141611095
H,0,-0.8213588188,-1.9841076525,0.6674275734
H,0,0.9549509351,-1.8910030143,0.7209685995
H,0,1.0527914089,-2.5978107142,-1.6600916394
H,0,-0.7063906438,-2.697983854,-1.7076961926

OEt cyanomethyl carbonate

E (total electronic) = -549.850592
E (total electronic) + ZPVE = -549.735434
Internal Thermal Energy = -549.725344
Enthalpy = -549.724400
Gibbs Free Energy = -549.772531

O,0,-0.0641820692,-0.9936408169,-0.1939933172
C,0,0.0705929012,-0.0952553462,0.7482107569
O,0,0.3707761857,-0.2745825585,1.8990727299
O,0,-0.1907058654,1.1206042819,0.2212253694
C,0,-0.0524774763,2.1989187795,1.1288661016
C,0,0.1753611349,-2.3726397213,0.2045347939
C,0,-0.0280348662,-3.2788882179,-1.0058257068
O,0,0.1831976171,-4.5823391997,-0.6698856694
C,0,-1.1537607121,2.2241080958,2.1082149281
N,0,-2.0140860743,2.2606417796,2.8628972325
H,0,0.8936796878,2.1461833497,1.6654333237
H,0,-0.0901600363,3.1074975961,0.533414354
H,0,-0.5240623601,-2.6245630166,1.0027103218
H,0,1.1960120914,-2.4477041736,0.5821399528
H,0,0.6523044636,-2.8956170211,-1.7988801629
H,0,-1.0526136218,-3.0654488109,-1.3845230081

OEt nitromethyl carbonate

E (total electronic) = -662.1138987
E (total electronic) + ZPVE = -661.994043

Internal Thermal Energy = -661.983369
Enthalpy = -661.982425
Gibbs Free Energy = -662.032610

O,0,-0.4523111138,-0.766429264,-0.9170830683
C,0,-0.4816404061,0.31794482,-0.1929144886
O,0,-0.5369692287,0.4142809414,1.0022880136
O,0,-0.4331996959,1.3906020397,-1.0309562155
C,0,-0.4713276516,2.6161862617,-0.400762698
C,0,-0.4895956706,-2.0238340979,-0.18125201
C,0,-0.438595572,-3.1779196583,-1.1778511245
O,0,-0.4674648082,-4.3743749011,-0.5275356556
N,0,-1.8774305617,2.9325810527,0.0799361337
O,0,-1.9881532537,3.9747144246,0.685770307
O,0,-2.7674363036,2.1592263151,-0.1699722938
H,0,-0.2315513983,3.3899081592,-1.1233310251
H,0,0.1500094499,2.6743919774,0.4887084693
H,0,-1.4102649276,-2.049020862,0.4029676118
H,0,0.367795036,-2.0490866387,0.4923295839
H,0,0.4735873649,-3.0144174036,-1.7941451216
H,0,-1.2870802588,-3.0193971661,-1.8803194182

OEt difluoromethyl carbonate

E (total electronic) = -656.1173186
E (total electronic) + ZPVE = -656.016145
Internal Thermal Energy = -656.006358
Enthalpy = -656.005414
Gibbs Free Energy = -656.053279

O,0,-0.0983281962,-0.3139557551,0.1634537813
C,0,-0.1187337138,0.9680590591,0.4009566664
O,0,-0.1947434132,1.5278710878,1.4593538589
O,0,-0.0357041002,1.6197929674,-0.7931909498
C,0,-0.0673877648,2.9969526626,-0.707800684
C,0,-0.1708877886,-1.1776933775,1.3359188207
C,0,-0.1200597258,-2.6331365588,0.8824105837
O,0,-0.1775074321,-3.4669136042,1.9581908205
F,0,1.1613562168,3.4539678318,-0.3993595283
F,0,-0.356906768,3.4348987017,-1.9383143145
H,0,-0.7868911492,3.3660678443,0.0168395869
H,0,-1.1031346579,-0.9622781124,1.8592158616
H,0,0.6725026479,-0.9408101508,1.9854961319
H,0,0.8045482654,-2.736657532,0.2718869573
H,0,-0.9543424204,-2.7635290639,0.1575754073

OEt dichloromethyl carbonate

E (total electronic) = -1376.8101343
E (total electronic) + ZPVE = -1376.712809
Internal Thermal Energy = -1376.702218
Enthalpy = -1376.701274
Gibbs Free Energy = -1376.751881

O,0,1.0085561619,-0.3158149579,-0.0473839095
C,0,0.0009652528,0.5081305234,0.025537683
O,0,0.0171833321,1.6955969016,0.1893104325
O,0,-1.1454230464,-0.2225145291,-0.1200777219
C,0,-2.3165061641,0.512957913,-0.0869628626
C,0,2.330636657,0.2855387024,0.0863336518
C,0,3.3860145498,-0.8072724765,-0.0516655381
O,0,4.6359268209,-0.2777745263,0.0606146143
H,0,-2.2629615762,1.3448819179,0.6038901406
H,0,2.3882530205,0.7652739609,1.0639942448
H,0,2.4408084666,1.0387865686,-0.6944469377
H,0,3.1873745386,-1.3097636793,-1.0245038371
H,0,3.1430085664,-1.5737604099,0.7176518255
Cl,0,-3.6098170881,-0.5789704305,0.420763065
Cl,0,-2.6747332018,1.1918065917,-1.7018285909

OEt dibromomethyl carbonate

E (total electronic) = -5604.7419794

E (total electronic) + ZPVE = -5604.645946
Internal Thermal Energy = -5604.634891
Enthalpy = -5604.633947
Gibbs Free Energy = -5604.687275

O,0,1.0113177649,-0.3120871333,-0.0722718303
C,0,0.0048664443,0.5102369312,0.0204595922
O,0,0.019539052,1.6923017142,0.2170566222
O,0,-1.1433998306,-0.2168367486,-0.1496148596
C,0,-2.311349652,0.5148005384,-0.1055069816
C,0,2.3327247436,0.2824645851,0.0990668739
C,0,3.3883011616,-0.8075594368,-0.0580743596
O,0,4.6361481821,-0.2887388858,0.1131097116
H,0,-2.2520212376,1.3600326853,0.5669853901
H,0,2.3763896366,0.7296259141,1.0927511681
H,0,2.4544852282,1.0608770007,-0.6548864065
H,0,3.216673012,-1.2655057796,-1.0576673099
H,0,3.1213278524,-1.606037099,0.6695475462
Br,0,-2.732207126,1.2479197573,-1.8698906675
Br,0,-3.7175972615,-0.6527256932,0.5059738007

OEt dicyanomethyl carbonate

E (total electronic) = -642.0715882
E (total electronic) + ZPVE = -641.958145
Internal Thermal Energy = -641.946389
Enthalpy = -641.945444
Gibbs Free Energy = -641.997463

O,0,0.5230817922,-1.1125781131,-0.4967132923
C,0,0.7169246477,-0.0748258519,0.2618300047
O,0,1.0572045938,-0.0315526462,1.4118813918
O,0,0.4635844669,1.0466253194,-0.476632328
C,0,0.6303154258,2.2621752885,0.2088081511
C,0,0.7497702164,-2.4112245057,0.1339549186
C,0,0.4797045284,-3.5109988892,-0.8876172334
O,0,0.6838224788,-4.7344746655,-0.3252674849
C,0,2.0239610131,2.4783423516,0.655479355
N,0,3.10682724,2.6836228893,0.9598680551
C,0,-0.3036240867,2.4077721889,1.3468093087
N,0,-1.054651772,2.5574431281,2.1958957639
H,0,0.3915672652,3.0432274015,-0.5153031709
H,0,0.0762389648,-2.493400646,0.9874989002
H,0,1.7831598234,-2.4416526312,0.4805285939
H,0,1.13366259,-3.2931023026,-1.7610887302
H,0,-0.5557411877,-3.3443313157,-1.2593242032

OEt dinitromethyl carbonate

E (total electronic) = -866.5873152
E (total electronic) + ZPVE = -866.465312
Internal Thermal Energy = -866.452230
Enthalpy = -866.451286
Gibbs Free Energy = -866.507157

O,0,0.5144768087,-0.857067906,-0.4478024644
C,0,0.4087134102,0.1851800507,0.3114303919
O,0,0.3022656647,0.2637740082,1.4992623751
O,0,0.409462496,1.3002347485,-0.514312063
C,0,0.4901683727,2.5078570475,0.0798894889
C,0,0.5184565818,-2.1483098848,0.2438780192
C,0,0.657983623,-3.2612422905,-0.7894711005
O,0,0.6939628411,-4.4724965288,-0.1689434395
N,0,1.8695258802,2.7846301449,0.6717859908
O,0,2.6162724915,1.8508283723,0.8064089197
O,0,2.0956368239,3.9431464588,0.9136942224
N,0,-0.5552245876,2.6984069482,1.1931474151
O,0,-1.6678466682,2.3815596675,0.8608332233
O,0,-0.210822969,3.1646164158,2.2440997631
H,0,0.3067960879,3.2957542001,-0.6449140015
H,0,-0.4167463211,-2.2339590997,0.7975193815
H,0,1.35817916,-2.149545237,0.939097538

H,0,1.568133925,-3.0219562299,-1.383062166
H,0,-0.1875446206,-3.1352198859,-1.50150649

OEt tricyanomethyl carbonate (Point group: Cs)

E (total electronic) = -734.277579
E (total electronic) + ZPVE = -734.167071
Internal Thermal Energy = -734.153211
Enthalpy = -734.152267
Gibbs Free Energy = -734.209621

O,0,-1.587562034,0.5361006602,0.
C,0,-0.4914165578,-0.1490257707,0.
O,0,-0.3184896895,-1.3341360624,0.
O,0,0.5627951578,0.743296319,0.
C,0,1.8315387651,0.1458912619,0.
C,0,-2.8298580647,-0.2442130416,0.
C,0,-4.0106932621,0.7208013266,0.
O,0,-5.1817663444,0.0273704147,0.
C,0,2.0718563667,-0.6808592195,1.2132759349
N,0,2.290873243,-1.2809046672,2.1606142496
C,0,2.8050699999,1.2639710029,0.
N,0,3.5639615308,2.1174154042,0.
C,0,2.0718563667,-0.6808592195,-1.2132759349
N,0,2.290873243,-1.2809046672,-2.1606142496
H,0,-2.8286530058,-0.8711262872,0.8918716241
H,0,-2.8286530058,-0.8711262872,-0.8918716241
H,0,-3.8698346669,1.3847686412,-0.881549719
H,0,-3.8698346669,1.3847686412,0.881549719

OEt trinitromethyl carbonate

E (total electronic) = -1071.0486585
E (total electronic) + ZPVE = -1070.925668
Internal Thermal Energy = -1070.909766
Enthalpy = -1070.908822
Gibbs Free Energy = -1070.971389

O,0,0.00361028,-0.741688713,-0.7521021166
C,0,0.2378356123,0.1180490772,0.1733348512
O,0,0.3343640563,0.0069133089,1.3543697301
O,0,0.3601625006,1.3730408997,-0.4678057941
C,0,0.7720585682,2.3967370391,0.2601060788
C,0,-0.1935811662,-2.1289034571,-0.298345845
C,0,-0.4602287408,-3.0059654613,-1.516251907
O,0,-0.6482921718,-4.2946755838,-1.1232760588
N,0,0.0032356149,2.5908820958,1.5833539989
O,0,-1.1857651004,2.4912743325,1.4640379261
O,0,0.6450233691,2.8299997788,2.5659161287
N,0,2.2858433959,2.3552412431,0.5712864069
O,0,2.7979286927,1.274112667,0.5050166827
O,0,2.7925518018,3.4141127131,0.8277551066
N,0,0.5689954573,3.6832839641,-0.555368368
O,0,0.15551597,4.6368295082,0.0445639503
O,0,0.8774566371,3.5958599335,-1.7100443409
H,0,-1.0392676424,-2.1309725116,0.3889722197
H,0,0.712798274,-2.434285228,0.2240696359
H,0,0.4010624271,-2.8550320862,-2.2038331806
H,0,-1.3292038357,-2.55315452,-2.0426951049

AROMATIC CARBONATES

OEt 2-nitrophenyl carbonate

E (total electronic) = -853.824061
E (total electronic) + ZPVE = -853.652624
Internal Thermal Energy = -853.638609
Enthalpy = -853.637665
Gibbs Free Energy = -853.695756

C,0,-0.8512766202,-2.915150829,-0.6085038282
C,0,-0.7342186066,-3.8506125997,-1.8084116968

O,0,-0.8167663155,-5.1520913394,-1.4154296653
O,0,-0.772682752,-1.5403401672,-1.081681888
C,0,-0.8865521108,-0.6138177347,-0.1686521443
O,0,-1.042014762,-0.7554492498,1.0129832813
O,0,-0.7830908508,0.5928646153,-0.7870505989
C,0,-0.9936076313,1.7189997802,-0.0294244456
C,0,0.0085774639,2.6730928389,-0.0273357948
C,0,-0.1535566437,3.8550810346,0.6807414711
C,0,-1.3114409912,4.0851090118,1.4132027091
C,0,-2.3132438565,3.1298969497,1.4300266867
C,0,-2.1576552393,1.9633630548,0.6978284087
N,0,-3.2696011982,1.0119947612,0.7033375597
O,0,-3.970035739,0.9720581396,1.6929926158
O,0,-3.4458997677,0.331205119,-0.2885406044
H,0,-1.8076269797,-3.0464793511,-0.1005986496
H,0,-0.0392317088,-3.0806584401,0.1008647708
H,0,0.2207308345,-3.5864531997,-2.3154129519
H,0,-1.5290164105,-3.5373966433,-2.521787368
H,0,0.9118634838,2.4674806674,-0.5859235546
H,0,0.6355297159,4.5951467331,0.6655848993
H,0,-1.4360842237,5.0038749069,1.9691703058
H,0,-3.2262990907,3.2777209415,1.9893754822

OEt 2-cyanophenyl carbonate

E (total electronic) = -741.5735384
E (total electronic) + ZPVE = -741.406348
Internal Thermal Energy = -741.392919
Enthalpy = -741.391975
Gibbs Free Energy = -741.448538

C,0,-0.2160405696,-3.0094067943,-0.4450031256
C,0,-0.5473017536,-3.8291126934,-1.68873399
O,0,-0.3166579128,-5.1537419764,-1.469917793
O,0,-0.4850279347,-1.6072107597,-0.7275416106
C,0,-0.2479856942,-0.7701696123,0.2488193468
O,0,0.1660653479,-1.0154910573,1.3477567617
O,0,-0.5528414022,0.4800044302,-0.1920002342
C,0,-0.4092719231,1.5121157552,0.7148215532
C,0,0.6054717572,2.4288346818,0.5315989201
C,0,0.7085553766,3.5087937072,1.3998616237
C,0,-0.1952076956,3.6669807724,2.4438130669
C,0,-1.2141423576,2.745796673,2.6248240597
C,0,-1.3263814189,1.6621455217,1.754704705
C,0,-2.3773563187,0.6992895105,1.9108614542
N,0,-3.2162975177,-0.0761533372,2.0243976592
H,0,-0.8346157774,-3.3128878107,0.4007206228
H,0,0.8365582992,-3.1098512356,-0.1773176422
H,0,0.0540782148,-3.3918746337,-2.5169999333
H,0,-1.6023167095,-3.5861116413,-1.9469315971
H,0,1.2992385634,2.2900880079,-0.2867264269
H,0,1.5026542411,4.230039517,1.2581632029
H,0,-0.1083459991,4.5094471469,3.1161978911
H,0,-1.9273728152,2.8561648282,3.4304274856

OEt 2-methoxyphenyl carbonate

E (total electronic) = -763.8457744
E (total electronic) + ZPVE = -763.644118
Internal Thermal Energy = -763.629989
Enthalpy = -763.629045
Gibbs Free Energy = -763.687036

C,0,0.6988640453,-2.6300512885,-1.1296890887
C,0,0.4401056171,-3.2530050885,-2.4988072589
O,0,0.6101020518,-4.6045456296,-2.4588042906
O,0,0.4994851559,-1.1951081067,-1.2253993849
C,0,0.6898805615,-0.5126371723,-0.1193105862
O,0,0.9992698835,-0.9459525672,0.9570882363
O,0,0.4963965943,0.795510431,-0.3988489526
C,0,0.5111705893,1.6645057077,0.6834890317
C,0,1.5524245116,2.5530792039,0.8248806418
C,0,1.5339449184,3.4748782018,1.8690547843
C,0,0.4674805303,3.4793755798,2.7524024082

C,0,-0.5872201319,2.579838528,2.6082312957
C,0,-0.5760138699,1.6619650175,1.5641722373
O,0,-1.5405155912,0.7499048256,1.3117550836
C,0,-2.648602222,0.7120526064,2.1997119259
H,0,0.0073215868,-3.0257704236,-0.3844169917
H,0,1.7231976817,-2.815924885,-0.8028984767
H,0,1.1179661485,-2.7293723937,-3.2097528757
H,0,-0.5832809822,-2.9315313888,-2.7959755901
H,0,2.3680686409,2.5170563722,0.1138656899
H,0,2.3484227349,4.176966986,1.9848840925
H,0,0.442246977,4.1896986351,3.5688025626
H,0,-1.410691127,2.6040535355,3.3075363387
H,0,-3.2966530829,-0.0795526279,1.8356968735
H,0,-2.3228835705,0.4828467996,3.2160857333
H,0,-3.1868656512,1.6617041417,2.1894135607

OEt 2-chlorophenyl carbonate

E (total electronic) = -1108.9307126
E (total electronic) + ZPVE = -1108.771797
Internal Thermal Energy = -1108.758916
Enthalpy = -1108.757972
Gibbs Free Energy = -1108.814127

C,0,0.2159299919,-2.5915980369,1.1673955064
C,0,0.0402334762,-4.0297923509,0.6870030037
O,0,0.1168465321,-4.9053690439,1.7276480094
O,0,0.1146841585,-1.7069430336,0.018394616
C,0,0.2583358324,-0.4274409588,0.2605231067
O,0,0.4586859092,0.1015884279,1.3190705053
O,0,0.1503914102,0.2327346918,-0.9193673189
C,0,0.1853604048,1.6136756164,-0.8558405236
C,0,1.3239047956,2.277269173,-1.2750955486
C,0,1.3467304982,3.6652605862,-1.2830876283
C,0,0.2310573406,4.3807178182,-0.8678788709
C,0,-0.9120222728,3.7138850057,-0.4473247843
C,0,-0.9316829782,2.3287106617,-0.4446445105
Cl,0,-2.3570000202,1.4741963806,0.0637494469
H,0,-0.5625087399,-2.3186932881,1.8816091561
H,0,1.1943962625,-2.4483434335,1.6280288107
H,0,0.8117496594,-4.1874373474,-0.0997562515
H,0,-0.9288943353,-4.0547234105,0.1399245869
H,0,2.1775904647,1.6933750516,-1.5939686624
H,0,2.236508049,4.1848197032,-1.6126317058
H,0,0.2437953484,5.4625180582,-0.8719673582
H,0,-1.7887857873,4.2589357291,-0.1242995252

OEt 2-fluorophenyl carbonate

E (total electronic) = -748.5701358
E (total electronic) + ZPVE = -748.409708
Internal Thermal Energy = -748.397223
Enthalpy = -748.396279
Gibbs Free Energy = -748.450861

C,0,0.2616079855,-2.7784725899,-0.4728177021
C,0,0.1122120346,-3.7462282309,-1.6431705169
O,0,0.3153391477,-5.0305342953,-1.2369753235
O,0,0.0451800541,-1.424732472,-0.9566001171
C,0,0.131537429,-0.4737909884,-0.0591277001
O,0,0.3580802112,-0.5907422534,1.1135193795
O,0,-0.0722309164,0.7106577838,-0.6879697813
C,0,-0.0908385742,1.8370966768,0.1138213993
C,0,0.8982538678,2.7935530841,-0.0111795794
C,0,0.8280647555,3.9551030629,0.7494844026
C,0,-0.2265369149,4.1493095078,1.6316619055
C,0,-1.2231960598,3.1878315743,1.759051391
C,0,-1.1413315159,2.0446244502,0.9935083891
F,0,-2.0924264038,1.1032710262,1.0835114639
H,0,-0.474139234,-2.9879708615,0.3048763957
H,0,1.2635959417,-2.8347776491,-0.0449980102
H,0,0.8228941366,-3.3975461234,-2.4256899356
H,0,-0.8966700462,-3.5580689838,-2.0739587193
H,0,1.7095593781,2.6172067437,-0.7054927015

H,0,1.6007735529,4.7055887284,0.6515862065
H,0,-0.2803757292,5.052465913,2.2247606681
H,0,-2.0582321001,3.3129328968,2.4356224856

OEt 2-methylphenyl carbonate

E (total electronic) = -688.6392002
E (total electronic) + ZPVE = -688.442994
Internal Thermal Energy = -688.429676
Enthalpy = -688.428732
Gibbs Free Energy = -688.484749

C,0,0.5485085186,-2.9046457829,-0.5333043977
C,0,0.2270090937,-3.8874189446,-1.6561735868
O,0,0.550117065,-5.1620082202,-1.2985932487
O,0,0.1677650975,-1.5712095431,-0.9632126379
C,0,0.3898582148,-0.6010150867,-0.1057506878
O,0,0.8734905531,-0.6990199624,0.9905318918
O,0,-0.0200593924,0.5544795759,-0.6669776719
C,0,0.0820790957,1.704205009,0.1182060461
C,0,1.1064220092,2.5889947996,-0.1598116823
C,0,1.189722177,3.7750094387,0.5592189105
C,0,0.2461503023,4.0501136471,1.5397858237
C,0,-0.7764397968,3.144077233,1.7972110224
C,0,-0.8827530259,1.9487745731,1.0904371304
C,0,-1.981289103,0.9587847396,1.3536913059
H,0,-0.0106564762,-3.1492116191,0.3712658905
H,0,1.615671547,-2.9044284856,-0.306534534
H,0,0.7675853883,-3.5156748147,-2.5554810563
H,0,-0.8502914633,-3.7401066498,-1.8946370002
H,0,1.822307963,2.3435271129,-0.9339313666
H,0,1.9865561732,4.4769871398,0.3507863462
H,0,0.3015898184,4.9726911809,2.1033492855
H,0,-1.514086672,3.3664903393,2.5594846621
H,0,-2.4808152495,0.6731517681,0.4265288116
H,0,-1.5816757485,0.0479710971,1.8052650577
H,0,-2.7207980891,1.3805274551,2.0321566859

OEt 2-(trifluoromethyl)phenyl carbonate

E (total electronic) = -986.3889709
E (total electronic) + ZPVE = -986.215564
Internal Thermal Energy = -986.200425
Enthalpy = -986.199481
Gibbs Free Energy = -986.260550

C,0,0.1048037912,-3.0243248549,-0.1081650019
C,0,0.4274664268,-4.1053417825,-1.1357836305
O,0,0.1283705626,-5.3420617457,-0.6488495019
O,0,0.4234417341,-1.7270090743,-0.6828972826
C,0,0.1797829992,-0.6879085159,0.0759218306
O,0,-0.2619592449,-0.6795874527,1.1913572203
O,0,0.519040218,0.425119201,-0.6235239565
C,0,0.3574866557,1.6359295769,0.0325783336
C,0,-0.8825229276,2.241723291,0.0710260486
C,0,-1.0082903055,3.4846992223,0.6780126044
C,0,0.0994383335,4.1090079612,1.2362009424
C,0,1.3419012935,3.4916079284,1.1911701182
C,0,1.4734303343,2.2481635338,0.5887300017
C,0,2.8018962622,1.5570905383,0.5157442322
H,0,-0.9550719678,-3.0345636385,0.1496842159
H,0,0.6977081808,-3.1538633294,0.7984382972
H,0,1.4987660205,-3.9671436205,-1.4043815999
H,0,-0.1319337278,-3.8301383114,-2.0579152822
H,0,-1.7317731123,1.7382402091,-0.3722308193
H,0,-1.9770498102,3.9656587922,0.7119360161
H,0,-0.0013367674,5.0780501811,1.7058542325
H,0,2.2098451387,3.9710757399,1.6226794715
F,0,3.2349314432,1.4238087657,-0.7466043851
F,0,3.7497859274,2.222314128,1.1828055255
F,0,2.7555644716,0.319314947,1.0358837392

OEt 2-(dimethylamino)phenyl carbonate

E (total electronic) = -783.275059
E (total electronic) + ZPVE = -783.032822
Internal Thermal Energy = -783.017296
Enthalpy = -783.016352
Gibbs Free Energy = -783.077034

C,0,0.8576163672,-2.8326024915,0.191186875
C,0,0.4891934307,-3.9805979126,-0.7446557895
O,0,0.5712267537,-5.1797131797,-0.1021027653
O,0,0.7551494976,-1.5827855168,-0.5393095238
C,0,1.049129818,-0.4952702258,0.1379898107
O,0,1.3722075122,-0.4264146417,1.2923209068
O,0,0.95865366,0.5567112838,-0.7070034669
C,0,0.9530264664,1.8145132485,-0.1140955378
C,0,2.0677255516,2.612411244,-0.2526872168
C,0,2.0845914372,3.8767751041,0.328036631
C,0,0.9793733082,4.3068129883,1.044895464
C,0,-0.1471415804,3.4983313525,1.1656003912
C,0,-0.1932170046,2.2341396788,0.5763240516
N,0,-1.2928296375,1.3568599561,0.679377576
C,0,-2.2555985226,1.6807265369,1.7206321863
C,0,-1.9726700532,1.0940441906,-0.5919185771
H,0,0.1775425934,-2.7908319208,1.0434015383
H,0,1.8810919147,-2.9380736634,0.5547579817
H,0,1.1627182701,-3.8893091367,-1.6262714842
H,0,-0.5245979479,-3.7438604515,-1.1391214081
H,0,2.9195493988,2.2272971398,-0.7988853532
H,0,2.958162511,4.5071119672,0.2285997082
H,0,0.9814608497,5.2838239004,1.5113663408
H,0,-1.001021369,3.8615885057,1.7207605323
H,0,-2.8428489408,2.5807848537,1.4914952227
H,0,-2.946407622,0.843856474,1.8207882057
H,0,-1.743972846,1.8251649496,2.671584183
H,0,-2.6685315716,0.2662108349,-0.4539688326
H,0,-2.5375314257,1.9742666594,-0.927374425
H,0,-1.2557498191,0.820060272,-1.3610592252

OEt 3-nitrophenyl carbonate

E (total electronic) = -853.8288892
E (total electronic) + ZPVE = -853.657778
Internal Thermal Energy = -853.643544
Enthalpy = -853.642600
Gibbs Free Energy = -853.702735

C,0,0.039289811,-2.8528996096,-1.7524104531
C,0,0.1563740426,-3.2864531919,-3.210789744
O,0,0.0495426475,-4.6402169728,-3.3214749242
O,0,0.1522999633,-1.4044630364,-1.6843029552
C,0,0.0418221649,-0.87702017,-0.4904366707
O,0,-0.1401993682,-1.4482934281,0.549240649
O,0,0.1772234211,0.4667299061,-0.6174092222
C,0,0.0404791553,1.2271427913,0.5311699211
C,0,-1.1687720123,1.2796511448,1.2099301026
C,0,-1.2930401333,2.1064665906,2.3167334726
C,0,-0.2227830837,2.8819074427,2.7412905092
C,0,0.9611674557,2.802287148,2.03117596
C,0,1.1252996426,1.9835002825,0.9258321014
N,0,2.1036501004,3.6204358024,2.4633433534
O,0,3.1327168283,3.5436939486,1.8226642561
O,0,1.9583851304,4.3298096431,3.4382215786
H,0,-0.9264266482,-3.1417090521,-1.3357402881
H,0,0.8370642393,-3.2883092998,-1.1490053576
H,0,1.121142408,-2.8728762579,-3.5809728409
H,0,-0.6249939971,-2.7200928136,-3.765371633
H,0,-2.0004195395,0.6772831953,0.8688702473
H,0,-2.2323899112,2.1514693239,2.850356323
H,0,-0.3011665569,3.5355121649,3.5972013726

OEt 3-cyanophenyl carbonate

E (total electronic) = -741.5737736
E (total electronic) + ZPVE = -741.406631

Internal Thermal Energy = -741.393196
Enthalpy = -741.392252
Gibbs Free Energy = -741.449211

C,0,0.2422072959,-2.8161178455,-1.1828181325
C,0,0.3182949378,-3.4498944058,-2.568922242
O,0,0.3764271916,-4.8079367724,-2.4770254295
O,0,0.177525788,-1.3715225553,-1.3342366154
C,0,0.0894450016,-0.680619293,-0.2242413731
O,0,0.0560984317,-1.101735893,0.8993673026
O,0,0.0474221829,0.632697108,-0.5568704958
C,0,-0.094121966,1.5435402505,0.477857645
C,0,-1.2591670689,1.5868130323,1.2285179492
C,0,-1.3985821202,2.5576533958,2.2096516838
C,0,-0.3872707136,3.480259931,2.4344662104
C,0,0.7717689406,3.4195474606,1.6634628459
C,0,0.9305302863,2.4459916249,0.6773313664
C,0,1.8239957644,4.3737409254,1.8853535367
N,0,2.6623559767,5.1371470671,2.0651247034
H,0,-0.650870801,-3.1464388749,-0.6506431333
H,0,1.1254867193,-3.0611663049,-0.5911567294
H,0,1.1972148317,-2.9886411443,-3.072618465
H,0,-0.5624785507,-3.0678311387,-3.1321571167
H,0,-2.0441502405,0.8659309361,1.0409661778
H,0,-2.3040926897,2.5978251215,2.7997248611
H,0,-0.4916158317,4.2423233347,3.1945683913
H,0,1.8273896337,2.3931800398,0.0752580591

OEt 3-methoxyphenyl carbonate

E (total electronic) = -763.8471966
E (total electronic) + ZPVE = -763.645836
Internal Thermal Energy = -763.631661
Enthalpy = -763.630716
Gibbs Free Energy = -763.689500

C,0,0.6959591826,-2.7440812693,-1.0960279936
C,0,0.3741133442,-3.5313846804,-2.363293242
O,0,0.7669721775,-4.8306723607,-2.2415462888
O,0,0.2606402842,-1.3706308469,-1.2768464768
C,0,0.4678746433,-0.5622579234,-0.2623052594
O,0,0.973215186,-0.837216237,0.7927847739
O,0,0.011886442,0.6611254116,-0.6036483356
C,0,0.1387281718,1.6628886875,0.3584536339
C,0,1.2121169285,2.5236232629,0.283696374
C,0,1.2860763576,3.5575584783,1.215483668
C,0,0.3115484794,3.7104571379,2.1830673816
C,0,-0.7673394968,2.8231824909,2.2354831297
C,0,-0.8602622078,1.7855073274,1.3131935115
O,0,-1.6773776914,3.0469982832,3.2132037684
C,0,-2.7851153479,2.1629413919,3.2943390319
H,0,0.1734472117,-3.1618007776,-0.234072188
H,0,1.7691806223,-2.7432374124,-0.8991156957
H,0,0.8630043872,-2.984089211,-3.2002814421
H,0,-0.7170886764,-3.4004414195,-2.5397654703
H,0,1.9636214013,2.3882556502,-0.4821119679
H,0,2.116918479,4.2503781727,1.1807814111
H,0,0.3605602056,4.5112059081,2.9094284137
H,0,-1.6764873711,1.0775084669,1.3131319478
H,0,-3.3842198722,2.5079102963,4.1318567215
H,0,-2.4532577346,1.1390957118,3.4784103111
H,0,-3.3797061063,2.1990174607,2.3792272822

OEt 3-chlorophenyl carbonate

E (total electronic) = -1108.9312891
E (total electronic) + ZPVE = -1108.772474
Internal Thermal Energy = -1108.759617
Enthalpy = -1108.758673
Gibbs Free Energy = -1108.814813

C,0,0.241410675,-2.809194852,-0.8048989093
C,0,-0.0492749858,-3.6812976648,-2.0231397943

O,0,0.0802149339,-5.0025022508,-1.7165826193
O,0,0.0786090694,-1.4154017717,-1.1819762079
C,0,0.2788443723,-0.5341649656,-0.2311271431
O,0,0.5827315512,-0.7494796793,0.910366017
O,0,0.0892365482,0.6962785756,-0.7616381745
C,0,0.2027158213,1.7818107693,0.0965415279
C,0,-0.7368005151,1.9940711212,1.0915122963
C,0,-0.6269944698,3.1302176747,1.8795804209
C,0,0.4004347715,4.0433362774,1.6730327384
C,0,1.317235142,3.7978703829,0.6647666216
C,0,1.2383492103,2.6687569806,-0.1351462105
Cl,0,2.6098876228,4.9373349493,0.3858409651
H,0,-0.4525098288,-3.0296321597,0.0074932052
H,0,1.2641159584,-2.9548180193,-0.4537330942
H,0,0.636980121,-3.3298263249,-2.8260219424
H,0,-1.0651827996,-3.391736876,-2.3741600505
H,0,-1.5354093889,1.2797928465,1.2409724986
H,0,-1.3514375275,3.3123764683,2.6623313282
H,0,0.4860957151,4.9326966871,2.2819984843
H,0,1.955187003,2.4795198309,-0.9223259574

OEt 3-fluorophenyl carbonate

E (total electronic) = -748.5728441
E (total electronic) + ZPVE = -748.412634
Internal Thermal Energy = -748.400156
Enthalpy = -748.399212
Gibbs Free Energy = -748.454068

C,0,0.2066162583,-2.8104631456,-0.6235221151
C,0,0.008808212,-3.7173997303,-1.8348417044
O,0,0.171336509,-5.0260678865,-1.4920150939
O,0,0.0118878874,-1.4312252364,-1.0372312672
C,0,0.1407096242,-0.5251198986,-0.0970742316
O,0,0.4041022113,-0.7082326782,1.0601587033
O,0,-0.0704064413,0.6875434027,-0.6578620656
C,0,-0.0237010725,1.7879078444,0.189192676
C,0,-1.0569214904,2.0263459192,1.0798346118
C,0,-1.0126622728,3.1713473994,1.8629238264
C,0,0.044182755,4.0678258518,1.7549342573
C,0,1.0470406235,3.7857866205,0.8494528996
C,0,1.0448630223,2.6556302195,0.054115638
F,0,2.0757470555,4.644825343,0.7301930053
H,0,-0.5178762452,-3.0410594017,0.158828445
H,0,1.2151537757,-2.9109498689,-0.2197903959
H,0,0.7209108148,-3.3574974402,-2.6109448651
H,0,-0.9983683577,-3.4742528377,-2.2416372882
H,0,-1.8764309132,1.3241085071,1.1535626052
H,0,-1.8117002531,3.3717139216,2.5642237675
H,0,0.0947682301,4.9676703772,2.3526156368
H,0,1.8441430671,2.4607827179,-0.6477245455

OEt 3-methylphenyl carbonate

E (total electronic) = -688.637386
E (total electronic) + ZPVE = -688.441606
Internal Thermal Energy = -688.428038
Enthalpy = -688.427094
Gibbs Free Energy = -688.484946

C,0,0.2943395851,-2.7330992998,-0.8346348429
C,0,0.4203715929,-3.5013325072,-2.1474953229
O,0,0.3189807238,-4.8439989946,-1.9386126669
O,0,0.4267606142,-1.3145544912,-1.1132482661
C,0,0.3494973478,-0.5119430075,-0.0755511979
O,0,0.1763516426,-0.8262495949,1.0713940571
O,0,0.4937261253,0.7539088345,-0.5179875436
C,0,0.4794561072,1.7653723174,0.4423106516
C,0,1.5787731366,1.9522398125,1.2634389011
C,0,1.5545380257,3.009711407,2.1603418099
C,0,0.4534849996,3.8580274885,2.2211282862
C,0,-0.6446094294,3.6667048979,1.3867815155
C,0,-0.6213161377,2.5975182222,0.4905211292
C,0,-1.828361114,4.595105157,1.4253372769

H,0,-0.6781417013,-2.9065603972,-0.3712443477
H,0,1.0807247315,-3.0236312088,-0.1363154408
H,0,1.3864119586,-3.1822196832,-2.599256667
H,0,-0.3584740686,-3.0852725968,-2.8252659676
H,0,2.4248339807,1.2805221025,1.1976904326
H,0,2.3999256393,3.1747278127,2.816167598
H,0,0.4486216926,4.6809404121,2.9260781868
H,0,-1.4564025193,2.4107905168,-0.1746722559
H,0,-2.7644448135,4.0366922655,1.3926736093
H,0,-1.816762872,5.266350115,0.5638563257
H,0,-1.8187252479,5.2050794196,2.3276597396

OEt 3-(trifluoromethyl)phenyl carbonate

E (total electronic) = -986.3897011
E (total electronic) + ZPVE = -986.216424
Internal Thermal Energy = -986.201175
Enthalpy = -986.200231
Gibbs Free Energy = -986.263190

C,0,0.1032704007,-3.2195054378,-1.5938682883
C,0,-0.052508422,-3.8791400085,-2.9611999439
O,0,-0.0650675146,-5.2366522206,-2.8472765828
O,0,0.1006804872,-1.7769098664,-1.771079208
C,0,0.2299224364,-1.0629855162,-0.6789477522
O,0,0.3488818713,-1.464557456,0.4462259702
O,0,0.2149568131,0.2433876117,-1.0350891887
C,0,0.2961548538,1.1808393822,-0.0160323879
C,0,-0.7292124202,1.3120428254,0.9082103661
C,0,-0.6458863776,2.3062621192,1.8703564891
C,0,0.447246306,3.1645649913,1.9031224875
C,0,1.45595848,3.0127792367,0.964724267
C,0,1.3930968686,2.018562209,-0.0043640724
C,0,2.6215431475,3.9545701054,0.9468082798
F,0,3.7688519279,3.3294260155,0.6475908074
F,0,2.4672194479,4.9218981881,0.0255982823
F,0,2.7996047547,4.5685423655,2.1214457571
H,0,-0.7234258061,-3.4866618516,-0.933975177
H,0,1.0453925722,-3.5073221731,-1.1252109378
H,0,0.7744318679,-3.4817677983,-3.5915701968
H,0,-0.9777185205,-3.4500040155,-3.4071462424
H,0,-1.5761265002,0.6395452744,0.8692688884
H,0,-1.4384329076,2.4156364422,2.5983086284
H,0,0.5122202782,3.9417152421,2.6523937117
H,0,2.1779389554,1.8915163353,-0.7388429569

OEt 3-(dimethylamino)phenyl carbonate

E (total electronic) = -783.2779661
E (total electronic) + ZPVE = -783.036038
Internal Thermal Energy = -783.020099
Enthalpy = -783.019155
Gibbs Free Energy = -783.081771

C,0,0.6302304519,-3.58396083,-0.3529291232
C,0,0.6811998647,-4.6323180142,-1.4607641805
O,0,0.6894850327,-5.891543584,-0.9396116227
O,0,0.6154450311,-2.2657143591,-0.9595679892
C,0,0.5300193846,-1.2487427525,-0.1301386122
O,0,0.4712285967,-1.2981857775,1.0696035559
O,0,0.5169697667,-0.1162665305,-0.8592510839
C,0,0.4276712724,1.0840084289,-0.1482757597
C,0,1.5919857048,1.7233916826,0.2308330464
C,0,1.4597032748,2.9399321295,0.8901171668
C,0,0.2164816414,3.4923578027,1.1505211562
C,0,-0.9646897378,2.8394850102,0.7423179452
C,0,-0.8299728425,1.5992504163,0.0905536015
N,0,-2.2066268542,3.3957073457,0.9582703979
C,0,-3.3794791062,2.556743594,0.7845595836
C,0,-2.3138765626,4.5130042887,1.8804121108
H,0,-0.2718375889,-3.6982593929,0.2500089929
H,0,1.505504529,-3.65789127,0.2946896029
H,0,1.5754295778,-4.3886428193,-2.0773224524
H,0,-0.1859151565,-4.420915741,-2.1259556529

H,0,2.5556881549,1.2798718473,0.0216361138
H,0,2.3467267464,3.4705735522,1.213175087
H,0,0.166429978,4.4371842435,1.670664643
H,0,-1.6865876778,1.0285749396,-0.236716135
H,0,-3.3573854238,1.6730818587,1.4337056924
H,0,-4.2664708112,3.1390610205,1.0189580623
H,0,-3.4664515558,2.2225970042,-0.2502028882
H,0,-1.7472506998,5.3708921521,1.516530882
H,0,-3.3564989401,4.8113201633,1.9502762286
H,0,-1.9526960507,4.2593315909,2.8842316306

OEt 4-(trifluoromethyl)phenyl carbonate

E (total electronic) = -986.3904065
E (total electronic) + ZPVE = -986.217174
Internal Thermal Energy = -986.201885
Enthalpy = -986.200941
Gibbs Free Energy = -986.263953

C,0,0.3007595727,-3.5043824117,-0.5128031426
C,0,0.2113029875,-4.5594455357,-1.6116466716
O,0,0.4516385942,-5.802815298,-1.1096568473
O,0,0.0405195212,-2.1991800434,-1.0971384381
C,0,0.0653115295,-1.1835496678,-0.2682530332
O,0,0.2742950165,-1.2108011493,0.9136076546
O,0,-0.1807156261,-0.0604015027,-0.9836193337
C,0,-0.2593133758,1.137243693,-0.2901824977
C,0,0.6410596005,2.1297179313,-0.6273804883
C,0,0.5423055012,3.3702881683,-0.010449238
C,0,-0.4508681364,3.5873017474,0.9307286794
C,0,-1.3529881674,2.5799637638,1.262234612
C,0,-1.2614327255,1.3448999177,0.6474435985
C,0,-0.5870994119,4.9116721419,1.6148697171
F,0,-0.4754542883,4.8003767083,2.9494285977
F,0,0.3356080766,5.7941523192,1.2186585085
F,0,-1.7876153139,5.4716673663,1.3879041157
H,0,-0.4408824664,-3.6871511851,0.2659463488
H,0,1.2957999088,-3.4894469757,-0.0655657031
H,0,0.9252600953,-4.2416568021,-2.4042746112
H,0,-0.7942880383,-4.4402378804,-2.0736799003
H,0,1.4047349045,1.9296627678,-1.3667436145
H,0,1.2380203998,4.1581510823,-0.2643388947
H,0,-2.1280509616,2.7624808174,1.9962589729
H,0,-1.9540761967,0.5490720274,0.8857046092

OEt 2,4-dinitrophenyl carbonate

E (total electronic) = -1058.318802
E (total electronic) + ZPVE = -1058.144838
Internal Thermal Energy = -1058.128210
Enthalpy = -1058.127266
Gibbs Free Energy = -1058.192308

C,0,0.6170331093,-3.3730642063,-0.5727240858
C,0,0.8322995734,-4.3982316571,-1.6815172189
O,0,0.6027124315,-5.6570891932,-1.2156868481
O,0,0.8996999699,-2.0427457722,-1.1014677271
C,0,0.7860639034,-1.060480091,-0.255210256
O,0,0.4603887109,-1.0993667699,0.8977911528
O,0,1.1340291206,0.0910725723,-0.9067314477
C,0,0.982298922,1.269437304,-0.2382208477
C,0,2.0932128829,2.0971279884,-0.1687297989
C,0,2.0148327405,3.324830738,0.4618747316
C,0,0.8137316166,3.7001347958,1.0395380705
C,0,-0.3094693715,2.9003883886,0.9984172137
C,0,-0.2176788275,1.6912750131,0.338739001
N,0,0.7231473301,4.9966349345,1.7233922288
N,0,-1.4426772911,0.8901450069,0.2459525648
O,0,-0.3388038963,5.2964561388,2.2278782717
O,0,1.7170882978,5.6916857828,1.7439945365
O,0,-2.2458352277,0.9950908881,1.145990767
O,0,-1.5875516668,0.1928115198,-0.7367755589
H,0,-0.4141177071,-3.3843303972,-0.2174246504
H,0,1.2919774283,-3.555179312,0.2641949891

H,0,1.8654869854,-4.2318421301,-2.0601254277
H,0,0.1697085319,-4.0934435435,-2.5219373083
H,0,3.0174445808,1.7540936712,-0.6123603647
H,0,2.8729167133,3.9786348325,0.5178587077
H,0,-1.2394278606,3.2097014979,1.4524213049

OEt 2,4-dicyanophenyl carbonate

E (total electronic) = -833.8144152
E (total electronic) + ZPVE = -833.648623
Internal Thermal Energy = -833.633401
Enthalpy = -833.632457
Gibbs Free Energy = -833.693144

C,0,-0.38515807,-3.8663558405,-0.2765368983
C,0,-0.5477142637,-4.7612679531,-1.5013119212
O,0,-0.3787213597,-6.0701870193,-1.1645518212
O,0,-0.5744287116,-2.4794276481,-0.6832839783
C,0,-0.4541704534,-1.5873660603,0.2607359236
O,0,-0.2095131931,-1.7574825822,1.4215402843
O,0,-0.6531543885,-0.3578636469,-0.3016950451
C,0,-0.6208082736,0.7248708827,0.5419568878
C,0,0.4015235223,1.6440772228,0.4024664002
C,0,0.4110163145,2.7782177168,1.1960073253
C,0,-0.6059224351,2.9831560083,2.1289805173
C,0,-1.6385149451,2.0625812702,2.2704224111
C,0,-1.6461618078,0.9285526097,1.4683519367
C,0,-0.5918142265,4.1609976247,2.952199132
C,0,-2.7084599747,-0.0297706052,1.5725594231
N,0,-0.5780715708,5.1023705552,3.6080710622
N,0,-3.5561793635,-0.7996892552,1.640236624
H,0,-1.1301817034,-4.1023561362,0.4843949449
H,0,0.6135341688,-3.9629631042,0.1510728592
H,0,0.1777276997,-4.3866365078,-2.2576213593
H,0,-1.5482494874,-4.5244789214,-1.9274002576
H,0,1.1784596411,1.4622381072,-0.3271207251
H,0,1.205942164,3.504667497,1.0966482043
H,0,-2.4296872823,2.2240677857,2.9892700701

OEt 2,4-dimethoxyphenyl carbonate

E (total electronic) = -878.3633488
E (total electronic) + ZPVE = -878.128732
Internal Thermal Energy = -878.112068
Enthalpy = -878.111124
Gibbs Free Energy = -878.174757

C,0,0.8598794471,-3.8951038463,-0.954554917
C,0,0.6958530616,-4.8983764935,-2.0927546467
O,0,0.7590149282,-6.1759475399,-1.6218524154
O,0,0.8081948506,-2.5501977007,-1.4981941516
C,0,0.9457410472,-1.5747467271,-0.6280024924
O,0,1.0884295849,-1.6792263454,0.5601698188
O,0,0.9175366595,-0.4054958206,-1.303420511
C,0,0.9233716705,0.7480266313,-0.5284183635
C,0,2.0407153348,1.5410295708,-0.4826610492
C,0,2.0382054059,2.7354836065,0.2398264507
C,0,0.8831764479,3.1024179888,0.9158227693
C,0,-0.2609514886,2.2963950596,0.8713254653
C,0,-0.2485123755,1.1172635895,0.1474497673
O,0,-1.2910971255,0.2684669636,0.0299548207
C,0,-2.4880947074,0.607597166,0.7159439208
O,0,0.7571699229,4.2344734749,1.6538920646
C,0,1.8892935433,5.0849351295,1.7419057603
H,0,0.0588340482,-4.0034206467,-0.2216910069
H,0,1.8211687842,-4.0290919387,-0.4558468861
H,0,1.4807479919,-4.6486602121,-2.8414305571
H,0,-0.2644953906,-4.6453203959,-2.5953554929
H,0,2.9266030268,1.2252060417,-1.0189668847
H,0,2.9276746916,3.3462840348,0.2615751441
H,0,-1.1380657626,2.6234816651,1.4109283595
H,0,-3.1924248806,-0.1904289911,0.5013695273
H,0,-2.3135643434,0.6659057937,1.7918706707
H,0,-2.8860774594,1.5572732802,0.3536092942

H,0,1.5907995037,5.9189446127,2.3704445808
H,0,2.733006376,4.5644952228,2.1998509993
H,0,2.1773692069,5.4544218264,0.7555759607

OEt 2,4-dichlorophenyl carbonate

E (total electronic) = -1568.5313112
E (total electronic) + ZPVE = -1568.381854
Internal Thermal Energy = -1568.367868
Enthalpy = -1568.366924
Gibbs Free Energy = -1568.425428

C,0,0.6749890117,-3.2128590227,0.4942245133
C,0,0.4535616114,-4.5805125576,-0.1448281356
O,0,0.848532669,-5.5722222245,0.7021020473
O,0,0.2596230177,-2.1793128168,-0.4416202419
C,0,0.4069015175,-0.9457231896,-0.0290037314
O,0,0.8302271722,-0.5689512992,1.028523247
O,0,-0.0020948508,-0.1193370922,-1.0269823073
C,0,-0.0024510084,1.2298169903,-0.7352831407
C,0,0.9825259395,2.0372810591,-1.272692916
C,0,0.963040006,3.4051757083,-1.0450638105
C,0,-0.0529121851,3.9411387343,-0.270839802
C,0,-1.0486666543,3.1478616597,0.2756401588
C,0,-1.0160346576,1.7845186327,0.0355382724
Cl,0,-0.0889642638,5.6576044101,0.0267082102
Cl,0,-2.2498241028,0.7616272585,0.6950752856
H,0,0.0846286701,-3.1071895452,1.4054835983
H,0,1.7291890461,-3.0592102492,0.7286371918
H,0,0.9997640751,-4.5625946791,-1.114324291
H,0,-0.6222404698,-4.6228488858,-0.426764562
H,0,1.7611860978,1.5834967126,-1.8714465115
H,0,1.7283312493,4.0448051438,-1.4617866432
H,0,-1.8378738909,3.5780142525,0.8761755683

OEt 2,4-difluorophenyl carbonate

E (total electronic) = -847.8122759
E (total electronic) + ZPVE = -847.660191
Internal Thermal Energy = -847.646833
Enthalpy = -847.645889
Gibbs Free Energy = -847.702825

C,0,0.126723715,-3.0737856725,-0.5565141254
C,0,-0.1254410409,-4.0134907308,-1.7318522992
O,0,0.0947312987,-5.3082364844,-1.3696523681
O,0,-0.1128918296,-1.7066140714,-0.9907011504
C,0,0.0710947113,-0.7781465507,-0.0855295046
O,0,0.4031290978,-0.9226684195,1.0583658786
O,0,-0.1741577658,0.4240810596,-0.6672383061
C,0,-0.0784862376,1.5309135829,0.1542242689
C,0,0.9211658939,2.4624433913,-0.0478226233
C,0,0.974168137,3.6093311777,0.7343191598
C,0,0.0134563641,3.7832833692,1.7095945295
C,0,-1.0007274996,2.8712369436,1.9390989796
C,0,-1.0277469949,1.7474447264,1.1412540198
F,0,-1.9924509872,0.8380935369,1.3115396355
F,0,0.0557992526,4.8866580399,2.4744821445
H,0,-0.5467776167,-3.2940675465,0.2729207845
H,0,1.1590526273,-3.1482693786,-0.2118844256
H,0,0.5253433264,-3.6545361318,-2.5604196073
H,0,-1.1629416051,-3.8065770902,-2.0776574441
H,0,1.6539725542,2.2829897403,-0.8232150391
H,0,1.7450238533,4.3541253831,0.5948850943
H,0,-1.7450012542,3.0297901258,2.7070843981

OEt 3,5-dinitrophenyl carbonate

E (total electronic) = -1058.3221485
E (total electronic) + ZPVE = -1058.148408
Internal Thermal Energy = -1058.131641
Enthalpy = -1058.130696
Gibbs Free Energy = -1058.196701

C,0,-0.1548151846,-3.1780860092,-0.8430043961
C,0,0.0648319696,-4.0470958648,-2.0776634736
O,0,-0.0900513767,-5.3650311951,-1.7708118106
O,0,0.0150348095,-1.7812751373,-1.220201609
C,0,-0.1424436678,-0.9073864567,-0.2626753996
O,0,-0.4093627252,-1.1096009105,0.8883648144
O,0,0.0613246432,0.3295111561,-0.7987942719
C,0,-0.087544244,1.4201807067,0.024146695
C,0,0.9519831978,2.3323982591,0.0513772207
C,0,0.7922576726,3.4774624775,0.8115466622
C,0,-0.3452646916,3.745070304,1.5446621469
C,0,-1.3500639566,2.7991482423,1.4804034856
C,0,-1.2582558459,1.6394806589,0.7340038562
N,0,-2.5887755697,3.044820291,2.2401373921
O,0,-3.4611601776,2.2054464352,2.1790617241
O,0,-2.6602135791,4.0720457765,2.8798666633
N,0,1.8919942178,4.4567812591,0.8438661652
O,0,1.7399759415,5.449616146,1.522662594
O,0,2.88243824,4.2104651257,0.1896920853
H,0,-1.1636487148,-3.3044523768,-0.4477624296
H,0,0.5713917191,-3.4125408797,-0.0635996272
H,0,1.0740227604,-3.78374849,-2.4660269796
H,0,-0.6424470147,-3.6715391927,-2.8505654453
H,0,1.8584749278,-2.1531467815,-0.5086426147
H,0,-0.4459777574,4.6436953765,2.1333504152
H,0,-2.0749595937,0.9335655166,0.706740137

OEt 3,5-dicyanophenyl carbonate

E (total electronic) = -833.8135017
E (total electronic) + ZPVE = -833.647825
Internal Thermal Energy = -833.632553
Enthalpy = -833.631609
Gibbs Free Energy = -833.692915

C,0,-0.3379376996,-3.0152059973,-0.0568165907
C,0,-0.3423172118,-4.1575908127,-1.0682595166
O,0,-0.3766393493,-5.3622468698,-0.4335531387
O,0,-0.3083127606,-1.7526309095,-0.7813562198
C,0,-0.2990969495,-0.6710587645,-0.0474975686
O,0,-0.3107294092,-0.5904752576,1.1488733787
O,0,-0.264787941,0.3969746562,-0.8908594344
C,0,-0.2869568104,1.6570767126,-0.3350164442
C,0,0.7157261911,2.5291793449,-0.7143133119
C,0,0.6858907434,3.8387726809,-0.2380677018
C,0,-0.3248192407,4.271671635,0.611571488
C,0,-1.3188665661,3.3678537029,0.9737120556
C,0,-1.3141576197,2.0575385239,0.5031905371
C,0,1.720117863,4.7574102453,-0.6314188093
C,0,-2.3783764303,3.7978598928,1.8462794
N,0,-3.2235296383,4.1417788007,2.5414633711
N,0,2.5442396931,5.4910837351,-0.9451518859
H,0,-1.2371025376,-3.0342370459,0.5606244611
H,0,0.542665883,-3.0628702433,0.5852157955
H,0,0.5535349248,-4.0051542137,-1.7108587864
H,0,-1.2083781124,-3.9712160818,-1.7420022892
H,0,1.5031245551,2.1899412634,-1.3736268319
H,0,-0.3404913407,5.2874764413,0.9803330847
H,0,-2.0957102361,1.3655955611,0.7839269576

OEt 3,5-dimethoxyphenyl carbonate

E (total electronic) = -878.3654305
E (total electronic) + ZPVE = -878.131106
Internal Thermal Energy = -878.114405
Enthalpy = -878.113460
Gibbs Free Energy = -878.177588

C,0,0.9511522589,-3.4633767783,0.2143426715
C,0,0.850298325,-4.7457359769,-0.6067984656
O,0,1.0626378416,-5.8386272278,0.1793371725
O,0,0.7211712964,-2.324948179,-0.6576244794

C,0,0.7587565611,-1.144833346,-0.0814686482
O,0,0.9595860196,-0.911029593,1.0799301701
O,0,0.5322810497,-0.2101756423,-1.0283145917
C,0,0.5108078552,1.115812421,-0.5977747233
C,0,1.6512101348,1.8650227561,-0.7393438039
C,0,1.6048003244,3.2137921944,-0.3639856301
C,0,0.4361432784,3.7656832739,0.1348133999
C,0,-0.7051448939,2.9649894215,0.261684464
C,0,-0.684222056,1.6261870538,-0.1048344453
O,0,-1.7978552734,3.5929775022,0.7558919303
C,0,-2.9837201086,2.8264441168,0.9047199255
O,0,2.7577598034,3.903830849,-0.5258321995
C,0,2.7608949842,5.2746517211,-0.1562770387
H,0,0.2008334168,-3.4492469031,1.0061480915
H,0,1.9426942038,-3.3628268259,0.6586190474
H,0,1.5764930258,-4.6374874945,-1.4433062039
H,0,-0.1494150724,-4.7237120932,-1.0956551136
H,0,2.562186796,1.4335222428,-1.1303233026
H,0,0.3656941585,4.8017071989,0.4315147904
H,0,-1.5447343777,0.9796094812,-0.0231988499
H,0,-3.7295042088,3.5033987747,1.3107685463
H,0,-2.8260133052,1.996727231,1.5965352384
H,0,-3.3226240707,2.443437494,-0.0598656441
H,0,2.5352249476,5.39145525,0.9054880117
H,0,3.7643905058,5.6373117515,-0.3583297197
H,0,2.0399295796,5.839174326,-0.7508245999

OEt 3,5-dichlorophenyl carbonate

E (total electronic) = -1568.5314774
E (total electronic) + ZPVE = -1568.382374
Internal Thermal Energy = -1568.368242
Enthalpy = -1568.367297
Gibbs Free Energy = -1568.427186

C,0,0.2500740447,-2.7766289827,-0.6826574597
C,0,0.2608302085,-3.6711263421,-1.9186469045
O,0,0.3135588223,-4.9850302895,-1.5616013963
O,0,0.1982544638,-1.3871508998,-1.1094996507
C,0,0.1927936418,-0.4942141297,-0.1510799977
O,0,0.2195388732,-0.6891017504,1.0327702273
O,0,0.1577175476,0.7332635731,-0.7276669517
C,0,0.1129585552,1.8232848082,0.1253136581
C,0,1.2186545539,2.6522708077,0.1679358294
C,0,1.1506097959,3.782327563,0.9670692218
C,0,0.0237910003,4.0894776789,1.7106184031
C,0,-1.0587174139,3.2261781277,1.6342975016
C,0,-1.0387534105,2.0886521833,0.8469224968
Cl,0,2.5251019577,4.8475032026,1.0417596698
Cl,0,-2.4895167487,3.590996233,2.5561960443
H,0,-0.6239505793,-2.977949588,-0.0616010515
H,0,1.1541718553,-2.9198793754,-0.0893767762
H,0,1.1203674345,-3.3320229561,-2.5391040737
H,0,-0.6407742677,-3.3946798548,-2.5098433559
H,0,2.1016192574,2.4179229781,-0.4099179633
H,0,-0.0122350821,4.974755442,2.3291632184
H,0,-1.8901355098,1.4245243778,0.7926893107

OEt 3,5-difluorophenyl carbonate

E (total electronic) = -847.814852
E (total electronic) + ZPVE = -847.663028
Internal Thermal Energy = -847.649661
Enthalpy = -847.648717
Gibbs Free Energy = -847.706059

C,0,0.0338046755,-2.9033420314,-0.757015992
C,0,0.0982766358,-3.7759053704,-2.0072749198
O,0,0.0408339585,-5.0968843592,-1.6792048175
O,0,0.0798403272,-1.5076926875,-1.1618729495
C,0,0.0336410718,-0.6258371131,-0.1937990868
O,0,-0.0378144245,-0.8362380883,0.9853251709
O,0,0.0911194288,0.6061947639,-0.7576821447
C,0,0.0042984911,1.7025040069,0.0820298036

C,0,1.0736505439,2.5805263777,0.0850151325
C,0,0.9577218166,3.7193335798,0.8591837506
C,0,-0.1581644709,4.0076123664,1.6187779957
C,0,-1.1902000349,3.0889179893,1.5724669941
C,0,-1.1469229766,1.9344436147,0.8177989568
F,0,1.9800582569,4.5870865513,0.87439609
F,0,-2.2922368248,3.337348704,2.2955807856
H,0,-0.8952732666,-3.0727121916,-0.2106406312
H,0,0.8802863505,-3.0994005524,-0.097288469
H,0,1.0268161951,-3.4789495204,-2.5443750597
H,0,-0.7305971686,-3.4327345832,-2.6660713408
H,0,1.9621020323,2.3862548206,-0.4987957505
H,0,-0.223493204,4.9056418073,2.2163439603
H,0,-1.978754413,1.2446289155,0.8078795214

OEt 3,5-dimethylphenyl carbonate

E (total electronic) = -727.9455561
E (total electronic) + ZPVE = -727.722202
Internal Thermal Energy = -727.706898
Enthalpy = -727.705953
Gibbs Free Energy = -727.767380

C,0,-0.4423264825,-2.9286498268,-0.9670188515
C,0,-0.3892788237,-3.7728862227,-2.2370350561
O,0,-0.5079236251,-5.098746033,-1.9438235166
O,0,-0.3226707124,-1.5282259681,-1.3300415135
C,0,-0.3539177354,-0.6709808388,-0.3337828844
O,0,-0.4686753941,-0.9258018507,0.8352752225
O,0,-0.2285282041,0.5693043163,-0.8463098698
C,0,-0.2707865067,1.6301672596,0.0605951298
C,0,0.9107136036,2.2654907097,0.3781961775
C,0,0.8817395404,3.3739570199,1.2268118984
C,0,-0.3429686282,3.7963620844,1.7306180216
C,0,-1.5376319427,3.147728804,1.4091360007
C,0,-1.4936318097,2.0517605237,0.5561443962
C,0,-2.8422378204,3.6167614455,1.9954128216
C,0,2.1579502069,4.0965517016,1.5652124852
H,0,-1.3899583505,-3.0709063606,-0.4453618936
H,0,0.3782388769,-3.183538249,-0.2945329818
H,0,0.5610988588,-3.5029708891,-2.7497830631
H,0,-1.1901880674,-3.3803255369,-2.9030558928
H,0,1.8430183243,1.9027845237,-0.0383255068
H,0,-0.3739726993,4.6572488402,2.3905810989
H,0,-2.3968423387,1.5231126153,0.2751964799
H,0,-3.6893573593,3.2479460319,1.4182651779
H,0,-2.8877785904,4.7056814744,2.0246237432
H,0,-2.9517306773,3.2556529186,3.020508846
H,0,1.9977292918,4.826402748,2.3575759864
H,0,2.9278895886,3.3953915415,1.8900764197

OEt 3,5-di(trifluoromethyl)phenyl carbonate

E (total electronic) = -1323.4475666
E (total electronic) + ZPVE = -1323.269579
Internal Thermal Energy = -1323.250645
Enthalpy = -1323.249701
Gibbs Free Energy = -1323.322228

C,0,-2.7724079298,-1.1755813633,-1.4370068104
C,0,-3.9227356911,-0.7739184037,-2.3550364721
O,0,-4.849764532,-1.7700482947,-2.4235470654
O,0,-1.7963945354,-0.0964232766,-1.4037212565
C,0,-0.7443348964,-0.3027685206,-0.6534605829
O,0,-0.4958298599,-1.2674132773,0.0151716452
O,0,0.0607678173,0.7866147773,-0.7602539197
C,0,1.2218280394,0.7921625303,-0.0126569125
C,0,2.4173249843,0.9226961306,-0.6903103973
C,0,3.5958344492,1.0056716618,0.0409680998
C,0,3.5866640099,0.9558997152,1.4231667302
C,0,2.3672020164,0.8262818983,2.0754913714
C,0,1.1778444921,0.7446801523,1.3723785061
C,0,2.3414738181,0.7278590282,3.5732662156
C,0,4.8850955228,1.1811819316,-0.7071376849

F,0,2.4542139546,-0.544192137,3.9868243566
F,0,1.2013588432,1.200635186,4.087439767
F,0,3.3469774729,1.4062751002,4.1362471904
F,0,4.9925638535,2.4152788179,-1.2228832179
F,0,5.9530255596,0.9874118799,0.0704803779
F,0,4.979024147,0.3291832128,-1.7364462992
H,0,-3.1248573564,-1.3500196483,-0.4194842952
H,0,-2.2763214426,-2.0743424375,-1.8058388096
H,0,-3.4616118244,-0.5115731952,-3.3334236994
H,0,-4.3158643248,0.1892180675,-1.9597732741
H,0,2.419445733,0.9590294421,-1.772369344
H,0,4.5081064051,1.0212459407,1.9852597558
H,0,0.2295822742,0.6501380816,1.8843740249

OEt 3,4-dicyanophenyl carbonate

E (total electronic) = -833.8129619
E (total electronic) + ZPVE = -833.647365
Internal Thermal Energy = -833.632043
Enthalpy = -833.631099
Gibbs Free Energy = -833.692594

C,0,0.1144523119,-3.7055313451,-0.6685512573
C,0,-0.1433139199,-4.594613991,-1.8818375879
O,0,-0.1666550547,-5.9080021591,-1.5221463001
O,0,0.1124533424,-2.3156821618,-1.1030281682
C,0,0.2789982321,-1.421832091,-0.1642454924
O,0,0.4405431059,-1.6048187536,1.0093159834
O,0,0.2520014975,-0.1960934621,-0.7580570436
C,0,0.3148355309,0.9212692013,0.0396896586
C,0,-0.5427930231,1.1053422034,1.1150626756
C,0,-0.4862864388,2.2873508615,1.8331637965
C,0,0.4178374439,3.2816918935,1.4734832321
C,0,1.2722330054,3.0824366559,0.3799894096
C,0,1.2228175029,1.8962602371,-0.3386463124
C,0,0.4704533017,4.5090211973,2.2144899158
N,0,0.5151402507,5.4922773414,2.8043626671
C,0,2.2047064717,4.1064940301,-0.0005951654
N,0,2.9465215932,4.9290254816,-0.2988547028
H,0,-0.6674491426,-3.829287791,0.0818171533
H,0,1.0845652998,-3.9224479322,-0.2190149778
H,0,0.6433608133,-4.3386472059,-2.6263317425
H,0,-1.0914596492,-4.2286850948,-2.3355881702
H,0,-1.2491402404,0.3336083379,1.3852225394
H,0,-1.1491953452,2.4453039504,2.6725092232
H,0,1.8753271106,1.7287965961,-1.1841873341

OEt 3,4-dimethoxyphenyl carbonate

E (total electronic) = -878.3605991
E (total electronic) + ZPVE = -878.126034
Internal Thermal Energy = -878.109314
Enthalpy = -878.108370
Gibbs Free Energy = -878.173133

C,0,1.0531782894,-3.7478804918,-1.2109982714
C,0,0.8938032612,-4.5537938609,-2.4970266895
O,0,1.0926934937,-5.8823238182,-2.2653161666
O,0,0.8150162945,-2.3458994286,-1.5022841913
C,0,0.9191887293,-1.5213681406,-0.4836276814
O,0,1.1943685304,-1.8054118828,0.6513831488
O,0,0.662893924,-0.2744221222,-0.9283658217
C,0,0.7137956665,0.7490721616,0.0195673196
C,0,1.8155469808,1.5634529012,0.0651658275
C,0,1.8311558264,2.6274096113,0.9721564629
C,0,0.7551131204,2.852923473,1.8110781785
C,0,-0.3713194164,2.001138579,1.7468229215
C,0,-0.3871044481,0.9508780412,0.8464186681
O,0,-1.3789370718,2.2946198196,2.5997095937
C,0,-2.5213716637,1.4532022784,2.5666098638
O,0,0.6765327661,3.8542691542,2.7212466643
C,0,1.7871408932,4.7315546606,2.8128365686
H,0,0.3326583276,-4.0716087445,-0.4582628236
H,0,2.0619783722,-3.8511418352,-0.8083306196

H,0,1.601706405,-4.1086041846,-3.231741505
H,0,-0.1163972836,-4.306497806,-2.8937427061
H,0,2.6539827068,1.38312172,-0.5938046517
H,0,2.6970584514,3.2721404329,1.0085163652
H,0,-1.232297669,0.2819607219,0.76972474
H,0,-3.2032891751,1.8437373889,3.3161533165
H,0,-2.2534918677,0.4240214647,2.8146427262
H,0,-2.9989003345,1.4833385318,1.5850093812
H,0,1.5370939842,5.4527679347,3.5855193511
H,0,2.6912434877,4.1887135202,3.0969803633
H,0,1.9532014188,5.2509519199,1.8665516667

OEt 3,4-dichlorophenyl carbonate

E (total electronic) = -1568.5298091
E (total electronic) + ZPVE = -1568.380469
Internal Thermal Energy = -1568.366418
Enthalpy = -1568.365474
Gibbs Free Energy = -1568.424844

C,0,0.1430548986,-2.3198628643,-2.4383371957
C,0,-0.033582319,-2.4322152949,-3.9496506398
O,0,-0.0226906461,-3.7378623653,-4.34023618
O,0,0.1212419805,-0.9147326854,-2.0648690547
C,0,0.2523084193,-0.6616848408,-0.7855338855
O,0,0.3880980387,-1.453486057,0.1064296108
O,0,0.2153647071,0.6830886119,-0.6213232821
C,0,0.2998549874,1.1546568545,0.6794927808
C,0,-0.7563445015,0.9867352859,1.5592388801
C,0,-0.6618774315,1.5277301917,2.8292153635
C,0,0.4735531219,2.2313920574,3.2096584517
C,0,1.5213898908,2.39366237,2.3116806539
C,0,1.4372774966,1.8503492828,1.0375916607
Cl,0,2.9531446256,3.2671948792,2.7501503702
Cl,0,0.5528129101,2.8981974579,4.809223543
H,0,-0.6663837306,-2.827733477,-1.9118500961
H,0,1.0978200642,-2.7441522596,-2.1242785238
H,0,0.7727860346,-1.8136044405,-4.4033891621
H,0,-0.9752657158,-1.8909372297,-4.1929088681
H,0,-1.6378898179,0.4397433123,1.2533713196
H,0,-1.4714620423,1.4105699488,3.5364702951
H,0,2.2482550294,1.970490133,0.3325239584

OEt 3,4-difluorophenyl carbonate

E (total electronic) = -847.8093251
E (total electronic) + ZPVE = -847.657219
Internal Thermal Energy = -847.643851
Enthalpy = -847.642907
Gibbs Free Energy = -847.699953

C,0,-3.1097513946,0.040076304,0.412922746
C,0,-4.3755888441,-0.3392368933,-0.3502328622
O,0,-5.4878928304,0.0408758496,0.3387433626
O,0,-1.9538149483,-0.3696140432,-0.3672706953
C,0,-0.7825369543,-0.0801775339,0.1463394191
O,0,-0.5587829389,0.4737692509,1.1877930231
O,0,0.1669723248,-0.5228684223,-0.7115045632
C,0,1.4897625622,-0.288494685,-0.3635241203
C,0,2.2901552607,-1.3757588821,-0.0693100596
C,0,3.6369897739,-1.1742433215,0.2099677924
C,0,4.1432066246,0.1065457902,0.1922931948
C,0,3.3252402329,1.1850390746,-0.1046279959
C,0,1.9901271006,1.0045275295,-0.3898954429
F,0,3.8572193762,2.411701178,-0.1139738021
F,0,5.4350828183,0.3364864949,0.4585800007
H,0,-3.0561225487,1.1187015438,0.5665847473
H,0,-3.069385644,-0.463311827,1.3800747432
H,0,-4.3081383402,-1.4340789651,-0.5389391509
H,0,-4.2803987695,0.1270295725,-1.3564481353
H,0,1.8635417564,-2.3692099037,-0.0637628646
H,0,4.2957590961,-2.0001991828,0.4418336535
H,0,1.3620432864,1.853521072,-0.6238419906

OEt 3,4-dimethylphenyl carbonate

E (total electronic) = -727.9461468
E (total electronic) + ZPVE = -727.722431
Internal Thermal Energy = -727.707449
Enthalpy = -727.706505
Gibbs Free Energy = -727.766872

C,0,-0.4853871914,-2.1242962235,-2.7806940938
C,0,-0.7146211448,-2.1262988193,-4.2892866564
O,0,-0.6301646531,-3.390780158,-4.7914833771
O,0,-0.5872829523,-0.7614068775,-2.2917299246
C,0,-0.4028639142,-0.5987011184,-1.0000491374
O,0,-0.1603984857,-1.4546057097,-0.1914398199
O,0,-0.5297618572,0.7137997891,-0.7217258186
C,0,-0.3766523911,1.0851775285,0.6160469683
C,0,0.8352040527,1.5915110835,1.035328416
C,0,0.9515885175,2.0160119897,2.3545445597
C,0,-0.1170188688,1.9373236591,3.2414451477
C,0,-1.3427247302,1.4183142009,2.7918046181
C,0,-1.4601559462,0.9958981588,1.4723951496
C,0,-2.516845189,1.3223348034,3.726545494
C,0,0.0324329108,2.4036227312,4.6638306265
H,0,-1.2363280691,-2.7310638473,-2.2722393562
H,0,0.5074501853,-2.5057677337,-2.5376825303
H,0,0.0282842095,-1.4159268685,-4.716554406
H,0,-1.7003253321,-1.6359400672,-4.4537188933
H,0,1.665517947,1.6535761231,0.3437995862
H,0,1.8972956699,2.417782293,2.6992538513
H,0,-2.3966471711,0.5944730274,1.1026549538
H,0,-2.7896607907,2.306427029,4.1145760308
H,0,-3.3845797127,0.899649916,3.2227431551
H,0,-2.2799318874,0.6945164222,4.5885813517
H,0,-0.6750876621,3.2041604564,4.8923539261
H,0,1.0393476086,2.7752720457,4.8476066564
H,0,-0.1669871521,1.5920121663,5.3674855224

OEt 3,4-di(trifluoromethyl)phenyl carbonate

E (total electronic) = -1323.4430853
E (total electronic) + ZPVE = -1323.264644
Internal Thermal Energy = -1323.246116
Enthalpy = -1323.245172
Gibbs Free Energy = -1323.314136

C,0,-0.1883697002,-3.1494328502,-1.9242871731
C,0,0.0936497763,-3.7330358721,-3.3054309028
O,0,-0.1417685181,-5.0750262484,-3.3154136582
O,0,0.0943267707,-1.7220658578,-1.9476922522
C,0,-0.0622661634,-1.0924911998,-0.8109378882
O,0,-0.428195252,-1.5482451604,0.2364615989
O,0,0.2807930564,0.2075230849,-1.0081434864
C,0,0.1465108444,1.0746165488,0.0567011133
C,0,-1.0706519526,1.2804403274,0.6762064203
C,0,-1.151239029,2.2199327465,1.6916026291
C,0,-0.0367503169,2.9491427477,2.0835048885
C,0,1.1884149251,2.7247779,1.4467360072
C,0,1.2733000733,1.7859247752,0.4314476586
C,0,2.4500810747,3.4781221709,1.794723593
F,0,2.6165408113,3.6092080933,3.1146225353
F,0,3.5357116042,2.8516708722,1.3290959382
F,0,2.4638953898,4.7086033967,1.266535488
C,0,-0.2107426745,3.9391176915,3.2076912152
F,0,0.2395268825,3.4626392354,4.3766565518
F,0,-1.4995719407,4.2442774314,3.3940432338
F,0,0.4278132498,5.0920627878,2.9785339462
H,0,-1.2342081589,-3.2875512653,-1.6462553568
H,0,0.4489133227,-3.6112429773,-1.1692657715
H,0,1.1418044037,-3.4516294362,-3.5523035776
H,0,-0.5307997004,-3.1545465712,-4.0223609766
H,0,-1.9427138926,0.7187955165,0.3717702918
H,0,-2.0998666086,2.3914691493,2.1799157402
H,0,2.2093037229,1.596419963,-0.0745218063

OEt 2,4,6-trinitrophenyl carbonate

E (total electronic) = -1262.7985319
E (total electronic) + ZPVE = -1262.622100
Internal Thermal Energy = -1262.602813
Enthalpy = -1262.601869
Gibbs Free Energy = -1262.673328

C,0,0.1022536912,-3.5185121614,0.4660454054
C,0,0.137781178,-4.7857106136,-0.381570172
O,0,0.1467997838,-5.8865563333,0.4195501594
O,0,0.1179127053,-2.3563763861,-0.4221379673
C,0,0.1157045664,-1.1999611273,0.1642707838
O,0,0.0921843045,-0.9368349521,1.3315372871
O,0,0.1557575243,-0.2366006797,-0.8196275311
C,0,0.1262203051,1.0518110693,-0.4171447019
C,0,1.1772064547,1.8927172813,-0.7743926072
C,0,1.1772721999,3.244342124,-0.502609982
C,0,0.1085488743,3.7525974737,0.2063680185
C,0,-0.945232978,2.9659408673,0.6231430886
C,0,-0.932766117,1.6278023,0.2868768463
N,0,2.3617007209,1.3380012388,-1.4476030112
N,0,0.0948442713,5.1865521036,0.5348149248
N,0,-2.0988288882,0.8278585255,0.6912120668
O,0,-0.8519344046,5.6051332164,1.1633670342
O,0,1.0316904774,5.8531408395,0.1542228552
O,0,-2.6737343503,1.1719385783,1.6979415754
O,0,-2.4176030286,-0.1027774299,-0.0159773578
O,0,2.8582447997,2.0147629423,-2.3204850153
O,0,2.7735365736,0.26790874,-1.0626639135
H,0,-0.8056974565,-3.4684557133,1.0680556708
H,0,0.9760278538,-3.4565943618,1.1151371078
H,0,1.0284408356,-4.6922090651,-1.0419662456
H,0,-0.7343325479,-4.7267823222,-1.0698675916
H,0,1.9985667979,3.8736437242,-0.8159530865
H,0,-1.7702211467,3.3832241217,1.1828563589

OEt 2,4,6-tricyanophenyl carbonate

E (total electronic) = -926.0492667
E (total electronic) + ZPVE = -925.885179
Internal Thermal Energy = -925.867976
Enthalpy = -925.867032
Gibbs Free Energy = -925.932692

C,0,0.4824025818,-3.5794284941,-0.978472355
C,0,0.5107803937,-4.4342720353,-2.2412405942
O,0,0.6597432056,-5.7489025401,-1.9195182544
O,0,0.3299215942,-2.1779345407,-1.3634982623
C,0,0.3100840612,-1.3228009018,-0.3855864919
O,0,0.388943448,-1.515344424,0.7923793311
O,0,0.1858977627,-0.0658075276,-0.9371050532
C,0,0.0785056894,0.9796058649,-0.0717661587
C,0,1.0920524895,1.933505909,-0.0497883864
C,0,0.9837921365,3.0519963886,0.7688816746
C,0,-0.1422833609,3.2053536319,1.5694450237
C,0,-1.1623142768,2.2588119496,1.5535647339
C,0,-1.0511596521,1.1474626509,0.7282823023
C,0,-0.2567699595,4.3579341239,2.4207773658
C,0,-2.1020092949,0.1720371343,0.6721340787
N,0,-0.3477483599,5.27725178,3.1000200049
N,0,-2.9391581453,-0.6088609824,0.6103997518
C,0,2.2483443372,1.7463711677,-0.8798494783
N,0,3.175597679,1.6018325274,-1.5381860532
H,0,-0.3596500627,-3.8465944546,-0.3390056787
H,0,1.4122249899,-3.6752276618,-0.4170858331
H,0,1.3263967121,-4.0227279198,-2.8765751275
H,0,-0.4256029068,-4.2017480064,-2.7956589662
H,0,1.7732312822,3.7907139743,0.7807230717
H,0,-2.0400303438,2.3859413861,2.1720923549

OEt 2,4,6-trimethoxyphenyl carbonate

E (total electronic) = -992.878475
E (total electronic) + ZPVE = -992.610895
Internal Thermal Energy = -992.591540
Enthalpy = -992.590595
Gibbs Free Energy = -992.661189

C,0,0.0545603878,-3.9614629369,0.4341509049
C,0,0.1039987583,-5.2673973174,-0.3529080801
O,0,0.3478522141,-6.3191582485,0.4796534861
O,0,-0.2059353531,-2.8638242606,-0.4793496494
C,0,-0.2423714729,-1.6664827313,0.06164087
O,0,-0.0892684014,-1.3914021861,1.2212504004
O,0,-0.4844126223,-0.7710392253,-0.9194390668
C,0,-0.5503739277,0.5559315254,-0.5250939109
C,0,0.5928601453,1.3394723572,-0.5619312114
C,0,0.5262046106,2.6938455622,-0.223865929
C,0,-0.7018675579,3.2245618599,0.156194615
C,0,-1.8541684512,2.4401961105,0.2088605279
C,0,-1.7730338728,1.0970220618,-0.1303186643
O,0,-2.8109669461,0.2338748273,-0.1041139449
C,0,-4.0723814142,0.7436466836,0.3058114388
O,0,-0.8753204353,4.5245209008,0.5032460355
C,0,0.2616502557,5.3730430689,0.4843800421
O,0,1.7272973786,0.7044324084,-0.9295316674
C,0,2.9243619162,1.4683019543,-0.9795444581
H,0,-0.7424946327,-3.9880100343,1.1789084249
H,0,1.0057388641,-3.7756247422,0.9349686136
H,0,0.8731961907,-5.1252864127,-1.1447296339
H,0,-0.860116549,-5.3363298629,-0.904735215
H,0,1.4117784257,3.3063205715,-0.2560900484
H,0,-2.7806422831,2.9007789701,0.5168937723
H,0,-4.7607915812,-0.0950991635,0.2643421159
H,0,-4.0216676423,1.1281330526,1.3260389068
H,0,-4.4105763539,1.530999049,-0.3701502116
H,0,-0.0904272371,6.3523704315,0.7952722886
H,0,1.0236377467,5.0202424238,1.1823832189
H,0,0.683624455,5.4387852534,-0.5205374372
H,0,3.1671535515,1.8755106102,0.003544944
H,0,3.7035388416,0.7792675322,-1.2914661951
H,0,2.838842992,2.2781029072,-1.7063242822

OEt 2,4,6-trifluorophenyl carbonate

E (total electronic) = -947.0492985
E (total electronic) + ZPVE = -946.905181
Internal Thermal Energy = -946.891003
Enthalpy = -946.890059
Gibbs Free Energy = -946.948586

C,0,-0.0258034517,-3.0020918355,-0.7330091203
C,0,-0.1797933507,-3.9307043823,-1.9335414464
O,0,-0.0691848766,-5.2330891535,-1.5495973464
O,0,-0.1426376846,-1.6236499951,-1.1878810475
C,0,-0.0129327825,-0.7067438041,-0.2659879031
O,0,0.1807975019,-0.8566257767,0.9072886588
O,0,-0.1341370266,0.5099252458,-0.8710348578
C,0,-0.0569493124,1.601983542,-0.0424280933
C,0,1.0396117582,2.4454900058,-0.0942067947
C,0,1.1253459227,3.5912647441,0.6720515545
C,0,0.0652994401,3.8665949228,1.5129206654
C,0,-1.0543178583,3.0623183566,1.6139024581
C,0,-1.0890780969,1.9348686235,0.8204518788
F,0,0.1241387637,4.9697191834,2.2697442003
F,0,2.0386962941,2.1282922588,-0.918103785
F,0,-2.1450175048,1.1220467049,0.8686592867
H,0,-0.8057654009,-3.1848981491,0.0073887825
H,0,0.9520947754,-3.1254880036,-0.2659834264
H,0,0.5836627646,-3.6068402948,-2.6757650544
H,0,-1.1562211128,-3.6739162631,-2.4018674851
H,0,1.9887137353,4.2386388367,0.614611344
H,0,-1.8696484971,3.3030602335,2.2810315315

OEt 2,4,6-trimethylphenyl carbonate

E (total electronic) = -767.2563075
E (total electronic) + ZPVE = -767.004973
Internal Thermal Energy = -766.988059
Enthalpy = -766.987115
Gibbs Free Energy = -767.051734

C,0,-0.0302383769,-3.0599824983,-1.54902913
C,0,-0.039388284,-3.7462455103,-2.9122007573
O,0,-0.0510935362,-5.1017278804,-2.7705236085
O,0,-0.0179021786,-1.6216433471,-1.745222242
C,0,-0.0090259285,-0.8922804215,-0.651407017
O,0,-0.01005354,-1.2916529837,0.483336196
O,0,0.001677571,0.4058401046,-1.0098495596
C,0,0.0122656081,1.337570611,0.0338520461
C,0,1.2387144986,1.7831053692,0.5060115147
C,0,1.2255834082,2.7565689807,1.5010713696
C,0,0.0337865089,3.2675824726,2.0090043942
C,0,-1.1691388489,2.7777817348,1.5064357084
C,0,-1.2039704293,1.8047427094,0.5114829474
C,0,-2.4952481367,1.2581360906,-0.0291866086
C,0,0.0456837509,4.3443240935,3.061882713
C,0,2.5176715511,1.2137297167,-0.0404142524
H,0,-0.9203825902,-3.3230713706,-0.9754597179
H,0,0.8576577443,-3.3388640273,-0.9794495671
H,0,0.8442164063,-3.3534722226,-3.4635478209
H,0,-0.9183553496,-3.3378389337,-3.4595877841
H,0,2.1710997622,3.1208403683,1.8891317641
H,0,-2.1063061956,3.1587298356,1.8987131383
H,0,-2.5741247541,0.1853216331,0.1618694434
H,0,-3.3453595231,1.7517995419,0.4385101718
H,0,-2.5592171825,1.4009228872,-1.109149559
H,0,-0.8385228593,4.2828535001,3.6962338193
H,0,0.9314835224,4.2671580807,3.6922838623
H,0,0.05343338,5.3344478083,2.600116282
H,0,2.5783862252,0.1396786991,0.1503299208
H,0,2.5793226329,1.3554020715,-1.120658622
H,0,3.3784811435,1.6922368862,0.4234509551

OEt 2,4,6-tri(trifluoromethyl)phenyl carbonate

E (total electronic) = -1660.5015577
E (total electronic) + ZPVE = -1660.318415
Internal Thermal Energy = -1660.296127
Enthalpy = -1660.295183
Gibbs Free Energy = -1660.373753

C,0,0.2501373837,-2.5148967307,-2.6022471174
C,0,0.2285746307,-2.5722226833,-4.1263109053
O,0,0.3486350246,-3.8600460879,-4.553753027
O,0,0.1181947412,-1.1250088325,-2.180363075
C,0,0.1206034108,-0.9232674163,-0.8928910233
O,0,0.2168837907,-1.7216483061,-0.0071905351
O,0,-0.0120036585,0.4274156407,-0.6858080885
C,0,-0.0275632458,0.829217249,0.6287446353
C,0,1.1615349732,1.1828371225,1.2542372576
C,0,1.1426462603,1.6269432658,2.5639322435
C,0,-0.0666220973,1.7185065568,3.2377855036
C,0,-1.2560461184,1.3880189173,2.613106546
C,0,-1.2352696302,0.9435717364,1.2998994378
C,0,-2.5156002314,0.6257842698,0.5752420555
C,0,-0.0555820324,2.1761044137,4.6681096965
C,0,2.4503211659,1.1219041554,0.479320995
F,0,-2.5113486619,-0.6112745752,0.0642536554
F,0,-2.721967104,1.4674281918,-0.443956907
F,0,-3.5713420578,0.7160838812,1.3848232835
F,0,0.4624036325,1.2423391795,5.4784139528
F,0,-1.2809417372,2.4533127206,5.1173381302
F,0,0.6905240818,3.2761875217,4.8254383991
F,0,2.6726118097,-0.094579166,-0.0324946015
F,0,3.4972890773,1.4262612571,1.246962152
F,0,2.4446295777,1.9810574548,-0.5459759926
H,0,-0.580645242,-3.0789047486,-2.1766580548
H,0,1.190933893,-2.9012532131,-2.2083973756

H,0,1.0412304868,-1.896639826,-4.4748944498
H,0,-0.7126723469,-2.0704643714,-4.4435029789
H,0,2.0673072115,1.9061237509,3.0523039976
H,0,-2.1968879876,1.478232672,3.1380421906

OEt pentacyanophenyl carbonate

E (total electronic) = -1110.5028534
E (total electronic) + ZPVE = -1110.342439
Internal Thermal Energy = -1110.321348
Enthalpy = -1110.320404
Gibbs Free Energy = -1110.394954

C,0,0.220328001,-2.9374579528,-2.3090054271
C,0,0.3087472933,-3.2536473268,-3.7980571316
O,0,0.3457050226,-4.6008845619,-3.9884002119
O,0,0.1930779559,-1.4822546616,-2.137476847
C,0,0.1226693813,-1.0626088222,-0.9156465449
O,0,0.0687963533,-1.6742109599,0.1086019455
O,0,0.1276522618,0.3271687667,-0.9567576681
C,0,-0.011684818,0.9802599788,0.2167249171
C,0,1.0160638055,1.8282634275,0.6218909016
C,0,0.8844887524,2.5798225655,1.7916426572
C,0,-0.2724393444,2.4754108657,2.564953344
C,0,-1.3012773039,1.6251206007,2.1542340099
C,0,-1.1770814355,0.8842602511,0.9777306794
C,0,1.9431881743,3.4566467318,2.2014532345
C,0,-2.4974957047,1.5206066636,2.9393509081
C,0,2.2045667554,1.9176178375,-0.1745172558
C,0,-0.4080499784,3.2422505825,3.7683786082
C,0,-2.2543702289,0.0539184078,0.5269695096
N,0,3.1612057277,1.9970364129,-0.7996757809
N,0,-3.1230558533,-0.5943995091,0.1558879023
N,0,-3.4523993712,1.4372316701,3.5667109559
N,0,-0.5162696117,3.8555124702,4.7300921698
N,0,2.7885468346,4.1568684397,2.529268784
H,0,-0.6925120719,-3.3418440517,-1.8708107574
H,0,1.0878277,-3.3201887911,-1.771089135
H,0,1.202426807,-2.7113506388,-4.1790202992
H,0,-0.557919104,-2.7461433963,-4.2768124682

OEt pentamethoxyphenyl carbonate

E (total electronic) = -1221.8836979
E (total electronic) + ZPVE = -1221.552309
Internal Thermal Energy = -1221.526648
Enthalpy = -1221.525704
Gibbs Free Energy = -1221.610895

C,0,0.0108705366,-3.9512197771,1.0544363778
C,0,-0.1480206328,-5.3348165962,0.4310254524
O,0,-0.1879222871,-6.2978735101,1.3945611517
O,0,0.0380618413,-2.9584614473,-0.0057836452
C,0,0.162762738,-1.7110789141,0.3814331732
O,0,0.2524992011,-1.3031961465,1.5071538351
O,0,0.1916101461,-0.9328249355,-0.7263967385
C,0,0.1623242009,0.4303013781,-0.5117899304
C,0,1.2631885236,1.1900095706,-0.8757730327
C,0,1.2180138334,2.5768959832,-0.7259330784
C,0,0.0797559432,3.1844522849,-0.1962740148
C,0,-1.0295474345,2.4075296712,0.1546758081
C,0,-0.9841292154,1.020903221,0.010801473
O,0,-2.036268901,0.2105681347,0.303513346
C,0,-2.5232181096,0.276619927,1.649975995
O,0,0.0499804019,4.5438115871,-0.1002859631
C,0,-0.0490491923,5.0516235427,1.2347906017
O,0,2.3948292361,0.5810905019,-1.3300369617
C,0,2.488250318,0.5690032785,-2.7575398921
O,0,-2.1530951876,3.0258643234,0.6267997184
O,0,2.2790299065,3.3212656665,-1.1531492318
C,0,-3.2383248214,3.0237012069,-0.3066381861
C,0,3.1540862136,3.7254655589,-0.0994617925
H,0,-0.8258498793,-3.7241739589,1.7168753945
H,0,0.9431590458,-3.8806517994,1.6169404694

H,0,0.6906666528,-5.4478536988,-0.2919573735
H,0,-1.0620108359,-5.2859690559,-0.2023427299
H,0,-3.0642463285,-0.6512492646,1.8189612541
H,0,-1.685888777,0.3444240254,2.3445927515
H,0,-3.1900121868,1.1280594638,1.7791287137
H,0,0.0835616112,6.1280548044,1.1597776784
H,0,-1.0222768922,4.8221520087,1.6646260654
H,0,0.7403300835,4.6271001948,1.8589640604
H,0,2.4880926046,1.589533503,-3.1433753197
H,0,3.4271894487,0.0792822943,-3.0029556749
H,0,1.6546260122,0.0069639466,-3.1836261071
H,0,-4.0549728505,3.5586098619,0.1715624378
H,0,-2.9435546718,3.537987669,-1.2231798566
H,0,-3.5459944773,2.0021735502,-0.536096686
H,0,3.5289853236,2.8508957034,0.4359523148
H,0,3.9809002726,4.254359095,-0.5671644372
H,0,2.636899586,4.3922211475,0.5921605799

OEt pentachlorophenyl carbonate

E (total electronic) = -2947.3163157
E (total electronic) + ZPVE = -2947.195715
Internal Thermal Energy = -2947.177965
Enthalpy = -2947.177021
Gibbs Free Energy = -2947.245288

C,0,0.6856441109,-2.8314348797,-1.162701451
C,0,0.488744562,-3.6629599843,-2.4262541122
O,0,0.9195565786,-4.9394333294,-2.2239805379
O,0,0.2161272855,-1.4733845151,-1.410575696
C,0,0.3246901894,-0.6460672776,-0.4085563523
O,0,0.7588236751,-0.8525894837,0.6890714003
O,0,-0.1578717792,0.5678987476,-0.8137984647
C,0,-0.1171979048,1.5607646426,0.1268595276
C,0,0.9939450967,2.386649682,0.2069878827
C,0,1.010716828,3.4409626754,1.1144800619
C,0,-0.088482019,3.6554726821,1.9445881796
C,0,-1.1983418624,2.8152014778,1.8704903516
C,0,-1.2070034866,1.7631855777,0.9602253832
Cl,0,-2.5413482747,0.6835153216,0.8438175827
Cl,0,-2.5549568034,3.0716731616,2.8970816546
Cl,0,-0.0735624266,4.9601063611,3.0680476002
Cl,0,2.3855936817,4.4711858774,1.206267012
Cl,0,2.3327077425,2.0641980379,-0.8242506699
H,0,0.112734986,-3.2421586029,-0.3305583271
H,0,1.7397155525,-2.7812951161,-0.8873804884
H,0,1.0217658199,-3.123732152,-3.2407610798
H,0,-0.5893085521,-3.5800989043,-2.6893804571

OEt pentafluorophenyl carbonate

E (total electronic) = -1145.5040146
E (total electronic) + ZPVE = -1145.375575
Internal Thermal Energy = -1145.359478
Enthalpy = -1145.358533
Gibbs Free Energy = -1145.421401

C,0,0.2740399783,-2.8827596932,-1.1034354279
C,0,0.2515294901,-3.663425209,-2.4137250604
O,0,0.4653389556,-4.9886741272,-2.1833277189
O,0,0.0486952168,-1.4716356828,-1.3941960612
C,0,0.0604691368,-0.6711296248,-0.365392725
O,0,0.2248314896,-0.9381502597,0.7901121122
O,0,-0.1532627334,0.6007967226,-0.8290996449
C,0,-0.2039619172,1.5817792777,0.1224844918
C,0,0.7964348073,2.5369866892,0.1756233798
C,0,0.7300485459,3.5779726363,1.0844275693
C,0,-0.33965858,3.6630889193,1.9555366244
C,0,-1.343902278,2.7119192495,1.9137173584
C,0,-1.2733064718,1.6797468186,0.9982832943
F,0,1.6920295108,4.4911441792,1.1241772003
F,0,-2.3712762855,2.7967032892,2.7492662354
F,0,1.8313685787,2.4615514455,-0.6508140076
F,0,-0.4055647477,4.6572657715,2.8298855025

F,0,-2.2425370296,0.7748038199,0.9559306365
H,0,-0.5144673955,-3.221004958,-0.4299908956
H,0,1.2405436187,-2.9769970027,-0.6071324445
H,0,1.0104717881,-3.185448401,-3.072532753
H,0,-0.7254636781,-3.4347708602,-2.8951286658

OEt pentamethylphenyl carbonate

E (total electronic) = -845.8651853
E (total electronic) + ZPVE = -845.557378
Internal Thermal Energy = -845.537612
Enthalpy = -845.536667
Gibbs Free Energy = -845.607066

C,0,-0.1495176068,-3.4340295163,0.6188726085
C,0,0.3043725733,-4.7663240496,0.0287427285
O,0,-0.0143500438,-5.7965311912,0.862480425
O,0,0.2070102635,-2.365466352,-0.2958700992
C,0,-0.1244312818,-1.1493547256,0.0831666614
O,0,-0.6869196255,-0.8406897151,1.1008607818
O,0,0.274776741,-0.2889302152,-0.8693930948
C,0,0.0033913067,1.06700768,-0.6358775099
C,0,0.9677152053,1.8234091308,0.0171502553
C,0,0.7147351338,3.1886804727,0.1945929078
C,0,-0.4664061619,3.7540057269,-0.3041082508
C,0,-1.4345404903,2.9506629688,-0.9211553508
C,0,-1.1966490627,1.5837205918,-1.1064312325
C,0,-2.2008274474,0.6922421551,-1.7913952493
C,0,-2.7385637055,3.5576706241,-1.3797813158
C,0,-0.6978716829,5.241059379,-0.1754568009
C,0,1.712063708,4.0505473145,0.930658911
C,0,2.2392987922,1.183956816,0.5135968761
H,0,-1.2312388059,-3.4213485857,0.7613563971
H,0,0.3390367415,-3.2474536988,1.5765194042
H,0,1.3944344425,-4.6626018762,-0.1712248845
H,0,-0.1624070627,-4.8350107374,-0.9794134003
H,0,-1.7728715053,-0.2788123138,-2.028240273
H,0,-3.0766749481,0.5300116691,-1.1581919392
H,0,-2.5499259046,1.1416515214,-2.7216649829
H,0,-2.6244479619,4.068008093,-2.340917925
H,0,-3.5129853406,2.8034774481,-1.4970907977
H,0,-3.1005273019,4.2940729069,-0.6625973809
H,0,-1.3094420375,5.6184791742,-0.9929260531
H,0,-1.2106256771,5.4871968292,0.7597897606
H,0,0.2417796083,5.7902649571,-0.18767027
H,0,2.3384845395,4.6176067652,0.2354675099
H,0,1.2067082705,4.7710796036,1.5733934386
H,0,2.3713567422,3.4551305032,1.5576432946
H,0,2.2452080049,1.1193729826,1.6045450466
H,0,2.359140621,0.1787815848,0.1167979526
H,0,3.1108019599,1.7685420788,0.2169778509

OEt penta(trifluoromethyl)phenyl carbonate

E (total electronic) = -2334.562927
E (total electronic) + ZPVE = -2334.369778
Internal Thermal Energy = -2334.341513
Enthalpy = -2334.340568
Gibbs Free Energy = -2334.429355

C,0,-0.4071623018,-3.4348573438,0.5980565769
C,0,-0.2138744768,-4.7622315295,-0.1277187456
O,0,-0.4700689229,-5.8008866743,0.7151430109
O,0,-0.125757548,-2.3423548099,-0.3297642016
C,0,-0.2519139977,-1.1446003083,0.1579752087
O,0,-0.5657696495,-0.8019769639,1.2592240882
O,0,0.050059365,-0.2544397417,-0.8497010528
C,0,-0.0283602807,1.0706849017,-0.5217825638
C,0,1.122119618,1.7293609991,-0.0930073001
C,0,1.0730427663,3.1080084105,0.1186431713
C,0,-0.144550808,3.7870493099,-0.0038712804
C,0,-1.255059855,3.1366236301,-0.553741989
C,0,-1.215018825,1.7580888109,-0.7680041507
C,0,-2.4277406974,0.9673191898,-1.2637065624

C,0,-2.4343504807,3.9675474701,-1.0799953742
 C,0,-0.3156456334,5.167667408,0.647304743
 C,0,2.369828735,3.9084935865,0.3075085957
 C,0,2.394097555,0.9080476043,0.1289114071
 H,0,-1.4340326492,-3.3237431984,0.9478802599
 H,0,0.2773659428,-3.3447921484,1.4421511728
 H,0,0.8215409005,-4.7471408468,-0.5349620234
 H,0,-0.872161002,-4.7263164021,-1.0241163901
 F,0,3.092652005,0.7829227442,-0.9977666046
 F,0,3.1760199536,1.4575467686,1.0559787576
 F,0,2.1350330934,-0.3226953181,0.5717643578
 F,0,3.3320604504,3.3925156277,-0.4607800838
 F,0,2.8059266389,3.9484017269,1.5599134834
 F,0,2.2153428416,5.1640663323,-0.1113419581
 F,0,-0.0782772148,6.2149896839,-0.1300183348
 F,0,0.4883091118,5.257809321,1.7111894917
 F,0,-1.5606894882,5.282991677,1.119418847
 F,0,-2.0519272835,5.2165191376,-1.3437752097
 F,0,-3.4699088574,4.0255423757,-0.2526197515
 F,0,-2.8503211167,3.4685114048,-2.2463254014
 F,0,-3.5707953074,1.5404745198,-0.8925924076
 F,0,-2.4726302327,-0.2660610464,-0.7590130094
 F,0,-2.4207778431,0.8507093509,-2.5901283859

Transition states

ALIPHATIC CARBONATES

TS-OEt hydrogen carbonate

E (total electronic) = -418.2908564
 E (total electronic) + ZPVE = -418.205511
 Internal Thermal Energy = -418.198130
 Enthalpy = -418.197186
 Gibbs Free Energy = -418.238802

O,0,0.1201493791,0.6896598645,-0.2502551368
 C,0,0.1421404576,0.9411663526,0.9905908832
 O,0,0.1528983354,0.1504434328,1.931983457
 O,0,0.1546250686,2.2868722129,1.254831808
 C,0,0.1026585946,-1.1806021076,-0.6245348733
 C,0,0.0776618776,-1.384153455,-2.0643719348
 O,0,0.0754989209,-2.7295631038,-1.7023732443
 H,0,0.171026565,2.3774283395,2.215715553
 H,0,-0.8117071423,-1.3481718683,-0.0801568935
 H,0,1.0323977681,-1.3593276253,-0.1105953791
 H,0,0.9679766149,-1.0401213618,-2.6040579817
 H,0,-0.8257524396,-1.0292716805,-2.5744512577

TS-OEt ethenyl carbonate (Point group: Cs)

E (total electronic) = -495.6594951
 E (total electronic) + ZPVE = -495.541745
 Internal Thermal Energy = -495.532003
 Enthalpy = -495.531059
 Gibbs Free Energy = -495.578824

O,0,0.3974589496,-0.6429538101,0.
 C,0,-0.5722660773,0.1667996008,0.
 O,0,-0.5604371101,1.3877413693,0.
 O,0,-1.7833456436,-0.5238515915,0.
 C,0,2.0831946078,0.2312851081,0.
 C,0,3.1458487716,-0.7634232816,0.
 O,0,3.9783536655,0.352344074,0.
 H,0,1.8933168699,0.756030051,0.9219603159
 H,0,1.8933168699,0.756030051,-0.9219603159
 H,0,3.1965409235,-1.393307151,-0.8964379381
 H,0,3.1965409235,-1.393307151,0.8964379381
 C,0,-2.9382466806,0.2057109619,0.
 C,0,-4.1186787207,-0.3934053014,0.

H,0,-2.8003610834,1.2783032999,0.
 H,0,-5.0169464323,0.2060493087,0.
 H,0,-4.2067606137,-1.4720540479,0.

TS-OEt ethynyl carbonate

E (total electronic) = -494.3994627
 E (total electronic) + ZPVE = -494.305998
 Internal Thermal Energy = -494.296563
 Enthalpy = -494.295619
 Gibbs Free Energy = -494.342662

O,0,0.004381966,-0.6412274319,-0.0000527168
 C,0,0.9748555856,0.1531582707,-0.0000199546
 O,0,1.0405468378,1.3592518669,0.0000185778
 O,0,2.2017928292,-0.603852878,-0.000033697
 C,0,-1.6413516475,0.2470598745,-0.0000221692
 C,0,-2.7299387254,-0.7240234145,0.0000233902
 O,0,-3.5657212462,0.3857131809,0.0000269677
 H,0,-1.458377271,0.7778104453,-0.9209584872
 H,0,-1.4583282444,0.7778433202,0.920885415
 H,0,-2.7809329344,-1.3563281707,0.8956519856
 H,0,-2.7809812671,-1.3563582747,-0.8955812324
 C,0,3.3127088173,0.0738210574,-0.0000035867
 C,0,4.3698462121,0.6331749387,0.0000220571
 H,0,5.3090224279,1.1331998453,0.0000441303

TS-OEt propyl carbonate

E (total electronic) = -536.190111
 E (total electronic) + ZPVE = -536.019692
 Internal Thermal Energy = -536.008193
 Enthalpy = -536.007249
 Gibbs Free Energy = -536.059330

O,0,-0.6768585358,-0.904818556,-0.4957598204
 C,0,-0.6171466662,-0.1996282337,0.5596153343
 O,0,-0.5630613522,-0.5865267931,1.7244297692
 O,0,-0.6165597683,1.1389618832,0.2778702787
 C,0,-0.5544880538,2.0200251097,1.4009100944
 C,0,-0.6176129506,-2.7881644894,-0.1392997004
 C,0,-0.6727319784,-3.5135495738,-1.3976714344
 O,0,-0.5953989151,-4.619820865,-0.5528827998
 C,0,-0.5176171308,3.4413626098,0.8783852964
 C,0,0.7301769205,3.7368623957,0.0527820494
 H,0,0.3410973542,1.7964748113,1.9859680313
 H,0,-1.4255109663,1.8551598557,2.0378271923
 H,0,-1.5076780437,-2.7654105226,0.4667615215
 H,0,0.3339118989,-2.7226343715,0.3611506711
 H,0,0.1833867731,-3.3670600559,-2.0665128194
 H,0,-1.6073914415,-3.4121478804,-1.9615495166
 H,0,-0.5636856448,4.1111002776,1.7407909916
 H,0,-1.4174117078,3.6250401093,0.2853036833
 H,0,0.7777010201,3.0909697979,-0.8244718701
 H,0,0.73978748,4.7727692724,-0.2878040147
 H,0,1.6324307084,3.5680902188,0.6451230623

TS-OEt fluoromethyl carbonate

E (total electronic) = -556.8304348
 E (total electronic) + ZPVE = -556.723733
 Internal Thermal Energy = -556.714412
 Enthalpy = -556.713468
 Gibbs Free Energy = -556.760367

O,0,0.042319901,-0.0140072493,-0.8090435631
 C,0,0.0986008991,0.7027091978,0.228477553
 O,0,0.2083035968,0.3710830642,1.3980669083
 O,0,0.0204397523,2.0579343132,-0.1019630667
 C,0,0.0415856644,2.9443788896,0.9558618848
 C,0,0.1282945044,-1.870656943,-0.4278210611

C,0,0.0684691157,-2.6225966812,-1.6726755591
O,0,0.1594851816,-3.7272599005,-0.8306134341
F,0,-1.2266652469,3.0329452315,1.5108177155
H,0,0.7152343594,2.6215023966,1.7445421936
H,0,0.2894470077,3.9233323861,0.5546578812
H,0,-0.7553105593,-1.8603122698,0.1891415855
H,0,1.0836363227,-1.8023763415,0.0661356111
H,0,0.9171759592,-2.4716755518,-2.3508471126
H,0,-0.8708944583,-2.5277675418,-2.2309075363

TS-OEt chloromethyl carbonate

E (total electronic) = -917.1856956
E (total electronic) + ZPVE = -917.080895
Internal Thermal Energy = -917.071226
Enthalpy = -917.070282
Gibbs Free Energy = -917.118906

O,0,0.8682708964,0.7500954795,-0.2669315048
C,0,-0.1586150997,0.2857894349,0.2998129547
O,0,-0.2757609262,-0.6725649918,1.0445953322
O,0,-1.2865567257,1.0489188486,-0.0254304745
C,0,-2.4850275341,0.619806421,0.498081399
C,0,2.4315856759,-0.2445505343,0.1224901954
C,0,3.5658908017,0.3357557222,-0.5821269213
O,0,4.2792449987,-0.6927095154,0.025942936
H,0,-2.3821891736,0.1929161017,1.488734009
H,0,-3.1892766843,1.4416439896,0.456147245
H,0,2.0297619411,-1.168410178,-0.2605048175
H,0,2.3686243042,-0.0755472282,1.1851282984
H,0,3.8386207221,1.3513555552,-0.2700557736
H,0,3.5075382191,0.29028717,-1.6765105758
Cl,0,-3.2184558554,-0.702277095,-0.5247545123

TS-OEt bromomethyl carbonate

E (total electronic) = -3031.1532187
E (total electronic) + ZPVE = -3031.049091
Internal Thermal Energy = -3031.039216
Enthalpy = -3031.038272
Gibbs Free Energy = -3031.088275

O,0,0.1083900472,-0.5280458683,-0.5767620925
C,0,0.6657638965,0.4377408078,0.0115758831
O,0,0.9488568711,0.5843290153,1.1875230982
O,0,0.9799875211,1.4529247801,-0.9047372613
C,0,1.5454916787,2.5879393663,-0.3876548522
Br,0,0.1528839118,3.849050606,0.3005338921
H,0,2.1798123519,2.4007358738,0.469713032
H,0,2.0298860285,3.1358934386,-1.1852199179
C,0,-0.3130842066,-1.9505455756,0.5941443353
C,0,-0.937268776,-3.032952789,-0.1542841173
O,0,-0.9909867437,-3.6640158514,1.0843864217
H,0,-0.9522901061,-1.3494840502,1.2201665223
H,0,0.7061589588,-2.0938968958,0.9142180116
H,0,-0.294550324,-3.5115405463,-0.9034574291
H,0,-1.9071001092,-2.7882553113,-0.604730526

TS-OEt cyanomethyl carbonate

E (total electronic) = -549.8197632
E (total electronic) + ZPVE = -549.707178
Internal Thermal Energy = -549.696890
Enthalpy = -549.695946
Gibbs Free Energy = -549.745349

O,0,0.4621555799,-0.7798696947,-0.0030616894
C,0,-0.5778967478,-0.0765207659,-0.135504681
O,0,-0.6936336173,1.1364054434,-0.234960641
O,0,-1.7186805597,-0.8698639041,-0.161408339
C,0,-2.9268869625,-0.1709392198,-0.3423202601

C,0,2.0472696153,0.2568048578,0.0289775388
C,0,3.2011504671,-0.6225604129,0.1522406136
O,0,3.9220636992,0.5673852433,0.1221963853
H,0,-2.8672955917,0.5348982638,-1.1699264949
H,0,-3.694753657,-0.913719908,-0.5494776139
H,0,1.7542551088,0.8161267246,0.9024432882
H,0,1.865434493,0.7040961482,-0.9345197909
H,0,3.3652672694,-1.2983001583,-0.6960590348
H,0,3.2585054546,-1.188417966,1.0901353387
C,0,-3.3198808736,0.573690015,0.8709416863
N,0,-3.6456856477,1.1353669735,1.815001784

TS-OEt nitromethyl carbonate

E (total electronic) = -662.084848
E (total electronic) + ZPVE = -661.967716
Internal Thermal Energy = -661.956734
Enthalpy = -661.955790
Gibbs Free Energy = -662.008078

O,0,1.1267724328,0.7671956712,-0.3448398346
C,0,0.0643470357,0.4133542631,0.2296275648
O,0,-0.1377577358,-0.4659482864,1.0498911941
O,0,-1.0169719271,1.203742593,-0.1924354777
C,0,-2.2179578527,0.88954231,0.3820066269
C,0,2.6182039101,-0.260902719,0.180465892
C,0,3.8098491468,0.2228914476,-0.5038602281
O,0,4.4561310588,-0.7874779074,0.2001121668
N,0,-2.7915591107,-0.3980032805,-0.2003210052
O,0,-3.7859964856,-0.8188387453,0.3514834492
O,0,-2.2558619578,-0.8986761417,-1.1574610465
H,0,-2.1716695035,0.7016479667,1.4509992826
H,0,-2.9495089308,1.6537797775,0.1315259312
H,0,2.1975927614,-1.1935455492,-0.1593939308
H,0,2.5187553773,-0.0221375103,1.2270095586
H,0,4.1086809375,1.2466993836,-0.2464770784
H,0,3.7971932936,0.1081076371,-1.5948843447

TS-OEt difluoromethyl carbonate

E (total electronic) = -656.0889905
E (total electronic) + ZPVE = -655.990583
Internal Thermal Energy = -655.980536
Enthalpy = -655.979591
Gibbs Free Energy = -656.028890

O,0,-0.1115988965,-0.3813746092,-0.6637778733
C,0,-0.0844603951,0.6125514011,0.1059158781
O,0,-0.115575075,0.6758801128,1.3214370122
O,0,-0.0028673679,1.8060326406,-0.6385528822
C,0,0.0182481507,2.9558704871,0.0898244629
C,0,-0.2383275987,-2.0155009539,0.2602238155
C,0,-0.2673792866,-3.1156946478,-0.6950520321
O,0,-0.3587985936,-3.920653267,0.4347453449
F,0,-0.3545200369,3.9499374758,-0.7411387668
F,0,1.2891286086,3.2395658012,0.473944057
H,0,-0.6185761169,2.9367154679,0.9684681513
H,0,-1.1653052566,-1.7635370858,0.7496851356
H,0,0.6731785456,-1.8705984344,0.8176963522
H,0,0.6464442159,-3.2352704594,-1.2904917422
H,0,-1.1408898971,-3.1286399289,-1.3589749132

TS-OEt dichloromethyl carbonate

E (total electronic) = -1376.7825194
E (total electronic) + ZPVE = -1376.687897
Internal Thermal Energy = -1376.677047
Enthalpy = -1376.676102
Gibbs Free Energy = -1376.728307

O,0,-0.1264153309,-0.3856713537,-0.6600410941

C,0,-0.1122555815,0.6086851098,0.1075186319
O,0,-0.1826978577,0.6850536031,1.3184037271
O,0,0.0083688685,1.8008095834,-0.6513012397
C,0,0.065019888,2.954701223,0.0697970941
C,0,-0.278175985,-2.0147339228,0.2622433368
C,0,-0.2383882363,-3.1195892303,-0.6879750546
O,0,-0.376003304,-3.9262022678,0.4353516183
H,0,-0.4937353595,2.9120274207,0.9956385016
H,0,-1.2342562141,-1.7782020995,0.7014098972
H,0,0.5991341541,-1.8548954418,0.868580673
H,0,0.7077436597,-3.2238168877,-1.2340019617
H,0,-1.0746392721,-3.1477516349,-1.3979664056
Cl,0,-0.5898259061,4.2714491345,-0.9320106038
Cl,0,1.7668076571,3.3475367941,0.5273139994

TS-OEt dibromomethyl carbonate

E (total electronic) = -5604.7148379
E (total electronic) + ZPVE = -5604.621495
Internal Thermal Energy = -5604.610163
Enthalpy = -5604.609218
Gibbs Free Energy = -5604.663880

O,0,-0.0767399716,-0.3914073699,-0.6541489009
C,0,-0.0990290628,0.6035434325,0.1110607191
O,0,-0.2212352642,0.6870745484,1.3162022275
O,0,0.0510630616,1.7969163341,-0.6496597269
C,0,0.0690994265,2.9501784547,0.0628134631
C,0,-0.2659035971,-2.0161980519,0.2623872827
C,0,-0.2526321045,-3.120583898,-0.6896526371
O,0,-0.4044169057,-3.9283618576,0.4307648562
H,0,-0.49717609,2.9068197844,0.9832398298
H,0,-1.2155113782,-1.7605008806,0.7048732211
H,0,0.6157562219,-1.8791306401,0.8681329332
H,0,0.6891817636,-3.2432427565,-1.2394364018
H,0,-1.0913567394,-3.1278432894,-1.3973663028
Br,0,-0.6703018799,4.3703602548,-1.0376193501
Br,0,1.9093894498,3.4223035551,0.6107656768

TS-OEt dicyanomethyl carbonate

E (total electronic) = -642.0453874
E (total electronic) + ZPVE = -641.934622
Internal Thermal Energy = -641.922631
Enthalpy = -641.921687
Gibbs Free Energy = -641.975534

O,0,-0.02844223,-0.4618281768,-0.7525081713
C,0,0.0359904397,0.6116504238,-0.1039619973
O,0,0.0665367976,0.8255108717,1.0949822133
O,0,0.0767102562,1.7147750724,-0.9774222689
C,0,0.149458122,2.9644504562,-0.3594297815
C,0,-0.086011944,-1.9777753522,0.3487397708
C,0,-0.1596487099,-3.1784855883,-0.4753746942
O,0,-0.1738388515,-3.8623691196,0.7340610318
C,0,-1.0368853737,3.2724704024,0.4730906098
N,0,-1.9746015338,3.5565720046,1.0636995312
C,0,1.3874559916,3.1511884537,0.4329510418
N,0,2.3678299089,3.3393299175,0.9918016379
H,0,0.1729337244,3.700542958,-1.1656460706
H,0,-0.9850063442,-1.6803425462,0.8648013579
H,0,0.8546769368,-1.7722954434,0.8343931256
H,0,0.7179289705,-3.3550368191,-1.1102571141
H,0,-1.0709061605,-3.2656275146,-1.0806882222

TS-OEt dinitromethyl carbonate

E (total electronic) = -866.5638906
E (total electronic) + ZPVE = -866.444501
Internal Thermal Energy = -866.431262
Enthalpy = -866.430317

Gibbs Free Energy = -866.487143

O,0,1.6520805478,-0.1874680175,0.8224435933
C,0,0.5600242775,0.07111347,0.2719208152
O,0,0.2698941922,0.4269563463,-0.8481909559
O,0,-0.5055338633,-0.0814937514,1.2270425779
C,0,-1.7582033178,-0.0234067328,0.768369671
C,0,3.1027525246,0.0539783827,-0.316855816
C,0,4.3438480622,-0.2509090344,0.3892265603
O,0,4.9834274295,0.0680373676,-0.8005632256
N,0,-2.0398517084,1.2234546296,-0.0942330988
O,0,-2.620992515,1.1040393717,-1.1390463665
O,0,-1.6769915414,2.2505384485,0.4206497463
N,0,-2.1615483358,-1.252740319,-0.05279718
O,0,-3.3495983093,-1.4010031276,-0.2062353603
O,0,-1.2868180001,-1.9888257145,-0.4279790609
H,0,-2.472709911,0.0249565069,1.5866647566
H,0,2.8986612361,1.0944911934,-0.5164128467
H,0,2.7719160279,-0.6620086804,-1.0530379326
H,0,4.4379728975,-1.2955183509,0.7137246413
H,0,4.5596423069,0.4120460118,1.2373174812

TS-OEt tricyanomethyl carbonate (Point group:

Cs)
E (total electronic) = -734.25541
E (total electronic) + ZPVE = -734.147279
Internal Thermal Energy = -734.133373
Enthalpy = -734.132429
Gibbs Free Energy = -734.189916

O,0,1.501457662,0.8080936391,0.
C,0,0.4961301815,0.0646264075,0.
O,0,0.3661788445,-1.1425056152,0.
O,0,-0.691839605,0.8534093177,0.
C,0,-1.8742523525,0.1176806336,0.
C,0,3.0954611838,-0.1409829078,0.
C,0,4.2270868748,0.7832401166,0.
O,0,5.0322391304,-0.3467928727,0.
H,0,2.8992646613,-0.6690057042,-0.9203840722
H,0,2.8992646613,-0.6690057042,0.9203840722
H,0,4.2961258724,1.4156169309,0.8949542095
H,0,4.2961258724,1.4156169309,-0.8949542095
C,0,-2.0292762555,-0.7338264832,-1.2133716503
N,0,-2.1990181676,-1.3444451936,-2.1646210398
C,0,-2.9786000656,1.1100781505,0.
N,0,-3.8307805828,1.8709967227,0.
C,0,-2.0292762555,-0.7338264832,1.2133716503
N,0,-2.1990181676,-1.3444451936,2.1646210398

TS-OEt trinitromethyl carbonate

E (total electronic) = -1071.030467
E (total electronic) + ZPVE = -1070.910237
Internal Thermal Energy = -1070.894090
Enthalpy = -1070.893146
Gibbs Free Energy = -1070.957050

O,0,0.0786501616,-1.0218276041,-0.4404520122
C,0,-0.200776609,-0.1076005544,0.3511940673
O,0,-0.5223846317,-0.0443578863,1.5057125653
O,0,-0.1124771447,1.1801830247,-0.3946740853
C,0,-0.179850477,2.2879972711,0.2892666929
C,0,-0.0346834586,-2.680108973,0.3269949338
C,0,0.2833749708,-3.7138467309,-0.6603995963
O,0,0.0707855266,-4.6552075766,0.3323307405
N,0,1.1092030061,2.609828321,1.0941178915
O,0,1.8160641311,1.6734953362,1.338410288
O,0,1.2851219114,3.7686976945,1.3678845695
N,0,-1.3804110966,2.3857330311,1.2601729112
O,0,-1.1756265058,2.8052793343,2.3649636715
O,0,-2.4202416038,2.0355211343,0.7750520255

N,0,-0.3251935363,3.4783523879,-0.6799847027
O,0,-1.1101541221,4.3357738183,-0.3770939452
O,0,0.3914206955,3.4300207134,-1.6408082113
H,0,-1.0700107449,-2.6020218277,0.624069862
H,0,0.7048863806,-2.5051507438,1.0942036111
H,0,1.3095574776,-3.6561336264,-1.0489826018
H,0,-0.4161503308,-3.7495305695,-1.5070196754

AROMATIC CARBONATES

TS-OEt 2-nitrophenyl carbonate

E (total electronic) = -853.7945724
E (total electronic) + ZPVE = -853.625648
Internal Thermal Energy = -853.611476
Enthalpy = -853.610531
Gibbs Free Energy = -853.669338

C,0,-0.4668753109,-2.9460629295,0.7280467186
C,0,-1.5193473778,-3.9210269175,0.9815665005
O,0,-0.5444436345,-4.5722176595,1.7298228137
O,0,-1.1329276112,-1.5642058059,-0.3683133946
C,0,-0.2807548268,-0.6635217883,-0.582630747
O,0,0.8796314805,-0.5731452072,-0.2237819564
O,0,-0.8356223503,0.3506765421,-1.3850040196
C,0,-0.0906230317,1.4624550441,-1.6309171504
C,0,0.0826173674,1.8406101654,-2.9554884661
C,0,0.8007168735,2.9820808877,-3.2773294006
C,0,1.3826983985,3.7560593512,-2.279639285
C,0,1.2327550786,3.3849717141,-0.9549454088
C,0,0.4855561452,2.2599097625,-0.6410457936
N,0,0.305575985,1.952513096,0.7768164544
O,0,-0.756693123,1.4795891028,1.1299287818
O,0,1.2199782036,2.2159658231,1.5315007121
H,0,-0.2013519427,-2.2842642457,1.5365649275
H,0,0.3133507738,-3.2295546939,0.0402431089
H,0,-1.8760051321,-4.4600641428,0.0950410954
H,0,-2.3775432621,-3.5400004923,1.5489280719
H,0,-0.3542822454,1.2152880961,-3.7228370714
H,0,0.9156960992,3.2617678567,-4.3164651462
H,0,1.9489557795,4.6423403235,-2.5302381035
H,0,1.6710916639,3.9627161174,-0.1530102419

TS-OEt 2-cyanophenyl carbonate

E (total electronic) = -741.5434621
E (total electronic) + ZPVE = -741.378800
Internal Thermal Energy = -741.365202
Enthalpy = -741.364258
Gibbs Free Energy = -741.421669

C,0,-0.0809309743,-2.9528666249,-1.0587935834
C,0,-0.2462807991,-3.7918637036,-2.2379837949
O,0,0.0263963681,-4.8345591634,-1.3581567935
O,0,-0.3418777826,-1.141244443,-1.5257747869
C,0,-0.1983637298,-0.3627463797,-0.545747905
O,0,0.0911028249,-0.5983669925,0.6132966353
O,0,-0.4168897864,0.9700411535,-0.942184461
C,0,-0.360544649,1.9288091305,0.0326683894
C,0,0.6833148012,2.8370975984,0.0371615566
C,0,0.7079651928,3.8529832853,0.9838233304
C,0,-0.3042247634,3.9652234757,1.9308139997
C,0,-1.3522716157,3.0596980189,1.9297339173
C,0,-1.3836046741,2.0410381503,0.977544457
C,0,-2.4668373851,1.1018664189,0.9511036222
N,0,-3.3392143607,0.355415526,0.9230419184
H,0,-0.8760915767,-2.960382418,-0.3308055701
H,0,0.9231918636,-2.7992406075,-0.6983882172
H,0,0.4964676666,-3.6326644039,-3.0294978364
H,0,-1.2532609309,-3.7890403973,-2.6731462922
H,0,1.4650644721,2.7367467487,-0.7041811867
H,0,1.5265965849,4.561074234,0.9824513197

H,0,-0.2780829551,4.7574247919,2.6665430317
H,0,-2.1504707913,3.1326906018,2.6563442495

TS-OEt 2-methoxyphenyl carbonate

E (total electronic) = -763.812596
E (total electronic) + ZPVE = -763.613390
Internal Thermal Energy = -763.599138
Enthalpy = -763.598193
Gibbs Free Energy = -763.657027

C,0,0.9733222317,-2.7152794233,-1.8756413984
C,0,0.8228609945,-3.1121823707,-3.2674479479
O,0,0.9571714941,-4.3966396274,-2.7460651052
O,0,0.8815308789,-0.8201816384,-1.7421889204
C,0,1.0195728938,-0.4052328576,-0.5560011809
O,0,1.2018059057,-1.0380083738,0.4714289214
O,0,0.965600601,0.9888441021,-0.5117682705
C,0,0.9320183303,1.5678891809,0.7364507622
C,0,2.0212746969,2.2774436315,1.1950074923
C,0,1.9682042003,2.9234166467,2.4290170616
C,0,0.8149880394,2.8403303897,3.1899404002
C,0,-0.291498222,2.1256480514,2.7317958886
C,0,-0.242378364,1.487393888,1.4981709199
O,0,-1.2567998703,0.7800592278,0.9477113611
C,0,-2.4502628675,0.6597942333,1.705065883
H,0,0.1321689109,-2.8709115763,-1.2204951586
H,0,1.9601811095,-2.7692031224,-1.4464288979
H,0,1.6272416088,-2.7860400942,-3.9376888093
H,0,-0.1500913066,-2.8824626418,-3.7182337593
H,0,2.9081298178,2.3179835887,0.5747582861
H,0,2.8241045722,3.4809151364,2.7855717147
H,0,0.7601279673,3.3343850102,4.1516377346
H,0,-1.1834997333,2.0766465303,3.3399980324
H,0,-3.1274672101,0.0583243603,1.1055913977
H,0,-2.2588689099,0.1585159008,2.6561519876
H,0,-2.8964117693,1.6392668479,1.889738605

TS-OEt 2-chlorophenyl carbonate

E (total electronic) = -1108.8992984
E (total electronic) + ZPVE = -1108.742770
Internal Thermal Energy = -1108.729818
Enthalpy = -1108.728874
Gibbs Free Energy = -1108.785062

C,0,-3.384337992,-0.0634251925,0.4710373423
C,0,-4.6158604791,-0.3394652757,-0.2546022637
O,0,-5.2239605155,0.0201397617,0.9445784928
H,0,-3.131698073,0.9698253589,0.6445194974
H,0,-3.0701751415,-0.7852183623,1.207141506
H,0,-4.7526519797,-1.3834876299,-0.5618153374
H,0,-4.8152961624,0.3239671089,-1.1049621789
O,0,-1.8986770683,-0.3768964021,-0.6624315652
C,0,-0.7933547082,-0.1831260963,-0.0856396987
O,0,-0.5567148893,0.1933622873,1.0492360891
O,0,0.270512503,-0.4837361352,-0.9475156503
C,0,1.5324724462,-0.2104814818,-0.4867073925
C,0,2.3529326667,-1.2505799607,-0.0789931201
C,0,3.6564658502,-0.9953133744,0.3248031166
C,0,4.1420574437,0.3060548785,0.3255312294
C,0,3.3259769958,1.353553301,-0.0814418723
C,0,2.0278892991,1.0892590168,-0.4862680362
Cl,0,0.9994268771,2.3927219493,-1.0097534888
H,0,1.9508513772,-2.2557130183,-0.0869663442
H,0,4.2904993093,-1.8134634885,0.640374136
H,0,5.156629132,0.5120209529,0.6399686727
H,0,3.6897061086,2.3725018023,-0.0892081337

TS-OEt 2-fluorophenyl carbonate

E (total electronic) = -748.5386452

E (total electronic) + ZPVE = -748.380765
Internal Thermal Energy = -748.368092
Enthalpy = -748.367148
Gibbs Free Energy = -748.422982

C,0,1.048819306,-2.8476281814,1.4890369837
C,0,1.7867850348,-4.0675189677,1.1951209388
O,0,1.4954327089,-4.3814672521,2.5196131113
H,0,-0.0243273007,-2.9200179373,1.5572676818
H,0,1.5390399396,-2.1060165292,2.0983701985
H,0,2.8495561031,-3.9261717752,0.9637589356
H,0,1.3292253648,-4.719806935,0.4413569297
O,0,1.0124366979,-1.7430648888,-0.0513157394
C,0,0.3975684281,-0.6580806164,0.1420329768
O,0,-0.1834125161,-0.253924122,1.1344023594
O,0,0.4546821725,0.1491384526,-1.002233624
C,0,-0.250123018,1.3251808153,-0.9646525019
C,0,0.4093717833,2.5422907947,-0.9647436722
C,0,-0.3161506595,3.7284450575,-0.9963345435
C,0,-1.7039214952,3.6973150819,-1.0216781266
C,0,-2.3754550736,2.478928314,-1.0222669307
C,0,-1.6378463438,1.3148810643,-0.997261556
F,0,-2.2662607962,0.1274838106,-1.0129886156
H,0,1.4917849376,2.5431851863,-0.9420165372
H,0,0.20657326,4.6757403993,-0.9984533595
H,0,-2.2706742333,4.6186608011,-1.0435582214
H,0,-3.4558316999,2.4204396677,-1.0455870478

TS-OEt 2-methylphenyl carbonate

E (total electronic) = -688.6061497
E (total electronic) + ZPVE = -688.412544
Internal Thermal Energy = -688.399026
Enthalpy = -688.398081
Gibbs Free Energy = -688.455347

C,0,-3.4165255357,-0.0719074552,0.3680484056
C,0,-4.6232171946,-0.1010691965,-0.44465429
O,0,-5.260347854,0.0460678622,0.7847630188
O,0,-1.892264314,-0.2438434846,-0.7563731904
C,0,-0.8039905535,-0.2446311723,-0.1123842163
O,0,-0.6171899237,-0.1527428719,1.0914092526
O,0,0.2814118324,-0.3794403778,-0.9733484293
C,0,1.5443281752,-0.3056112388,-0.4132644388
C,0,2.2622005558,-1.476609766,-0.2412372917
C,0,3.5599614674,-1.4213089371,0.2538358009
C,0,4.1220757479,-0.1922013174,0.570692437
C,0,3.3865069712,0.9743553171,0.3883922102
C,0,2.0860877461,0.942583509,-0.1072739135
C,0,1.278757848,2.1926289752,-0.3110430049
H,0,-3.1046957259,0.8811949812,0.7624346595
H,0,-3.1820120224,-0.9528438829,0.9424145387
H,0,-4.8131919083,-1.046076476,-0.967633828
H,0,-4.7392819929,0.7371429562,-1.1422355181
H,0,1.796543152,-2.4197870711,-0.498963831
H,0,4.1253826052,-2.334519467,0.3891619845
H,0,5.1325372733,-0.1382478024,0.9556444698
H,0,3.8298022031,1.9333179132,0.6319978082
H,0,0.8950532766,2.2466291958,-1.3314120704
H,0,0.4179259675,2.2080896934,0.3610579508
H,0,1.8839454432,3.0772509734,-0.1184998541

TS-OEt 2-trifluoromethylphenyl carbonate

E (total electronic) = -986.3578923
E (total electronic) + ZPVE = -986.187029
Internal Thermal Energy = -986.171719
Enthalpy = -986.170775
Gibbs Free Energy = -986.232712

C,0,3.7961195462,0.273645402,-0.3390149375

C,0,4.9505305013,-0.1981784186,0.412683587
O,0,5.6555977524,0.1669508775,-0.7303872361
O,0,2.230812612,0.0750801766,0.7075155457
C,0,1.1996514974,0.5123505302,0.1273369854
O,0,1.0726787201,1.0128589189,-0.9761250675
O,0,0.0728970058,0.3579527741,0.949658091
C,0,-1.1320328517,0.7717821512,0.4354150408
C,0,-1.4853996119,2.1102354143,0.4576356554
C,0,-2.7335928501,2.4978619934,-0.0093783267
C,0,-3.628001548,1.5517638111,-0.4954473914
C,0,-3.2726036536,0.210772639,-0.5147940749
C,0,-2.022826154,-0.1800132932,-0.0513781502
C,0,-1.6163137482,-1.6220437366,-0.053084875
F,0,-2.5375574622,-2.4021676966,-0.633147948
F,0,-0.466269511,-1.8284696075,-0.7144824529
F,0,-1.4335339517,-2.1023660716,1.1873375123
H,0,3.6783586156,1.339164809,-0.449174121
H,0,3.4341608805,-0.354197026,-1.1368788556
H,0,4.9484133542,-1.2697198701,0.6469702603
H,0,5.1836137241,0.3760810155,1.3177142401
H,0,-0.7757001694,2.8327691039,0.8394780244
H,0,-3.0087689627,3.5446347873,0.0079302401
H,0,-4.6010519149,1.8559314741,-0.8568941342
H,0,-3.9617473999,-0.5338833579,-0.8893380616

TS-OEt 2-(dimethylamino)phenyl carbonate

E (total electronic) = -783.2413578
E (total electronic) + ZPVE = -783.001722
Internal Thermal Energy = -782.985975
Enthalpy = -782.985031
Gibbs Free Energy = -783.047252

C,0,0.2961252006,-2.8895660827,-0.5828690996
C,0,0.1143727183,-3.8571028865,-1.653968277
O,0,0.3180882938,-4.7801792094,-0.6311996876
O,0,0.131545889,-1.1281601337,-1.2872083249
C,0,0.2753472821,-0.2341424712,-0.4042042379
O,0,0.4955751766,-0.354180225,0.7901223927
O,0,0.1867809853,1.0378574415,-0.9719295137
C,0,0.0552297875,2.0973689439,-0.0993021422
C,0,1.142336496,2.9217936144,0.1120984232
C,0,1.0440396908,4.0058761621,0.9792542242
C,0,-0.155627363,4.2422417958,1.6304617338
C,0,-1.255939285,3.4201546987,1.402788963
C,0,-1.1816054511,2.3364033326,0.5256617011
N,0,-2.2619359277,1.4621194176,0.2795237389
C,0,-2.7478416894,1.4799109115,-1.1015815517
C,0,-3.3707551423,1.5543322559,1.2147131684
H,0,-0.515055362,-2.7595392941,0.1142437498
H,0,1.2982434158,-2.7281509793,-0.2213610175
H,0,0.8816574322,-3.8401316912,-2.4372725003
H,0,-0.8818779825,-3.8688477293,-2.1121525226
H,0,2.0700229731,2.6892582382,-0.3962513591
H,0,1.9004471179,4.6453857064,1.1486134994
H,0,-0.2492311041,5.0751867704,2.3159775122
H,0,-2.1846915818,3.6333620952,1.9139021555
H,0,-3.4392891154,0.6486878549,-1.2428870975
H,0,-3.2792371679,2.4163131785,-1.3218044156
H,0,-1.9211151398,1.3671692701,-1.7968784215
H,0,-3.9405349173,2.4887618868,1.110173115
H,0,-4.0500097775,0.7234477446,1.0245473833
H,0,-3.0063764522,1.4772693833,2.238674408

TS-OEt 3-nitrophenyl carbonate

E (total electronic) = -853.797961
E (total electronic) + ZPVE = -853.629348
Internal Thermal Energy = -853.614939
Enthalpy = -853.613995
Gibbs Free Energy = -853.674778

C,0,-0.0710571334,-3.6963852579,-1.2182245365
C,0,-0.1885220108,-4.46504041,-2.4491954011
O,0,-0.1193660425,-5.5620645064,-1.5958603222
O,0,-0.0930846967,-1.8476520724,-1.623728247
C,0,-0.0195933068,-1.1202170489,-0.5959447839
O,0,0.0644316601,-1.4309281705,0.5790760979
O,0,-0.0293705383,0.2347996418,-0.9589729558
C,0,-0.0412379379,1.1740333611,0.039109201
C,0,-1.0596606115,1.2205447056,0.986350161
C,0,-1.0768554626,2.2334826893,1.9334708521
C,0,-0.0901202537,3.2102976935,1.943472863
C,0,0.9020699808,3.1356925764,0.982895224
C,0,0.9551253546,2.1339118984,0.0269289197
N,0,1.9525526001,4.1628157122,0.9704712861
O,0,2.8075486745,4.0950297618,0.1093956222
O,0,1.9139581083,5.0289646984,1.8219817744
H,0,-0.9384448354,-3.6462213224,-0.580412029
H,0,0.8977405412,-3.6602369479,-0.7471628876
H,0,0.6487526751,-4.3549131463,-3.1492048745
H,0,-1.1364214288,-4.3411106029,-2.9871308009
H,0,-1.8298728858,0.4613985165,0.9728294558
H,0,-1.869666804,2.2671268036,2.6683988741
H,0,-0.0894115308,4.0100026366,2.6688113824
H,0,1.7443928842,2.1010457901,-0.7096898751

TS-OEt 3-cyanophenyl carbonate

E (total electronic) = -741.5425044
E (total electronic) + ZPVE = -741.377954
Internal Thermal Energy = -741.364289
Enthalpy = -741.363345
Gibbs Free Energy = -741.421567

C,0,-0.1762372317,-3.4469989313,-1.3083601608
C,0,-0.3479116104,-4.1479812225,-2.5726999296
O,0,-0.1630014493,-5.2865413214,-1.7940101847
O,0,-0.3151770766,-1.5801648917,-1.5978210588
C,0,-0.168874293,-0.9074604611,-0.5403966793
O,0,0.0326069133,-1.2806230646,0.6021120597
O,0,-0.2518957348,0.4630291081,-0.821357324
C,0,-0.1892678502,1.3457364823,0.22742048
C,0,-1.12700274,1.3237291518,1.2539603182
C,0,-1.07519901,2.2820189904,2.2553003464
C,0,-0.0991219676,3.2683337357,2.2387390081
C,0,0.8290037752,3.2800314414,1.1998644019
C,0,0.7938379918,2.318139832,0.1899923727
C,0,1.8430337655,4.2983486284,1.1642291381
N,0,2.6520867486,5.1128910814,1.1371899905
H,0,-0.9958061331,-3.4778793706,-0.609090519
H,0,0.8218209165,-3.3870304507,-0.905973579
H,0,0.4289898543,-3.9546152731,-3.3224612515
H,0,-1.3379669415,-4.043580652,-3.0331497358
H,0,-1.8880846434,0.5550769455,1.2595604583
H,0,-1.8052916327,2.2633576143,3.0534448106
H,0,-0.0556524898,4.0211001436,3.0139214663
H,0,1.514579839,2.3257194841,-0.6165684285

TS-OEt 3-methoxyphenyl carbonate

E (total electronic) = -763.8142777
E (total electronic) + ZPVE = -763.615458
Internal Thermal Energy = -763.601113
Enthalpy = -763.600169
Gibbs Free Energy = -763.659650

C,0,-3.3537062661,0.1415453307,0.4314072807
C,0,-4.5701642476,0.1890900229,-0.3655676963
O,0,-5.1657771831,0.496109129,0.8552329953
H,0,-2.9305394541,1.0799138004,0.7499262112
H,0,-3.2091484755,-0.7154167566,1.0683631405
H,0,-4.8737279634,-0.7641396609,-0.8148698632
H,0,-4.6039802057,0.9818710249,-1.1225631256

O,0,-1.8806033089,-0.2890462029,-0.6906276997
C,0,-0.788126442,-0.3741410578,-0.0600352367
O,0,-0.563282369,-0.2037623886,1.1281617103
O,0,0.2520812004,-0.7176855302,-0.9207389222
C,0,1.5129907671,-0.840786799,-0.3678103481
C,0,1.9690869026,-2.0891726226,0.0087064242
C,0,3.2671639742,-2.2014804181,0.5018250961
C,0,4.0825643222,-1.0903381608,0.6126964936
C,0,3.6037562363,0.163735955,0.2247648526
C,0,2.310439008,0.2936458587,-0.2706466346
O,0,4.4681116373,1.2008557282,0.3630340215
C,0,4.0128202677,2.4889541834,-0.0191995743
H,0,1.3193482052,-2.9491207443,-0.0845432306
H,0,3.6442819064,-3.1708802306,0.8022959467
H,0,5.092866536,-1.1675678109,0.9930425813
H,0,1.9010923959,1.2440111747,-0.5821273593
H,0,4.8389559116,3.1685723857,0.1689875602
H,0,3.7540899497,2.5126159142,-1.0798716716
H,0,3.148388695,2.7899238756,0.5763580481

TS-OEt 3-chlorophenyl carbonate

E (total electronic) = -1108.8993359
E (total electronic) + ZPVE = -1108.743126
Internal Thermal Energy = -1108.730032
Enthalpy = -1108.729088
Gibbs Free Energy = -1108.786639

C,0,-0.0160470219,-3.3963409357,-0.4554902441
C,0,-0.1676624002,-4.3822297459,-1.5156414289
O,0,-0.06650392,-5.295058051,-0.4693625018
O,0,-0.0624894976,-1.6521636079,-1.1993486299
C,0,0.0612384855,-0.7464277511,-0.3280589593
O,0,0.2012603058,-0.8410848233,0.8794722683
O,0,0.035571902,0.5162684018,-0.9289518544
C,0,0.0822247889,1.6196782946,-0.1088162511
C,0,1.1704280176,2.4694109592,-0.2332915469
C,0,1.1932598924,3.6279463689,0.5270727574
C,0,0.1708616956,3.9492966091,1.4026523609
C,0,-0.9083234312,3.0783402099,1.510173282
C,0,-0.9619337773,1.9153557636,0.7575347711
Cl,0,2.5572486371,4.7110626862,0.3697703305
H,0,-0.863902094,-3.2245703285,0.1870664433
H,0,0.9666215711,-3.2701275273,-0.0313987404
H,0,0.6474043912,-4.4090505056,-2.2490228172
H,0,-1.1323857181,-4.3629794331,-2.0370543114
H,0,1.9742026407,2.2255553213,-0.9146038727
H,0,0.2147899178,4.8597944168,1.9841007752
H,0,-1.7172810967,3.3170944635,2.1883692551
H,0,-1.7992552885,1.2348532141,0.8351779145

TS-OEt 3-fluorophenyl carbonate

E (total electronic) = -748.540765
E (total electronic) + ZPVE = -748.383138
Internal Thermal Energy = -748.370455
Enthalpy = -748.369511
Gibbs Free Energy = -748.426203

C,0,-0.8124878233,-3.1835935318,-0.3506627584
C,0,-0.7849689533,-4.1384833721,-1.4487893331
O,0,-1.123069807,-5.0534627293,-0.4553814131
H,0,-1.777758058,-2.8865549551,0.025367432
H,0,0.0109974975,-3.2015951761,0.3442479641
H,0,0.1964604559,-4.2861700678,-1.9155877739
H,0,-1.5427371991,-3.9797985991,-2.2256364375
O,0,-0.3920694893,-1.4532421974,-1.006733965
C,0,-0.3968042636,-0.5732823179,-0.1006824931
O,0,-0.6241855587,-0.6858979338,1.0924509347
O,0,-0.0740841372,0.6788010493,-0.6309224924
C,0,-0.0994834971,1.7556207603,0.2272215103
C,0,1.1074232697,2.3370270437,0.583021757

C,0,1.0686360638,3.4607227324,1.3863226135
C,0,-0.1078238698,4.0165355585,1.8455910846
C,0,-1.3030035727,3.4104051707,1.4725567867
C,0,-1.3072055938,2.2837840773,0.6632803667
F,0,2.2376724122,4.0350610529,1.7344232168
H,0,2.0482010272,1.9269228329,0.2414015823
H,0,-0.0817855169,4.8974417769,2.4723525859
H,0,-2.2404842858,3.826744944,1.8174276875
H,0,-2.2328261007,1.8072618815,0.3687441443

TS-OEt 3-methylphenyl carbonate

E (total electronic) = -688.6041695
E (total electronic) + ZPVE = -688.411011
Internal Thermal Energy = -688.397196
Enthalpy = -688.396252
Gibbs Free Energy = -688.455859

C,0,3.6135809361,0.2728730639,-0.3126257491
C,0,4.8452290923,0.0227151761,0.4204485915
O,0,5.4264215118,0.709481261,-0.6424447836
O,0,2.1477266179,-0.4705092088,0.645343176
C,0,1.0368436995,-0.2596454353,0.0788317672
O,0,0.8023059489,0.3188854564,-0.9705043583
O,0,-0.0060208747,-0.8070086344,0.8219036409
C,0,-1.294977678,-0.6083433964,0.36382692
C,0,-2.0016876146,-1.6967050421,-0.118556451
C,0,-3.3258252977,-1.518655363,-0.5045008286
C,0,-3.9226927706,-0.269354475,-0.4116014046
C,0,-3.2079855756,0.8284678445,0.0716131929
C,0,-1.886499545,0.6428605723,0.4645755714
C,0,-3.8469542963,2.1898454249,0.1450983868
H,0,3.2131124519,1.2728123442,-0.2876309941
H,0,3.4301710792,-0.3177831051,-1.1950412161
H,0,5.1287919033,-1.0324165418,0.5149770444
H,0,4.9167654913,0.5137915006,1.3983775713
H,0,-1.5178572876,-2.6630977622,-0.1789770678
H,0,-3.893387358,-2.3624857286,-0.8767291236
H,0,-4.9563354561,-0.1410556584,-0.7117354009
H,0,-1.3039877064,1.4711416955,0.8516658061
H,0,-3.7692908462,2.701679837,-0.816966604
H,0,-4.9059275679,2.1123375212,0.3919133115
H,0,-3.3596038571,2.8141349234,0.8935450018

TS-OEt 3-trifluoromethylphenyl carbonate

E (total electronic) = -986.3580861
E (total electronic) + ZPVE = -986.187433
Internal Thermal Energy = -986.171983
Enthalpy = -986.171039
Gibbs Free Energy = -986.234775

C,0,-0.6251548396,-2.6830114517,-2.6905111288
C,0,-0.0961547986,-2.9709974821,-4.0159975136
O,0,-0.5911602473,-4.2482034613,-3.7689623115
O,0,-0.289550592,-0.8698336388,-2.2528562091
C,0,-0.643596263,-0.5799762399,-1.0761758633
O,0,-1.1686717271,-1.2778529563,-0.2255984173
O,0,-0.3370374925,0.7548066612,-0.7885076103
C,0,-0.7149177388,1.251913315,0.435875263
C,0,-2.0566797569,1.3562800824,0.7889656253
C,0,-2.4027344553,1.9317582415,1.9998090681
C,0,-1.4200862676,2.4104089347,2.8617502878
C,0,-0.0906995692,2.3017831378,2.4901235194
C,0,0.2743763464,1.7206612541,1.2796943305
C,0,1.0024284397,2.8079053393,3.3798432099
F,0,1.8740993498,1.8382087989,3.7055028505
F,0,0.5410425831,3.3177113156,4.526358018
F,0,1.7255391453,3.7730905468,2.7861142532
H,0,-1.6942455802,-2.5860588173,-2.593994627
H,0,-0.0799376728,-3.0673299914,-1.8441542849
H,0,0.9939989261,-2.8947322686,-4.1098325744

H,0,-0.5757929342,-2.4272599614,-4.8390047468
H,0,-2.8133447675,0.9835788153,0.1112208934
H,0,-3.4455073133,2.0134341515,2.2766835256
H,0,-1.6891820833,2.8629603956,3.8059656617
H,0,1.3134033086,1.6329992792,0.9867537805

TS-OEt 3-(dimethylamino)phenyl carbonate

E (total electronic) = -783.2443681
E (total electronic) + ZPVE = -783.004912
Internal Thermal Energy = -782.988844
Enthalpy = -782.987900
Gibbs Free Energy = -783.051116

C,0,4.2394109159,-0.3378183172,0.4114247236
C,0,5.4486134213,-0.5731685168,-0.3625053501
O,0,6.0026229675,-0.827227489,0.8900163811
O,0,2.8155005085,0.1300876569,-0.7633563094
C,0,1.7161048025,0.2912534886,-0.1579881395
O,0,1.471826476,0.1958959258,1.0353406501
O,0,0.7022110595,0.6156898682,-1.052113447
C,0,-0.5619469393,0.8295376418,-0.5270603071
C,0,-0.9151413202,2.0955860064,-0.0903347906
C,0,-2.2092198328,2.2779100804,0.3795567379
C,0,-3.1251932357,1.2374240457,0.4059751528
C,0,-2.769796663,-0.0437793682,-0.0592917926
C,0,-1.4519576471,-0.2286786168,-0.5158689515
N,0,-3.6839227465,-1.0811066138,-0.083190421
C,0,-4.904122856,-0.9360047626,0.691995015
C,0,-3.1819585518,-2.4317956047,-0.2668298922
H,0,3.7240575739,-1.1975825959,0.806287077
H,0,4.1751444131,0.5836000767,0.9663073811
H,0,5.8476827767,0.3023168483,-0.8885508417
H,0,5.4089927691,-1.4296137635,-1.0462054459
H,0,-0.1921667204,2.8999557652,-0.1119690843
H,0,-2.5150438358,3.2530286608,0.7388737992
H,0,-4.1179670649,1.4274265202,0.7855174034
H,0,-1.1000485591,-1.1873839482,-0.8678447359
H,0,-5.4944079595,-1.8429476298,0.5898238737
H,0,-4.7036861353,-0.7647282497,1.7568676128
H,0,-5.504713659,-0.1068286438,0.316962148
H,0,-2.45823473,-2.7166332499,0.506978823
H,0,-4.0184885742,-3.1250018693,-0.2340621347
H,0,-2.7034551733,-2.5372510655,-1.2410743352

TS-OEt 4-trifluoromethylphenyl carbonate

E (total electronic) = -986.3588936
E (total electronic) + ZPVE = -986.188209
Internal Thermal Energy = -986.172764
Enthalpy = -986.171820
Gibbs Free Energy = -986.235443

C,0,-4.8308501215,-0.4109593633,-0.2747450444
C,0,-6.0950397856,0.1186377848,0.2157714715
O,0,-6.6448552454,-0.9244101817,-0.5239253921
H,0,-4.4705862316,-1.3255112958,0.167244073
H,0,-4.5801334206,-0.2220010482,-1.3057375914
H,0,-6.3439997755,1.128936447,-0.1311687571
H,0,-6.2369986815,0.0566498144,1.3016312983
O,0,-3.4020256322,0.6334064095,0.4027118398
C,0,-2.2714166449,0.2118241361,0.0321055035
O,0,-1.9872176997,-0.7325748672,-0.6840509661
O,0,-1.254764433,1.0199505456,0.5558992455
C,0,0.0492376423,0.6492808763,0.3427209481
C,0,0.8899630969,1.5652688649,-0.2685576987
C,0,2.2359896251,1.2629687039,-0.4299033537
C,0,2.7214470521,0.0452961783,0.0187054984
C,0,1.8739838424,-0.8730444707,0.6343331231
C,0,0.5354376796,-0.5723880111,0.8003255796
C,0,4.163174665,-0.3162743448,-0.1394086167
H,0,0.4854577407,2.5086966969,-0.6104525592

H,0,2.8981398637,1.9738445507,-0.9052620636
H,0,2.2634046611,-1.8206263917,0.9864169248
H,0,-0.1374366595,-1.2719920646,1.2769057547
F,0,4.3256115908,-1.442090991,-0.8572786456
F,0,4.8725047871,0.6389748417,-0.7508618336
F,0,4.7591813344,-0.5460728101,1.044552912

TS-OEt 2,4-dinitrophenyl carbonate

E (total electronic) = -1058.2917544
E (total electronic) + ZPVE = -1058.120373
Internal Thermal Energy = -1058.103590
Enthalpy = -1058.102645
Gibbs Free Energy = -1058.168544

C,0,0.7811846004,-3.3928742754,-0.8504541483
C,0,0.8587405067,-4.34979923,-1.9478743714
O,0,0.7572468229,-5.3144853059,-0.9528606263
O,0,0.8697747931,-1.6465404183,-1.5264545213
C,0,0.8211341469,-0.7758475116,-0.6244919986
O,0,0.7276016131,-0.876399352,0.5827490904
O,0,0.9249278358,0.519228018,-1.1973227364
C,0,0.76026526,1.5939850896,-0.4005942275
C,0,1.7286701034,2.5926784551,-0.467471445
C,0,1.6218465583,3.7376246253,0.2962766906
C,0,0.5410466592,3.869423073,1.1546847671
C,0,-0.4378748678,2.9027796271,1.2582394035
C,0,-0.3270195318,1.7820068553,0.4604175879
N,0,0.4250689015,5.0734820795,1.9807934151
O,0,1.2834929152,5.9241724064,1.8628900465
O,0,-0.5214227841,5.1544006902,2.7375279342
N,0,-1.4255582682,0.8152512744,0.5263476864
O,0,-1.7398648181,0.2486283703,-0.4994248913
O,0,-1.9760186577,0.6660983838,1.5959479269
H,0,-0.1814942918,-3.2576434674,-0.3833946852
H,0,1.65363726,-3.2909882381,-0.2249066306
H,0,1.8054413954,-4.3379119665,-2.5028754589
H,0,0.0209511309,-4.3074806349,-2.6554823035
H,0,2.5704262442,2.4407631387,-1.1287670481
H,0,2.3698163993,4.5153352797,0.2431788961
H,0,-1.2773769267,3.0206650338,1.9276646478

TS-OEt 2,4-dicyanophenyl carbonate

E (total electronic) = -833.7861903
E (total electronic) + ZPVE = -833.623063
Internal Thermal Energy = -833.607622
Enthalpy = -833.606677
Gibbs Free Energy = -833.668539

C,0,-0.0893695292,-4.2695756706,0.0604429698
C,0,-0.2054942701,-5.2681843518,-0.9946300364
O,0,0.0756416608,-6.1798502041,0.0166929461
O,0,-0.3820222021,-2.5564425498,-0.6578546533
C,0,-0.3082257996,-1.6473205427,0.2069275222
O,0,-0.0834057729,-1.6963542485,1.4002011801
O,0,-0.5224112232,-0.3828557244,-0.3970539388
C,0,-0.5666453958,0.7022377116,0.4191302884
C,0,0.4090886019,1.6795816689,0.2958711881
C,0,0.3434129438,2.8236636779,1.0698197735
C,0,-0.7040401018,2.9924152289,1.9776898252
C,0,-1.6911761255,2.0218719509,2.1073822039
C,0,-1.6214574789,0.8775988799,1.3231330002
C,0,-0.7681762604,4.1801082193,2.7824587867
C,0,-2.6434843678,-0.1246058619,0.4164513759
N,0,-3.4684095287,-0.9201377566,1.4767558067
N,0,-0.8166716104,5.1304981007,3.4243080568
H,0,-0.8995377142,-4.205262239,0.7691661889
H,0,0.9024877921,-4.0436058619,0.4178677026
H,0,0.5484394767,-5.1920759629,-1.7882358133
H,0,-1.2028527986,-5.3507103455,-1.4444869765
H,0,1.2131876834,1.5278785675,-0.4110629261

H,0,1.1033660917,3.5877968659,0.9772030299
H,0,-2.5074520713,2.1541364606,2.8040654995

TS-OEt 2,4-dimethoxyphenyl carbonate

E (total electronic) = -878.329804
E (total electronic) + ZPVE = -878.097797
Internal Thermal Energy = -878.080938
Enthalpy = -878.079994
Gibbs Free Energy = -878.144836

C,0,1.2274880158,-4.1221946786,-1.5175006116
C,0,1.1782329989,-4.9172250358,-2.7347827939
O,0,1.2977133365,-5.9837053813,-1.8470325408
O,0,1.1019780506,-2.2755864221,-1.964653524
C,0,1.1328517589,-1.5236413143,-0.9481776578
O,0,1.2187498133,-1.8224419379,0.2324844085
O,0,1.075989102,-0.1824323892,-1.3239291278
C,0,0.9500965018,0.7416514561,-0.3086784416
C,0,2.00923053,1.5417119711,0.0420708603
C,0,1.8788345681,2.5302773451,1.0214026868
C,0,0.6512594445,2.6894454878,1.6451318331
C,0,-0.4371978699,1.8802927972,1.2972202399
C,0,-0.2947833608,0.9096649136,0.320968662
O,0,-1.2837159617,0.0870424465,-0.0945299496
C,0,-2.5492505682,0.2212764722,0.5330688273
O,0,0.3955078165,3.6107637721,2.6127170412
C,0,1.4641889042,4.4572458338,3.001265055
H,0,0.3463341242,-4.1035699388,-0.89770317
H,0,2.1833815608,-4.0114589554,-1.0327702868
H,0,2.0206468596,-4.7756866398,-3.4224155688
H,0,0.2343368144,-4.8664215671,-3.2906690331
H,0,2.9570746541,1.3926952506,-0.4601489447
H,0,2.7287431972,3.1460103565,1.2739797403
H,0,-1.3760651792,2.0423667647,1.8071142543
H,0,-3.1941028028,-0.5204354114,0.0709167686
H,0,-2.4740822575,0.0260263453,1.6047252433
H,0,-2.961482347,1.219039205,0.3691486955
H,0,1.0662723699,5.1114607727,3.7718403186
H,0,2.2950105269,3.8764219023,3.4077157769
H,0,1.8148703989,5.0563885792,2.1580662389

TS-OEt 2,4-dichlorophenyl carbonate

E (total electronic) = -1568.5005359
E (total electronic) + ZPVE = -1568.353774
Internal Thermal Energy = -1568.339542
Enthalpy = -1568.338598
Gibbs Free Energy = -1568.398410

C,0,-0.027267063,-2.9955130857,-2.2355606465
C,0,-0.0983768021,-3.3871334358,-3.6361003339
O,0,-0.0337184341,-4.6798010816,-3.1251353018
O,0,-0.0691090703,-1.1082745862,-2.1061877277
C,0,-0.0151930313,-0.6996514088,-0.914741498
O,0,0.0511295199,-1.3240148108,0.1290573696
O,0,-0.0249823219,0.7049642468,-0.8765350039
C,0,-0.0912542776,1.2844937817,0.3609080683
C,0,1.0353069262,1.8859463889,0.8985398067
C,0,0.9743650159,2.5393526087,2.1205362648
C,0,-0.2317272217,2.5769777761,2.79999045
C,0,-1.3731611717,1.9835578893,2.2864057943
C,0,-1.2914943533,-1.3404111034,1.0628477334
Cl,0,-2.7101302126,0.601423487,0.3886338279
Cl,0,-0.3271737515,3.3942434083,4.3387462907
H,0,-0.9124051187,-3.1343545453,-1.6362706595
H,0,0.9274909021,-3.0859557538,-1.7436796288
H,0,0.7554649786,-3.0764061947,-4.2506369798
H,0,-1.0334364969,-3.1247917547,-4.1460924356
H,0,1.9626824707,1.8366173354,0.3428957294
H,0,1.8525225123,3.0107518953,2.5395699475
H,0,-2.3106679989,2.0214267365,2.8234659329

TS-OEt 2,4-difluorophenyl carbonate

E (total electronic) = -847.7811661
E (total electronic) + ZPVE = -847.631612
Internal Thermal Energy = -847.618100
Enthalpy = -847.617156
Gibbs Free Energy = -847.674914

C,0,3.7999343098,-0.0363739129,0.418260363
C,0,5.036999161,0.1968990147,-0.3129057676
O,0,5.6383393574,-0.2435328939,0.8625020252
O,0,2.3225682691,0.4069142407,-0.6809377156
C,0,1.2152544805,0.2344269707,-0.1016477965
O,0,0.9721966267,-0.1860194849,1.015986544
O,0,0.1582910539,0.622208093,-0.9387973213
C,0,-1.1104066472,0.4241379554,-0.4586336073
C,0,-1.9161726577,1.4985500241,-0.1254602262
C,0,-3.2256086803,1.2987292768,0.296745477
C,0,-3.6964350397,0.0051474727,0.3808641062
C,0,-2.9246549242,-1.0963441675,0.0583029883
C,0,-1.6334173885,-0.8585975519,-0.3627203975
F,0,-4.9611063444,-0.2047988394,0.7906902625
F,0,-0.8542638485,-1.8941116992,-0.6993350689
H,0,3.4903024927,-1.0594209777,0.5565394682
H,0,3.5363672956,0.6729695301,1.1857422368
H,0,5.2299792998,1.2426686215,-0.5816580619
H,0,5.1873341591,-0.4426408683,-1.1912521282
H,0,-1.5062674636,2.4970437478,-0.2028934047
H,0,-3.8693822063,2.1270843989,0.5579492939
H,0,-3.3142069451,-2.1026283909,0.1275704904

TS-OEt 3,5-dinitrophenyl carbonate

E (total electronic) = -1058.293252
E (total electronic) + ZPVE = -1058.122191
Internal Thermal Energy = -1058.105183
Enthalpy = -1058.104239
Gibbs Free Energy = -1058.171578

C,0,-0.5841953014,-3.5946293929,-0.879739986
C,0,-0.6189152427,-4.4945345042,-2.0254546
O,0,-0.8077607726,-5.4868089772,-1.0698650959
O,0,-0.3263892889,-1.8254090739,-1.4708733543
C,0,-0.2803174183,-0.9980348239,-0.5237239905
O,0,-0.3632304327,-1.16488953,0.6779184087
O,0,-0.0849531769,0.3041775874,-1.032917135
C,0,-0.07741659,1.3520619568,-0.1647205247
C,0,0.9584765968,2.266774273,-0.2806257568
C,0,0.949406462,3.3837682903,0.5367019999
C,0,-0.0349421439,3.6297033563,1.4711715451
C,0,-1.0445550519,2.6891442355,1.5489133936
C,0,-1.0998365069,1.5592510192,0.755100447
N,0,-2.1249273313,2.9101194133,2.5260464494
O,0,-3.0038576557,2.0773321414,2.5938729918
N,0,2.0478351778,4.3557929982,0.4087904566
O,0,-2.0723038993,3.9129221958,3.2065288046
O,0,2.0336303378,5.3223061821,1.1415854912
O,0,2.9030335932,4.1337552505,-0.4221265643
H,0,-1.5214002841,-3.3820007032,-0.3910693025
H,0,0.303220511,-3.6097964335,-0.2677490922
H,0,0.3171231871,-4.5554933673,-2.594656786
H,0,-1.4569704593,-4.3341135315,-2.7152214698
H,0,1.7512252166,2.1071335706,-0.9971558176
H,0,-0.0191587198,4.5045664569,2.1018917827

TS-OEt 3,5-dicyanophenyl carbonate

E (total electronic) = -833.7839961
E (total electronic) + ZPVE = -833.620969
Internal Thermal Energy = -833.605463

Enthalpy = -833.604519
Gibbs Free Energy = -833.667153

C,0,-0.7021556579,-3.3537964406,-0.9250264093
C,0,-0.7844120608,-4.2224552019,-2.0918070373
O,0,-0.8436692668,-5.246616851,-1.1527494418
O,0,-0.5844541826,-1.5556125334,-1.4812113932
C,0,-0.49862863,-0.7516788352,-0.5156196703
O,0,-0.468868145,-0.958628523,0.6829450719
O,0,-0.4148102287,0.5702767467,-0.9959737667
C,0,-0.3856997975,1.5939878724,-0.0950308856
C,0,0.6112597448,2.5445615479,-0.243104778
C,0,0.6341162564,3.6521898225,0.6032586953
C,0,-0.3193586167,3.8165656963,1.6001863775
C,0,-1.3099694245,2.8472368046,1.7277758213
C,0,-1.3571346239,1.7385793701,0.8872974026
C,0,-2.3126338222,2.9980847065,2.7480416229
C,0,1.6660018409,4.6411849452,0.4440864691
N,0,2.4888347771,5.4307324649,0.3170225207
N,0,-3.1122793231,3.1189558047,3.5619859154
H,0,-1.6059759161,-3.2028665127,-0.3571121991
H,0,0.2321583511,-3.3360246562,-0.3876183135
H,0,0.1039457521,-4.2195075525,-2.7356283487
H,0,-1.683218052,-4.0897021541,-2.7067824245
H,0,1.3576231387,2.4186608488,-1.0159045407
H,0,-0.2950176965,4.6748049111,2.256511078
H,0,-2.1365404168,0.9980157189,0.994224234

TS-OEt 3,5-dimethoxyphenyl carbonate

E (total electronic) = -878.3325105
E (total electronic) + ZPVE = -878.100957
Internal Thermal Energy = -878.083968
Enthalpy = -878.083024
Gibbs Free Energy = -878.148962

C,0,-3.8737105665,-0.5892286218,0.2359330011
C,0,-5.11737603,-0.6592480033,-0.5158724121
O,0,-5.69674027,-0.6335308051,0.7500657285
H,0,-3.6090760982,0.3595423405,0.672844968
H,0,-3.5458757435,-1.4823949239,0.741753845
H,0,-5.2675708137,-1.5828480975,-1.0878048616
H,0,-5.3297168171,0.208207125,-1.1523935464
O,0,-2.4085444091,-0.5857084912,-0.9760296947
C,0,-1.2866750195,-0.5623509679,-0.3936672475
O,0,-1.0335779433,-0.5267277706,0.8002011165
O,0,-0.2489853159,-0.5883172792,-1.3233631711
C,0,1.041518325,-0.541818857,-0.8317815093
C,0,1.7350449632,-1.7188704733,-0.675272895
C,0,3.0654097878,-1.6610085154,-0.2438534277
C,0,3.6694436108,-0.442142535,0.0190119119
C,0,2.9341279762,0.7369478207,-0.1524109416
C,0,1.6148673054,0.7027796385,-0.5796969606
O,0,3.6084745858,1.8806171905,0.1256636608
C,0,2.9124066075,3.1063900967,-0.0363779841
O,0,3.6898958719,-2.8572801022,-0.1114386901
C,0,5.0397686418,-2.8482314092,0.325333809
H,0,1.2677118717,-2.6722299785,-0.8809670745
H,0,4.6941239207,-0.3609127314,0.3502632527
H,0,1.0210893705,1.5931415579,-0.7221702763
H,0,3.6161558788,3.8894335519,0.2306885447
H,0,2.5925555318,3.238721027,-1.071972324
H,0,2.0447102572,3.152212242,0.6248411953
H,0,5.1255601852,-2.3987017597,1.3167185089
H,0,5.3487011599,-3.8886151075,0.3688663938
H,0,5.6739461757,-2.3068751611,-0.3796829198

TS-OEt 3,5-dichlorophenyl carbonate

E (total electronic) = -1568.5005625
E (total electronic) + ZPVE = -1568.354073
Internal Thermal Energy = -1568.339728

Enthalpy = -1568.338784
Gibbs Free Energy = -1568.399972

C,0,-0.0732796566,-3.3401536925,-0.513912967
C,0,-0.3477580401,-4.307272871,-1.5674581345
O,0,-0.0435874965,-5.2432915744,-0.5837638014
O,0,-0.3138063473,-1.5871863659,-1.1836459629
C,0,-0.0663963344,-0.6985693095,-0.3233324658
O,0,0.2887384709,-0.8084451311,0.8364772969
O,0,-0.2390328815,0.577469409,-0.8817349653
C,0,-0.0851012705,1.6698099881,-0.0692658582
C,0,0.8515277642,2.6208836557,-0.4447926627
C,0,0.9663572163,3.7713733574,0.3178511249
C,0,0.1850645248,3.9941217404,1.4383600631
C,0,-0.7386377851,3.0169226252,1.7788077808
C,0,-0.8945204645,1.8562172369,1.0445833636
H,0,-0.8141247413,-3.227746611,0.2607591362
H,0,0.9580579236,-3.1799252237,-0.245036717
H,0,0.340989653,-4.2744073556,-2.420574106
H,0,-1.3827468411,-4.3197936267,-1.9307193645
H,0,1.4691462667,2.4581966519,-1.3169608886
H,0,0.2886425148,4.8956127751,2.0247360709
H,0,-1.6206583571,1.1073355915,1.3263671528
Cl,0,-1.7411722622,3.2686015967,3.1840281917
Cl,0,2.1366794938,4.9780264535,-0.145310457

TS-OEt 3,5-difluorophenyl carbonate

E (total electronic) = -847.7836991
E (total electronic) + ZPVE = -847.634480
Internal Thermal Energy = -847.620902
Enthalpy = -847.619958
Gibbs Free Energy = -847.678458

C,0,-3.4139140055,0.0235382272,0.3849864891
C,0,-4.6117985653,-0.4793340702,-0.2726470007
O,0,-5.2764089908,0.2643728263,0.6976885963
H,0,-3.152425633,1.0554888529,0.2163478149
H,0,-3.152619578,-0.4085875221,1.3371336362
H,0,-4.7525316308,-1.5657661751,-0.216945182
H,0,-4.7519644349,-0.1428055033,-1.3071998191
O,0,-1.8789725021,-0.6475486192,-0.4966683237
C,0,-0.8023412907,-0.2688765019,0.0413506945
O,0,-0.621714862,0.4377068596,1.0167564707
O,0,0.2961379334,-0.8055842667,-0.646215111
C,0,1.5583446483,-0.4299699235,-0.2686585994
C,0,2.4579426728,-1.441457803,0.0368896392
C,0,3.7577915276,-1.0821210086,0.3349335508
C,0,4.1992145915,0.2255212746,0.3494650873
C,0,3.2585456987,1.1904133157,0.0382614069
C,0,1.9468785039,0.9045246747,-0.27550004
F,0,3.6495697022,2.4765352179,0.0382803249
F,0,4.6380686828,-2.0541449313,0.6284903417
H,0,2.1518191771,-2.4780719905,0.0367064212
H,0,5.2215352918,0.4813041533,0.5882546342
H,0,1.2490610629,1.694875913,-0.5107800319

TS-OEt 3,5-dimethylphenyl carbonate

E (total electronic) = -727.9121839
E (total electronic) + ZPVE = -727.691525
Internal Thermal Energy = -727.675945
Enthalpy = -727.675001
Gibbs Free Energy = -727.738132

C,0,-3.9311499568,0.05175451,0.3879722074
C,0,-5.1620063523,-0.1265948219,-0.3667680969
O,0,-5.7612799283,0.1533263669,0.858911785
O,0,-2.4422461724,-0.2033416219,-0.7697360964
C,0,-1.3310889052,-0.0753267315,-0.178928791
O,0,-1.1050523493,0.1768923265,0.9948173389
O,0,-0.2758858956,-0.2718895703,-1.0642622565

C,0,1.0072884204,-0.1326494279,-0.5645191812
C,0,1.7421437797,-1.2679636711,-0.2857325326
C,0,3.0637584971,-1.1489676227,0.1510417265
C,0,3.6063826431,0.1213741102,0.2979186179
C,0,2.865790593,1.2735722409,0.0178686278
C,0,1.5557025007,1.1355974774,-0.4202594722
C,0,3.4840011094,2.6345016666,0.2002840662
C,0,3.8733829143,-2.3843222437,0.4437165977
H,0,-3.6462132774,1.0584863311,0.6457254659
H,0,-3.6382360837,-0.7394045852,1.0583196147
H,0,-5.3308189741,-1.1373984101,-0.7570997028
H,0,-5.336944685,0.6102576172,-1.1598621268
H,0,1.2837681981,-2.2421101448,-0.4129642025
H,0,4.6326271252,0.224162343,0.6362070465
H,0,0.9494147697,2.0041548296,-0.6498542585
H,0,2.8332409461,3.418340993,-0.1853053935
H,0,3.6678865667,2.8354548991,1.2577748583
H,0,4.4438458931,2.698023399,-0.314656795
H,0,4.0289098747,-2.9688528203,-0.4653013528
H,0,4.849040291,-2.1270919982,0.854116154
H,0,3.3571754576,-3.0268764408,1.158964152

TS-OEt 3,5-di(trifluoromethyl)phenyl carbonate

E (total electronic) = -1323.4173176
E (total electronic) + ZPVE = -1323.242041
Internal Thermal Energy = -1323.222910
Enthalpy = -1323.221965
Gibbs Free Energy = -1323.295163

C,0,0.5798667242,-3.7608483049,-0.2861664675
C,0,0.7546707683,-4.8785461632,-1.2036237175
O,0,0.6927989041,-5.6503169742,-0.0478043213
O,0,0.5623923686,-2.1405946465,-1.2576326148
C,0,0.4650363512,-1.1277252677,-0.5138073238
O,0,0.3681056878,-1.0485968685,0.697373353
O,0,0.4972668136,0.0458331417,-1.2866470582
C,0,0.3303991894,1.2453212702,-0.6516581744
C,0,1.2881331978,2.2210375608,-0.8516747773
C,0,1.1076692065,3.4801484172,-0.2867372598
C,0,-0.0060439331,3.7696495108,0.4757818143
C,0,-0.9572637338,2.7706221865,0.6632512138
C,0,-0.8058099781,1.5151158046,0.1080330756
C,0,-2.1599874921,3.0922875108,1.5000464383
C,0,2.1629840435,4.5178932443,-0.5282496474
F,0,-1.8249178652,3.3290722166,2.7784043063
F,0,-2.7860517226,4.1957711398,1.0642972553
F,0,-3.0584548555,2.1044492852,1.5070538513
F,0,3.3615693856,4.1205790135,-0.0745520094
F,0,1.882396272,5.6804042939,0.0663661236
F,0,2.3196515236,4.7703265852,-1.8367241999
H,0,-0.4026754352,-3.6132085848,0.1319947796
H,0,1.4263953027,-3.4804906061,0.3192044261
H,0,1.713614756,-4.8972140328,-1.7360900331
H,0,-0.0648453591,-5.0268467835,-1.9176938892
H,0,2.1627157232,1.993482146,-1.4485285806
H,0,-0.1392754125,4.7502333772,0.9129944747
H,0,-1.5510284309,0.746174528,0.2533539624

TS-OEt 3,4-dicyanophenyl carbonate

E (total electronic) = -833.7836471
E (total electronic) + ZPVE = -833.620659
Internal Thermal Energy = -833.605115
Enthalpy = -833.604171
Gibbs Free Energy = -833.667291

C,0,0.0549713321,-3.8492138875,-1.4094743767
C,0,-0.0272085589,-4.5999400844,-2.6556199138
O,0,0.0151479852,-5.7157314735,-1.8268573598
O,0,0.0448915972,-2.0018779078,-1.7807740526

C,0,0.1114428873,-1.2964240796,-0.7400474572
O,0,0.1747227627,-1.6188561222,0.4304912807
O,0,0.1323501723,-0.0710063909,-1.0884523038
C,0,0.0794746423,1.0090908333,-0.105235042
C,0,-0.8771070812,0.9821415462,0.9058027644
C,0,-0.9277178846,2.0083755365,1.8320269588
C,0,-0.0303969422,3.0698351469,1.7546730864
C,0,0.9243032618,3.0929274474,0.7279963128
C,0,0.9807374595,2.0621780963,-0.1986927252
C,0,-0.0868447235,4.1336259283,2.7139246275
N,0,-0.1294956003,4.9868214499,3.4807758925
C,0,1.8520868405,4.1854601577,0.6334889586
N,0,2.5899529324,5.0612805849,0.5633193617
H,0,-0.830165561,-3.8137485423,-0.7951705275
H,0,1.0092153181,-3.8282001099,-0.9081876829
H,0,0.8301270255,-4.4757520026,-3.3289161916
H,0,-0.9584845002,-4.4623295959,-3.2191269055
H,0,-1.5764114849,0.1608157435,0.9612171643
H,0,-1.6698291245,1.9947944763,2.6184202663
H,0,1.7143692446,2.0703714675,-0.9928741355

TS-OEt 3,4-dimethoxyphenyl carbonate

E (total electronic) = -878.3272312
E (total electronic) + ZPVE = -878.095248
Internal Thermal Energy = -878.078349
Enthalpy = -878.077405
Gibbs Free Energy = -878.142879

C,0,-4.5415548675,0.0258151412,0.4749624463
C,0,-5.8034180318,-0.0223927871,-0.2473465687
O,0,-6.3435794141,0.2500090808,1.007048236
O,0,-3.111425714,-0.2987129302,-0.7382324247
C,0,-1.9762528491,-0.2706431237,-0.1807351173
O,0,-1.6958519878,-0.0664271032,0.9904350436
O,0,-0.9670775272,-0.5225765514,-1.105611035
C,0,0.3383175411,-0.4991147702,-0.6467125302
C,0,1.012170776,-1.6813534915,-0.4576090662
C,0,2.3545959577,-1.6512361447,-0.0663262864
C,0,3.0022531636,-0.4460233729,0.1331031183
C,0,2.2976503537,0.7623190514,-0.0646417663
C,0,0.9711616816,0.728397531,-0.4552067752
O,0,3.0063725408,1.8971631968,0.1495318819
C,0,2.3281940042,3.1282339421,-0.0410001083
O,0,4.3000772553,-0.3117766989,0.5115756744
C,0,5.0363244259,-1.5055546969,0.7149336572
H,0,-4.1700093873,0.99489145,0.7643931223
H,0,-4.2939924344,-0.8141018778,1.1029573585
H,0,-6.0630377977,-0.998849036,-0.6736454246
H,0,-5.9413043213,0.7598157813,-1.0034664062
H,0,0.5042035824,-2.6234130407,-0.6154583989
H,0,2.8802689578,-2.584140088,0.0776258621
H,0,0.4056639604,1.6353569827,-0.6145430318
H,0,3.0525982973,3.9074387093,0.1776345563
H,0,1.9827183076,3.2278546767,-1.0722753773
H,0,1.4790943822,3.215348712,0.6403011834
H,0,6.0357635445,-1.1969047404,1.0081189569
H,0,4.5918633456,-2.1091456231,1.509515024
H,0,5.0898925746,-2.0936604184,-0.2040709287

TS-OEt 3,4-dichlorophenyl carbonate

E (total electronic) = -1568.4984743
E (total electronic) + ZPVE = -1568.351721
Internal Thermal Energy = -1568.337469
Enthalpy = -1568.336525
Gibbs Free Energy = -1568.396655

C,0,-0.0801562247,-3.7595072685,-0.8527873512
C,0,-0.1529500048,-4.6194787534,-2.0253421147
O,0,-0.1063949395,-5.6471753995,-1.0880614297
O,0,-0.1027414045,-1.9457915264,-1.3975069336

C,0,0.0020796137,-1.143136691,-0.4293319429
O,0,0.1068465937,-1.3670248202,0.7639327319
O,0,0.0025909114,0.179766425,-0.8917272673
C,0,0.0394496321,1.1873338008,0.0392294628
C,0,-0.9919325359,1.371773105,0.9512591508
C,0,-0.9466390019,2.4468741396,1.8201553967
C,0,0.1172305968,3.3395916854,1.7804678767
C,0,1.1405349511,3.1488946671,0.8620648545
C,0,1.1050190778,2.069135399,-0.0088889719
Cl,0,0.1360401436,4.6804183996,2.8846925018
Cl,0,2.4867767929,4.2420288689,0.776691368
H,0,-0.9683644038,-3.6681942144,-0.2490678345
H,0,0.872395157,-3.6784856277,-0.3552024705
H,0,0.7067008275,-4.5566695293,-2.7037116901
H,0,-1.083080067,-4.5448283245,-2.6019263157
H,0,-1.8186820377,0.6753943646,0.9784233834
H,0,-1.7407073989,2.6059685539,2.5371173735
H,0,1.901165721,1.916599746,-0.7246987781

TS-OEt 3,4-difluorophenyl carbonate

E (total electronic) = -847.7776401
E (total electronic) + ZPVE = -847.628102
Internal Thermal Energy = -847.614519
Enthalpy = -847.613575
Gibbs Free Energy = -847.672117

C,0,0.4282586239,-3.1900836089,-1.4570734338
C,0,0.5435186767,-3.8070486605,-2.7704201627
O,0,0.4736658564,-4.9952868288,-2.0490220795
O,0,0.4499812246,-1.3035261151,-1.6432352467
C,0,0.3084069593,-0.6999690192,-0.5433884334
O,0,0.1810559989,-1.1502646025,0.5823909266
O,0,0.3200382851,0.6849286697,-0.7431021369
C,0,0.1296163812,1.4982151551,0.3489503741
C,0,1.1348999266,2.3894555938,0.6870090948
C,0,0.9450219304,3.2838138728,1.7345975258
C,0,-0.2446202362,3.26430369375,2.4277265294
C,0,-1.2431142412,2.3681262596,2.0824758984
C,0,-1.0743056139,1.4804790644,1.0439175922
F,0,-0.4620255892,4.1103337527,3.4460316888
F,0,-2.387363799,2.3823413122,2.7793186971
H,0,-0.5395962078,-3.2078511081,-0.9834700398
H,0,1.2971093889,-3.213591598,-0.8198156637
H,0,1.4911388389,-3.6233478743,-3.2913072956
H,0,-0.2945266435,-3.6153662588,-3.451563857
H,0,2.0595354245,2.383224059,0.126205551
H,0,1.7110846802,3.9927606337,2.0190996259
H,0,-1.8640718647,0.7879333638,0.7869598451

TS-OEt 3,4-dimethylphenyl carbonate

E (total electronic) = -727.912669
E (total electronic) + ZPVE = -727.691445
Internal Thermal Energy = -727.676311
Enthalpy = -727.675367
Gibbs Free Energy = -727.736302

C,0,-0.2797698274,-3.8018325053,-1.2705908336
C,0,-0.5611785149,-4.6844586834,-2.3921919181
O,0,-0.0536879566,-5.6606677318,-1.5381576959
O,0,-0.7716146602,-2.0215324146,-1.7308632302
C,0,-0.5498934388,-1.193071868,-0.8008074932
O,0,-0.0834462656,-1.3877203035,0.3115820593
O,0,-0.9138846452,0.0924931391,-1.1872487952
C,0,-0.7444823987,1.104377537,-0.2574001134
C,0,-1.7348345842,1.346684137,0.6826179663
C,0,-1.6144550986,2.3986554994,1.5836871591
C,0,-0.47705534,3.2215193628,1.533366289
C,0,0.5014340225,2.9604085516,0.5797996367
C,0,0.379142922,1.9061086206,-0.3190682208
C,0,-0.3251326452,4.3687406649,2.4953272279

C,0,-2.6925737923,2.6545104427,2.6013818723
H,0,-0.9462558546,-3.8430078986,-0.4249877399
H,0,0.7498111801,-3.5434614132,-1.0858167481
H,0,0.0267329954,-4.494372231,-3.2981570301
H,0,-1.6211078574,-4.7875158488,-2.6537536576
H,0,-2.6054979637,0.7008972621,0.7057447984
H,0,1.37964245,3.5947002052,0.5363955135
H,0,1.1421172435,1.7058103395,-1.0607583527
H,0,-1.1436521954,5.0849053087,2.3894972449
H,0,0.6124377424,4.8964686487,2.3258116321
H,0,-0.339017812,4.0211012303,3.5310893369
H,0,-3.10841444,3.6585726426,2.4890589847
H,0,-3.5036398679,1.9348416559,2.5011222597
H,0,-2.2968883971,2.5862876501,3.6175315083

TS-OEt 3,4-di(trifluoromethyl)phenyl

carbonate

E (total electronic) = -1323.4128667
E (total electronic) + ZPVE = -1323.237083
Internal Thermal Energy = -1323.218311
Enthalpy = -1323.217367
Gibbs Free Energy = -1323.287947

C,0,-0.7693566005,-3.7441953161,-1.373976227
C,0,-0.8729995617,-4.4919603573,-2.6195412689
O,0,-0.9592365763,-5.5986038752,-1.7809331665
O,0,-0.5994321555,-1.9017839703,-1.7553798109
C,0,-0.4822873701,-1.1979463625,-0.7163627725
O,0,-0.4782073555,-1.5228220116,0.4564196942
O,0,-0.3155605246,0.1541482389,-1.0667412975
C,0,-0.2738448017,1.0941811601,-0.0780070034
C,0,0.7699704122,2.0089582995,-0.1229860555
C,0,0.8372961995,3.0409427827,0.7982165749
C,0,-0.1535245578,3.1631578686,1.7785048146
C,0,-1.1880487678,2.2371104937,1.8114124142
C,0,-1.2585288875,1.2048205336,0.8905433433
C,0,-0.1467981596,4.2423330241,2.8285003326
F,0,0.7162728099,3.983213975,3.8224936898
F,0,0.1771050624,5.4428782458,2.3321337525
F,0,-1.3494886706,4.3770762015,3.4003896247
C,0,1.990186012,4.0057453491,0.6690247264
F,0,2.5295154203,4.3189686544,1.8524403662
F,0,2.9752909006,3.4957448528,-0.0786932096
F,0,1.6253070868,5.1544053698,0.0827099711
H,0,-1.66941967,-3.6226310938,-0.7934113245
H,0,0.1645892248,-3.801180837,-0.8387855613
H,0,0.0155478152,-4.4510769253,-3.2616134879
H,0,-1.7678760666,-4.2784040966,-3.2171162843
H,0,1.5264784113,1.8995735294,-0.8871660063
H,0,-1.9584522971,2.3276724869,2.5641042865
H,0,-2.0705333325,0.49284778,0.9230648851

TS-OEt 2,4,6-trinitrophenyl carbonate

E (total electronic) = -1262.7740879
E (total electronic) + ZPVE = -1262.600399
Internal Thermal Energy = -1262.580873
Enthalpy = -1262.579929
Gibbs Free Energy = -1262.652819

C,0,0.1110690371,-3.5307481306,-1.8388055378
C,0,0.0561489075,-4.0751156516,-3.1923578616
O,0,0.1103782269,-5.3214641705,-2.5833882939
O,0,0.065189323,-1.6705696796,-1.8997703441
C,0,0.1278852173,-1.1507279748,-0.7640900044
O,0,0.2322740548,-1.6235365882,0.3464637553
O,0,0.0747277479,0.2778002865,-0.8888746874
C,0,0.0543762449,1.0041933508,0.2294984998
C,0,0.9870169718,2.0315859343,0.3969429218
C,0,0.9767004934,2.8934743961,1.472055162
C,0,0.0330579794,2.6789884333,2.4559347249

C,0,-0.8980187053,1.6627710421,2.3739518501
C,0,-0.8898483561,0.8597836313,1.2538259844
N,0,0.0180737609,3.5613152027,3.6285209571
O,0,0.8325856052,4.4584825958,3.663788401
O,0,-0.8074978274,3.3372667498,4.4873684439
N,0,2.0547851187,2.2130434016,-0.5967957784
N,0,-1.9525524358,-0.1488282631,1.1561844623
O,0,-2.3150181281,-0.6672136535,2.188172007
O,0,-2.4163266078,-0.3721864116,0.0595728058
O,0,2.3348060753,3.3547592789,-0.8947817523
O,0,2.6018509197,1.2220831436,-1.0222890467
H,0,-0.7797809733,-3.6273334637,-1.2378063226
H,0,1.0590638461,-3.5899982579,-1.3274523815
H,0,0.9169973655,-3.8165594865,-3.822684313
H,0,-0.8708813594,-3.8520626483,-3.7364431039
H,0,1.7001915131,3.6928384558,1.5499130849

TS-OEt 2,4,6-tricyanophenyl carbonate

E (total electronic) = -926.0237542
E (total electronic) + ZPVE = -925.862371
Internal Thermal Energy = -925.844965
Enthalpy = -925.844021
Gibbs Free Energy = -925.910902

C,0,0.1888475015,-3.5574289478,-1.98354526
C,0,0.0578983895,-4.0923728462,-3.3346073285
O,0,0.1598495526,-5.3392723467,-2.7314223893
O,0,0.1376763906,-1.6905384856,-2.0356891598
C,0,0.2417339322,-1.1730719578,-0.8996996996
O,0,0.3453270897,-1.6542059535,0.207160286
O,0,0.2487414881,0.2565619668,-1.0211259301
C,0,0.2499239684,0.9760604511,0.1159530481
C,0,1.3385778991,1.8060376475,0.3922433127
C,0,1.3468209373,2.6165909242,1.5209278737
C,0,0.2596610265,2.5922473355,2.3872365575
C,0,-0.8350026749,1.7717285843,2.1284303219
C,0,-0.8381511485,0.970815286,0.9951639451
C,0,0.2632051666,3.4248894636,3.5577805671
C,0,-1.9745170638,0.1483707656,0.6938483551
C,0,2.4556768988,1.8063344408,-0.5091279473
N,0,3.3543267653,1.8114789846,-1.2214861714
N,0,-2.8897390784,-0.4948279131,0.4410154429
N,0,0.2662229016,4.0896915891,4.4925267209
H,0,-0.6644737781,-3.6580205463,-1.3313181035
H,0,1.1659544875,-3.609151897,-1.5296781701
H,0,0.8773742324,-3.8251735534,-4.0142094425
H,0,-0.902237876,-3.8772540971,-3.8210635188
H,0,2.1956199065,3.2559327126,1.7213868886
H,0,-1.682939915,1.7608623927,2.7995938012

TS-OEt 2,4,6-trimethoxyphenyl carbonate

E (total electronic) = -992.844809
E (total electronic) + ZPVE = -992.579895
Internal Thermal Energy = -992.560319
Enthalpy = -992.559375
Gibbs Free Energy = -992.630910

C,0,0.4017048534,-4.4162606512,-0.6752321738
C,0,0.4357220017,-5.3371927839,-1.8007310892
O,0,0.6082514135,-6.2915021715,-0.8009716888
O,0,0.1559891345,-2.6413848891,-1.3209078445
C,0,0.1252943667,-1.7816373127,-0.3935401965
O,0,0.2291299001,-1.9417899923,0.8127493286
O,0,-0.0557695584,-0.5018940413,-0.9131983948
C,0,-0.1006860963,0.5312929157,-0.0066681454
C,0,1.0610441593,1.2120978601,0.3308553854
C,0,1.0191548316,2.3051981593,1.20223894
C,0,-0.2085641083,2.6877169016,1.7298772184
C,0,-1.3824640056,2.0070317005,1.411126415
C,0,-1.3219838566,0.9248568095,0.5428348259

O,0,-2.3930961166,0.1863952573,0.1715226097
C,0,-3.6540414955,0.5504355171,0.7114888263
O,0,-0.3614390217,3.7348633183,2.5835744205
C,0,0.7984872859,4.4645554668,2.9471633729
O,0,2.1997704336,0.7419709145,-0.2312643306
C,0,3.4132443388,1.4076440707,0.0822196397
H,0,-0.492670865,-4.3955294363,-0.0748560661
H,0,1.336158792,-4.1853644018,-0.1910103771
H,0,1.2822426049,-5.2100562174,-2.4860964144
H,0,-0.4961862235,-5.4134122206,-2.3736147555
H,0,1.9225929131,2.8337576636,1.4571951883
H,0,-2.3096728767,-2.3410790735,1.8519671717
H,0,-4.3710339092,-0.1534844809,0.2990370823
H,0,-3.6485311559,0.4725743654,1.8004721761
H,0,-3.926026236,1.5658978017,0.4167191552
H,0,0.4626524126,5.244761507,3.6243339326
H,0,1.520134776,3.8237878934,3.4583511406
H,0,1.2661593916,4.9186064054,2.0708650892
H,0,3.6204356516,1.3594421286,1.153087112
H,0,4.1916720309,0.8811076721,-0.4623834848
H,0,3.3824842334,2.4500141969,-0.2412270688

TS-OEt 2,4,6-trifluorophenyl carbonate

E (total electronic) = -947.0196505
E (total electronic) + ZPVE = -946.878101
Internal Thermal Energy = -946.863765
Enthalpy = -946.862821
Gibbs Free Energy = -946.922133

C,0,0.7347514338,-3.3398887189,-0.5052507716
C,0,0.6804803045,-4.3818079059,-1.5214055501
O,0,1.2346643678,-5.1823298229,-0.5276815406
O,0,0.0600111676,-1.7274081477,-1.2191385597
C,0,0.0865577889,-0.7792352291,-0.3907851359
O,0,0.4505231651,-0.7517255462,0.7699454904
O,0,-0.3939089071,0.4042355059,-0.9893354266
C,0,-0.4609998888,1.5022372578,-0.1847849186
C,0,0.4262690758,2.5553531973,-0.3395377025
C,0,0.3516955372,3.7136292216,0.4105173654
C,0,-0.6546818704,3.7885223518,1.3520427318
C,0,-1.5691150818,2.7745579465,1.5648415997
C,0,-1.4471679507,1.6458899299,0.7805625026
F,0,-0.751006498,4.9001486404,2.0970652835
F,0,-2.3088800951,0.638293699,0.9423657701
F,0,1.3898064807,2.4344670397,-1.2574963455
H,0,0.0099496167,-3.3865564905,0.2914446387
H,0,1.7022444696,-2.9242386432,-0.2745527042
H,0,1.3147332129,-4.2079009604,-2.3994352539
H,0,-0.3291857134,-4.6607329666,-1.8473595547
H,0,1.0551064799,4.5209815583,0.2644167605
H,0,-2.3481110952,2.8584670833,2.3092303213

TS-OEt 2,4,6-trimethylphenyl carbonate

E (total electronic) = -767.2227402
E (total electronic) + ZPVE = -766.974288
Internal Thermal Energy = -766.957054
Enthalpy = -766.956110
Gibbs Free Energy = -767.023275

C,0,-3.9164809879,-0.0020886791,0.4846468518
C,0,-5.1457556992,0.0317531298,-0.2923351202
O,0,-5.7449271548,0.0447785454,0.9649215992
O,0,-2.4268581179,-0.0397897934,-0.7014067669
C,0,-1.3134950732,-0.0263073134,-0.1003184486
O,0,-1.0850957312,0.0002367366,1.1005363662
O,0,-0.2598012954,-0.0461612641,-1.0057270639
C,0,1.023274601,-0.0212062602,-0.4821552927
C,0,1.6700900461,-1.2272660025,-0.2390422874
C,0,2.9834265463,-1.1808571089,0.2216739132
C,0,3.6403503523,0.0276437546,0.4383846936

C,0,2.9485797448,1.2115116168,0.1932042463
C,0,1.6352902247,1.2088949924,-0.2682816035
C,0,0.8752033486,2.4805578302,-0.5207523865
C,0,5.0731126443,0.0551274124,0.9032836762
C,0,0.9475701112,-2.5264280622,-0.4603073538
H,0,-3.6024947987,0.9110779235,0.9625316291
H,0,-3.6517952174,-0.9328783693,0.9584852345
H,0,-5.341039152,-0.8587507108,-0.9017310277
H,0,-5.2936788377,0.9341551826,-0.897555103
H,0,3.5031355342,-2.1130875501,0.4189957574
H,0,3.4412279681,2.1627526208,0.3681722277
H,0,0.5478093831,2.5410748276,-1.5602890884
H,0,1.4929861066,3.3496362895,-0.2991858597
H,0,-0.0210465846,2.5241787594,0.1023339067
H,0,5.270771705,0.935200461,1.5156656465
H,0,5.7563800767,0.0865336588,0.0511460533
H,0,5.3142740688,-0.8335831331,1.4866593138
H,0,0.0523118459,-2.5816878815,0.1631879132
H,0,1.5904718482,-3.371290044,-0.2175631269
H,0,0.6229165941,-2.6218619388,-1.4980252094

TS-OEt 2,4,6-tri(trifluoromethyl)phenyl carbonate

E (total electronic) = -1660.47369
E (total electronic) + ZPVE = -1660.293340
Internal Thermal Energy = -1660.270798
Enthalpy = -1660.269853
Gibbs Free Energy = -1660.349656

C,0,-4.7089207155,0.0126622692,-0.9063419183
C,0,-6.0091721003,0.0049322708,-0.2475132968
O,0,-6.5205976683,0.0202710587,-1.5401428377
O,0,-3.342522212,-0.0031401032,0.3849308958
C,0,-2.1973679067,0.0011928486,-0.1311821446
O,0,-1.8370945724,0.0147981764,-1.2891902561
O,0,-1.2053785571,-0.0131536273,0.8919099404
C,0,0.087341572,-0.0108735671,0.4676582645
C,0,0.7632086111,1.1944999653,0.2918712673
C,0,2.0861313277,1.1986649007,-0.1099734843
C,0,2.7378500786,-0.006046358,-0.3328331747
C,0,2.0857594223,-1.2108145545,-0.1376580133
C,0,0.7592408991,-1.210561605,0.264469996
C,0,0.0402080615,-2.5045303597,0.5292117857
C,0,4.1782384777,0.0263183751,-0.7496176189
C,0,0.047620013,2.4836352698,0.5877194025
F,0,4.3777834128,0.8706409328,-1.770419403
F,0,4.9734449313,0.4418299973,0.2480581852
F,0,4.6212483547,-1.1740890099,-1.1304560537
F,0,0.8028778004,-3.5598593979,0.2278993919
F,0,-1.0865863569,-2.6190830951,-0.1820430499
F,0,-0.300805853,-2.6226149453,1.8191402856
F,0,-0.2946025127,2.5700178665,1.8796889389
F,0,-1.077614326,2.6190119768,-0.1220754893
F,0,0.814089474,3.5436226014,0.3138776063
H,0,-4.3901562583,-0.9031321322,-1.3780668271
H,0,-4.3899666017,0.9393752075,-1.3561210931
H,0,-6.2247296176,0.8936150258,0.3589513825
H,0,-6.2248220589,-0.8978361365,0.337739701
H,0,2.6062032057,2.1377447627,-0.249222393
H,0,2.6030324858,-2.1467036535,-0.2971309899

TS-OEt pentacyanophenyl carbonate

E (total electronic) = -1110.4803515
E (total electronic) + ZPVE = -1110.322596
Internal Thermal Energy = -1110.301319
Enthalpy = -1110.300375
Gibbs Free Energy = -1110.376339

C,0,-0.1529606051,-3.8981215426,-1.0987807651
C,0,-0.1892008151,-4.773774939,-2.2681660233

O,0,-0.2510338609,-5.8276767862,-1.3685024982
O,0,-0.0667530353,-2.1264688038,-1.6335114307
C,0,0.0125391363,-1.338885121,-0.6684037861
O,0,0.0620491299,-1.4952679866,0.5276758424
O,0,0.0682711023,0.0243057601,-1.1719526503
C,0,0.0540924813,1.0152780084,-0.2807355563
C,0,1.1166680297,1.9237426474,-0.2755154681
C,0,1.1194150117,3.0102127018,0.6003048133
C,0,0.0610946902,3.1971047374,1.4904280959
C,0,-1.0065076692,2.2961715129,1.4830167365
C,0,-1.0163948403,1.2163929634,0.5999967086
C,0,0.064376315,4.3071798402,2.396174419
C,0,-2.147172145,0.3373809414,0.5530386892
C,0,-2.1079343639,2.4923549819,2.3818665641
C,0,2.2171299572,3.9342791238,0.5912011946
C,0,2.2066952146,1.7181646516,-1.1831657671
N,0,0.0671887707,5.1953406356,3.1204354043
N,0,-2.9873316651,2.6503307868,3.0990703979
N,0,-3.0707056722,-0.3391733253,0.5014191955
N,0,3.0874399646,1.566802405,-1.9003910462
N,0,3.0935607503,4.6722131387,0.5850441326
H,0,-1.0727564502,-3.7898298821,-0.5446969915
H,0,0.7652285046,-3.8825992667,-0.5321480176
H,0,0.7141214805,-4.7334407394,-2.8912327835
H,0,-1.0730374165,-4.6411420526,-2.90620141

TS-OEt pentamethoxyphenyl carbonate

E (total electronic) = -1221.8514452
E (total electronic) + ZPVE = -1221.522509
Internal Thermal Energy = -1221.496769
Enthalpy = -1221.495825
Gibbs Free Energy = -1221.581105

C,0,4.8341369522,-0.1795035933,0.681095885
C,0,6.1194863973,0.0011630802,0.0229003806
O,0,6.6270941394,-0.4476838915,1.2391137419
O,0,3.4396018734,0.2926666941,-0.5174108021
C,0,2.2917991274,0.1790224587,-0.0027759312
O,0,1.9724249689,-0.1718872283,1.1206658257
O,0,1.3033377742,0.5493580736,-0.9210289842
C,0,0.0046107861,0.3206038049,-0.552147005
C,0,-0.8387690426,1.402880295,-0.3422228716
C,0,-2.1852222667,1.1915221658,-0.0374413514
C,0,-2.6774544756,-0.1081932819,0.0564964582
C,0,-1.8253314539,-1.1957364966,-0.1626201818
C,0,-0.4786419063,-0.9838367654,-0.4545968019
O,0,0.3851277158,-2.0057884976,-0.7111883102
C,0,0.5728427042,-2.9390188807,0.3586231309
O,0,-4.0065656976,-0.3128983817,0.2929045544
C,0,-4.290270842,-0.798619028,1.6062982033
O,0,-0.3521373308,2.6785327384,-0.4015178605
C,0,-0.369483139,3.214151002,-1.7264018538
O,0,-3.0255771685,2.2581558264,0.1113261902
O,0,-2.3397459275,-2.4602633606,-0.0772515979
C,0,-2.9129305111,2.8978515122,1.3836908036
C,0,-2.4587658067,-3.113768539,-1.343738327
H,0,4.4787041659,-1.1888734897,0.8088672776
H,0,4.5471434436,0.5495217778,1.4210018391
H,0,6.367863876,1.0360350652,-0.2420615161
H,0,6.3008809979,-0.6538798759,-0.8378037433
H,0,1.4785511367,-3.4917593228,0.1197330907
H,0,0.7092529763,-2.40075611,1.2964589082
H,0,-0.2729266151,-3.6220659321,0.4306084063
H,0,-5.3688183577,-0.9243609008,1.6631231701
H,0,-3.7954939214,-1.7551497781,1.7762401517
H,0,-3.9652114521,-0.0737043001,2.3556277375
H,0,-1.3917331842,3.2370359835,-2.1095006246
H,0,0.0229796614,4.2259890789,-1.6599180444
H,0,0.2618576853,2.6139238992,-2.3843047232
H,0,-3.6025371309,3.7385019777,1.3712682683
H,0,-3.1916409178,2.2058317244,2.1812563492
H,0,-1.894507459,3.2550187978,1.541647994
H,0,-2.8962155265,-4.0894861214,-1.1469532506

H,0,-3.115145375,-2.539565561,-2.0006279244
H,0,-1.4788512341,-3.2323210191,-1.8088408213

TS-OEt pentachlorophenyl carbonate

E (total electronic) = -2947.2881003
E (total electronic) + ZPVE = -2947.170293
Internal Thermal Energy = -2947.152246
Enthalpy = -2947.151302
Gibbs Free Energy = -2947.222271

C,0,0.1472973207,-2.8214227987,-2.3695184836
C,0,-0.0941452065,-3.2224887553,-3.7496865072
O,0,0.3293020949,-4.4758621906,-3.3219971284
O,0,-0.2622679728,-0.996940447,-2.1597077795
C,0,-0.0732927489,-0.5906906488,-0.9854046224
O,0,0.320138161,-1.169761011,0.0082445402
O,0,-0.3969390452,0.7854056935,-0.8864557442
C,0,-0.2345261626,1.3452820644,0.3374107342
C,0,0.973859787,1.9405444484,0.6784875482
C,0,1.1241728112,2.5768632201,1.9059292039
C,0,0.0581375529,2.6095558923,2.8028972749
C,0,-1.1509373628,2.0011303635,2.4712238474
C,0,-1.2899570594,1.3676687459,1.2409764495
Cl,0,-2.7578504023,0.582833461,0.7979508067
Cl,0,-2.4706295502,2.0305344794,3.5777748646
Cl,0,0.2358142845,3.4006503115,4.3236852661
Cl,0,2.6242192851,3.319820233,2.3118633742
Cl,0,2.2710372347,1.855429334,-0.451572075
H,0,-0.5622324882,-3.1528141401,-1.6283362877
H,0,1.1744433345,-2.7133361524,-2.0598539898
H,0,0.5477928928,-2.7323714075,-4.4924197329
H,0,-1.1408467603,-3.1596976955,-4.0728355592

TS-OEt pentafluorophenyl carbonate

E (total electronic) = -1145.4760043
E (total electronic) + ZPVE = -1145.350189
Internal Thermal Energy = -1145.333917
Enthalpy = -1145.332973
Gibbs Free Energy = -1145.396738

C,0,0.3471942794,-3.4450695795,-0.5395813781
C,0,0.4507845629,-4.4042953284,-1.6316874087
O,0,0.4942085649,-5.3552527655,-0.6183201124
O,0,0.242389373,-1.7027153822,-1.2399157043
C,0,0.1493260553,-0.8241535432,-0.3458001133
O,0,0.0999573684,-0.9159757902,0.864359736
O,0,0.1073456397,0.4653038488,-0.9373788875
C,0,-0.0400038256,1.5103979472,-0.0840543334
C,0,1.0083073351,2.3921046626,0.1262292679
C,0,0.8585057577,3.5002415803,0.940926376
C,0,-0.3500896467,3.7343067765,1.5681206797
C,0,-1.4060200925,2.8615803445,1.3738896679
C,0,-1.2467916177,1.7624834729,0.5526745397
F,0,-0.4997388735,4.7950308117,2.3528340451
F,0,-2.271599859,0.9370685291,0.3675540079
F,0,2.1814084097,2.1784982876,-0.4615564152
F,0,-2.5695706614,3.0872364551,1.9752538761
F,0,1.8743950324,4.3370377862,1.1256718053
H,0,-0.5964942896,-3.3873781574,-0.0210250169
H,0,1.2405321014,-3.2515654546,0.0323547244
H,0,1.3600663636,-4.3163540119,-2.2394686822
H,0,-0.4258399772,-4.4516954896,-2.2898776739

TS-OEt pentamethylphenyl carbonate

E (total electronic) = -845.8310596
E (total electronic) + ZPVE = -845.526138
Internal Thermal Energy = -845.506057
Enthalpy = -845.505113

Gibbs Free Energy = -845.577375

C,0,4.3368114055,-0.0151155508,0.5137049242
C,0,5.5832374213,0.0219877317,-0.2348532706
O,0,6.1506618198,0.0424256637,1.0371876814
O,0,2.8730662845,-0.0649989519,-0.7073571025
C,0,1.746046322,-0.043940819,-0.1298491994
O,0,1.4960659194,-0.0043578964,1.0667134025
O,0,0.7146266175,-0.0721722537,-1.0549926587
C,0,-0.5837838242,-0.033714258,-0.5618947092
C,0,-1.1832287455,1.2062953309,-0.3617920538
C,0,-2.515886848,1.2377901359,0.0642893492
C,0,-3.2209880432,0.0417027621,0.2533719457
C,0,-2.5787387253,-1.1921347556,0.0863491535
C,0,-1.2451140168,-1.237247041,-0.3372647295
C,0,-0.5293822764,-2.5474575852,-0.5485432034
C,0,-3.3252848044,-2.4742384061,0.3693875625
C,0,-4.6813986062,0.083540649,0.6386519588
C,0,-3.1937065604,2.5617750754,0.3265876126
C,0,-0.401837856,2.4734194481,-0.6000175355
H,0,4.0647175508,-0.9455779725,0.9838541345
H,0,4.0060043833,0.8981060517,0.9798151999
H,0,5.7416662931,0.9230502212,-0.8393173867
H,0,5.7978976806,-0.8697274724,-0.835802555
H,0,-0.3503061533,-3.0548827151,0.4028717241
H,0,-1.1197259338,-3.2226695372,-1.169923059
H,0,0.4316758332,-2.3933362603,-1.032702224
H,0,-3.9770451338,-2.7493145936,-0.4655461588
H,0,-3.9564280944,-2.373668547,1.2524065159
H,0,-2.6455406141,-3.3050331023,0.5428396677
H,0,-4.8109036161,0.10229043,1.7255870564
H,0,-5.2159435956,-0.7864753794,0.2613800476
H,0,-5.1715658539,0.968582772,0.236563798
H,0,-3.8224840756,2.8630392195,-0.5169435782
H,0,-2.4704028337,3.3557238702,0.4971418563
H,0,-3.836375714,2.5060289973,1.205137822
H,0,0.5386829987,2.2638818077,-1.1037074586
H,0,-0.9675812825,3.1750637586,-1.2146833965
H,0,-0.1737794924,2.9771775725,0.3429512067

TS-OEt penta(trifluoromethyl)phenyl carbonate

E (total electronic) = -2334.5366814
E (total electronic) + ZPVE = -2334.346374
Internal Thermal Energy = -2334.317852
Enthalpy = -2334.316908
Gibbs Free Energy = -2334.407147

C,0,-5.4622237374,0.0760304152,0.8948245549
C,0,-6.7627715253,0.1051415854,0.2350689233
O,0,-7.2854259468,0.099944602,1.5223642412
O,0,-4.0988346877,0.0670012022,-0.3882508875
C,0,-2.9581962631,0.042132257,0.1291328916
O,0,-2.5876106616,0.023339749,1.2821475833
O,0,-1.9609151097,0.0365042432,-0.9002701994
C,0,-0.6747468872,0.0102501975,-0.4816585805
C,0,-0.0207636899,-1.2172862544,-0.350472201
C,0,1.339477961,-1.2399530798,-0.0413581773
C,0,2.0107921002,-0.0428625654,0.2348933612
C,0,1.3803406763,1.1819197176,-0.014990577
C,0,0.0202225103,1.2118824659,-0.3240308661
C,0,-0.7509616605,2.5190273967,-0.5058866982
C,0,2.228748637,2.4561004745,-0.1254564544
C,0,3.3399772357,-0.0736209804,0.999979538
C,0,2.1444645559,-2.5393183769,-0.179856344
C,0,-0.835540524,-2.493403676,-0.5604404888
F,0,-0.2145826934,3.509163954,0.2096279597
F,0,-2.0142064078,2.4353958721,-0.0937627602
F,0,-0.778678091,2.8928086019,-1.7862445872
F,0,3.4990324707,2.158238456,-0.4016862932
F,0,1.806118835,3.1924333655,-1.1566089039
F,0,2.2195006312,3.2142532392,0.964387607
F,0,3.4081621683,0.9831041368,1.8171000663

F,0,3.3721793703,-1.1495859433,1.7938723524
F,0,4.4438202805,-0.0842257586,0.2636311603
F,0,3.4241718707,-2.2785280804,-0.4500108099
F,0,2.109257352,-3.3202784099,0.8932245599
F,0,1.6976093637,-3.2383496497,-1.2266391268
F,0,-0.3331139579,-3.5164157421,0.1331348115
F,0,-2.0953849478,-2.3761967849,-0.1460932682
F,0,-0.8754143694,-2.8380708099,-1.8486217768
H,0,-5.1324057617,0.9864742183,1.3699116253
H,0,-5.1634617864,-0.855135733,1.3498701879
H,0,-6.9890010531,-0.7801177696,-0.3729249691
H,0,-6.9588055468,1.0105438341,-0.3534358439

M06-2X/AUG-cc-pVDZ IEFPCM, Solvent = Water

Substrates

ALIPHATIC CARBONATES

OEt trifluoromethyl carbonate

E (total electronic) = -755.2367285
E (total electronic) + ZPVE = -755.144859
Internal Thermal Energy = -755.134406
Enthalpy = -755.133461
Gibbs Free Energy = -755.183671

O,0,-0.008817176,0.2646548041,-0.5525631533
C,0,-0.3950832776,-0.6507855815,0.2930734204
O,0,-0.4136510772,-0.619395638,1.4926195926
O,0,-0.8092177151,-1.7377999948,-0.455991049
C,0,-1.2678251449,-2.8246050596,0.231683875
C,0,0.4680135101,1.5140156993,0.041442777
C,0,0.82880764,2.483960674,-1.082459479
O,0,1.2699275942,3.667008307,-0.5657391505
F,0,-0.3392234014,-3.3523664144,1.0293906322
F,0,-1.6080740714,-3.7362300676,-0.6749695298
F,0,-2.3426642905,-2.544427067,0.9688726799
H,0,1.3414769441,1.2800926877,0.661700149
H,0,-0.3350720357,1.916515757,0.6697807822
H,0,-0.085293531,2.5741226397,-1.7223785007
H,0,1.5777670326,1.9550422539,-1.7248140461

OEt trichloromethyl carbonate (Point group: Cs)

E (total electronic) = -1836.2928562
E (total electronic) + ZPVE = -1836.206693
Internal Thermal Energy = -1836.194963
Enthalpy = -1836.194018
Gibbs Free Energy = -1836.248276

O,0,-1.8120456436,0.4582393989,0.
C,0,-0.7261556986,-0.2684955642,0.
O,0,-0.6126957075,-1.4621367134,0.
O,0,0.3333832212,0.6233093219,0.
C,0,1.6242817089,0.1504067494,0.
C,0,-3.0729720399,-0.2819900714,0.
C,0,-4.2229288393,0.7243486499,0.
O,0,-5.4255200057,0.0801208106,0.
Cl,0,1.9908423612,-0.8115280162,1.4613547422
Cl,0,2.6501818818,1.6052349154,0.
Cl,0,1.9908423612,-0.8115280162,-1.4613547422
H,0,-3.0957854822,-0.9126896408,0.8967413578
H,0,-3.0957854822,-0.9126896408,-0.8967413578
H,0,-4.0561957176,1.3868582233,-0.8869039795
H,0,-4.0561957176,1.3868582233,0.8869039795

OEt tribromomethyl carbonate (Point group: Cs)

E (total electronic) = -8178.2532402

E (total electronic) + ZPVE = -8178.169057

Internal Thermal Energy = -8178.156386

Enthalpy = -8178.155442

Gibbs Free Energy = -8178.212567

O,0,2.5526309692,-0.5505296532,0.
 C,0,1.4925542735,0.2129705321,0.
 O,0,1.4190176948,1.4096537557,0.
 O,0,0.4004330846,-0.64015775,0.
 C,0,-0.8730271363,-0.1301261673,0.
 C,0,3.836024356,0.1517050356,0.
 C,0,4.9607895322,-0.882110512,0.
 O,0,6.175598729,-0.2608484161,0.
 H,0,3.8762820583,0.7815693912,0.8966119642
 H,0,3.8762820583,0.7815693912,-0.8966119642
 H,0,4.7809425012,-1.5407759892,-0.8871310618
 H,0,4.7809425012,-1.5407759892,0.8871310618
 Br,0,-1.2489746041,0.9285181731,-1.6010001137
 Br,0,-2.0319529943,-1.6916804832,0.
 Br,0,-1.2489746041,0.9285181731,1.6010001137

Transition states**TS-OEt trifluoromethyl carbonate**

E (total electronic) = -755.2107572

E (total electronic) + ZPVE = -755.121485

Internal Thermal Energy = -755.110791

Enthalpy = -755.109847

Gibbs Free Energy = -755.161586

O,0,0.0044166757,0.2864763677,-0.7520058507
 C,0,0.0533828038,-0.5966072174,0.1444767789
 O,0,0.0034764529,-0.5288441538,1.3570263063
 O,0,0.1942303897,-1.883214758,-0.4792491495
 C,0,0.2652605848,-2.9667299356,0.3166801025
 C,0,-0.1791428499,2.0091735425,-0.05613908
 C,0,-0.2289150905,2.9785428368,-1.1508669902
 O,0,-0.3526620088,3.9277883599,-0.1396948091
 F,0,1.3208154377,-2.9537290919,1.1432333999
 F,0,0.3925458819,-4.0402858792,-0.4748943917
 F,0,-0.8312105396,-3.1517373948,1.0657321449
 H,0,0.7355274351,1.9695611999,0.5254812999
 H,0,-1.1103882925,1.7997217953,0.4590162472
 H,0,-1.1010913452,2.8767011114,-1.8192998402
 H,0,0.6926274649,3.0417372171,-1.754714168

TS-OEt trichloromethyl carbonate (Point group:

Cs)

E (total electronic) = -1836.2669122

E (total electronic) + ZPVE = -1836.183290

Internal Thermal Energy = -1836.171308

Enthalpy = -1836.170364

Gibbs Free Energy = -1836.225009

O,0,-1.7358834426,0.724059135,0.
 C,0,-0.7546809722,-0.0652046207,0.
 O,0,-0.6794076621,-1.2754876752,0.
 O,0,0.4554496515,0.7251527334,0.
 C,0,1.6684898433,0.1325876268,0.
 C,0,-3.3756281524,-0.1650361798,0.
 C,0,-4.4636802737,0.8135120881,0.
 O,0,-5.3019362184,-0.2980479461,0.
 H,0,-3.1925053928,-0.6970773829,0.9274586239
 H,0,-3.1925053928,-0.6970773829,-0.9274586239

H,0,-4.5131433664,1.448629356,-0.9011699064

H,0,-4.5131433664,1.448629356,0.9011699064

Cl,0,1.9628388628,-0.8732610511,1.4632766965

Cl,0,2.8668639802,1.464919459,0.

Cl,0,1.9628388628,-0.8732610511,-1.4632766965

TS-OEt tribromomethyl carbonate (Point group:

Cs)

E (total electronic) = -8178.2276926

E (total electronic) + ZPVE = -8178.146133

Internal Thermal Energy = -8178.133185

Enthalpy = -8178.132241

Gibbs Free Energy = -8178.190770

O,0,-2.454908893,0.8470158733,0.
 C,0,-1.5000728912,0.0271898385,0.
 O,0,-1.4578746066,-1.183664778,0.
 O,0,-0.2620325146,0.7819021419,0.
 C,0,0.9321949298,0.1646087086,0.
 C,0,-4.1178481752,0.0093044524,0.
 C,0,-5.1774704322,1.0191286767,0.
 O,0,-6.0511236125,-0.0642201915,0.
 H,0,-3.9525755358,-0.5290168886,0.9272939445
 H,0,-3.9525755358,-0.5290168886,-0.9272939445
 H,0,-5.2064760318,1.655937401,-0.9009922891
 H,0,-5.2064760318,1.655937401,0.9009922891
 Br,0,1.2351028485,-0.9407932057,1.6032599489
 Br,0,1.2351028485,-0.9407932057,-1.6032599489
 Br,0,2.2674043698,1.595024857,0.

5. References

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