Group Additivity Rules for Estimation of Thermochemistry of Furan Derivatives

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1 Characterization of Functional Groups

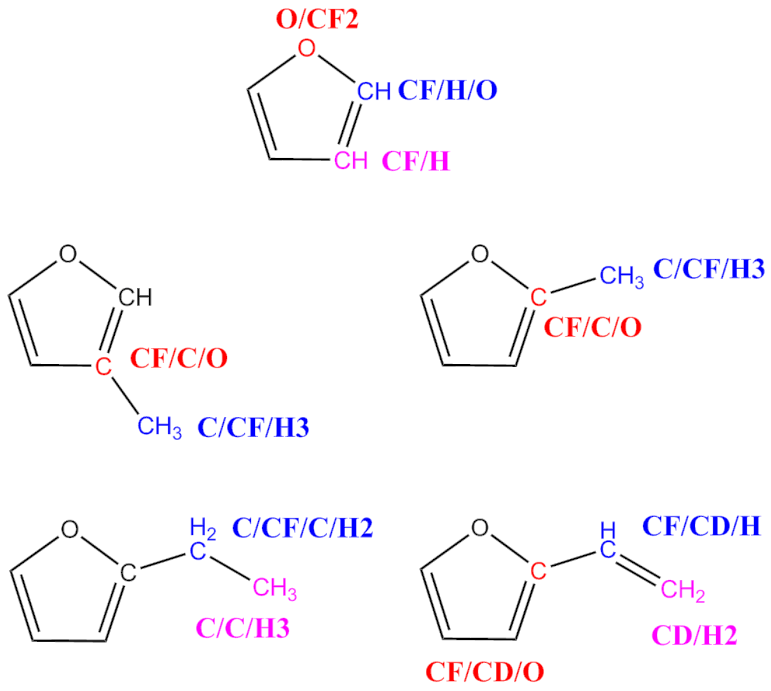

Figure 1: Functional groups assigned to furan and related methyl, ethyl and vinyl derivatives.

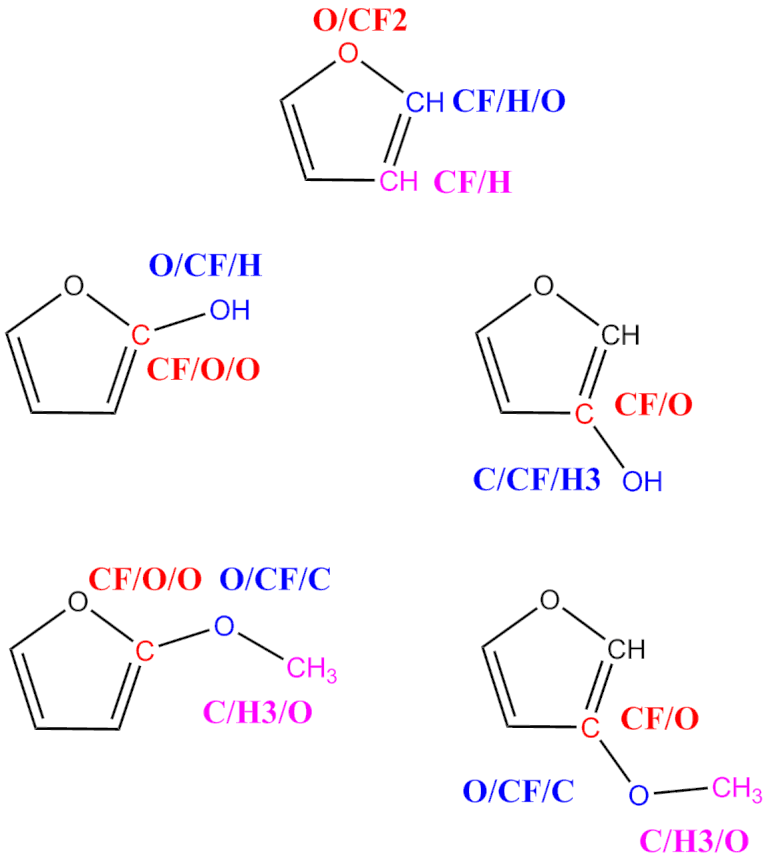

Figure 2: Functional groups assigned to furan and related alkoxy and methoxy derivatives.

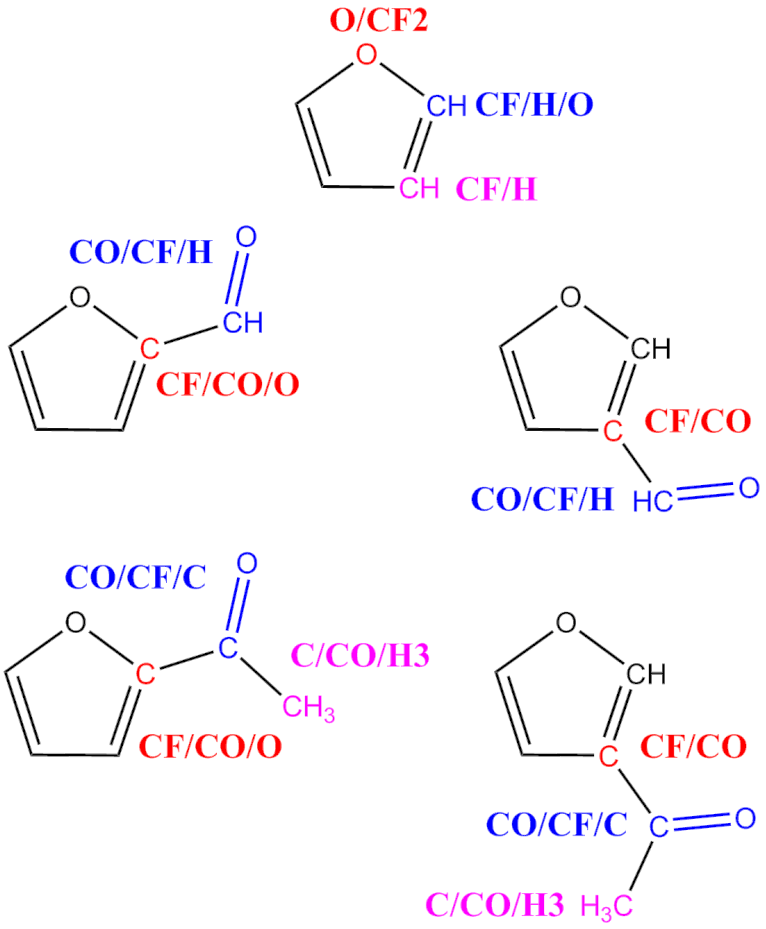

Figure 3: Functional groups assigned to furan and related formyl and acetyl derivatives.

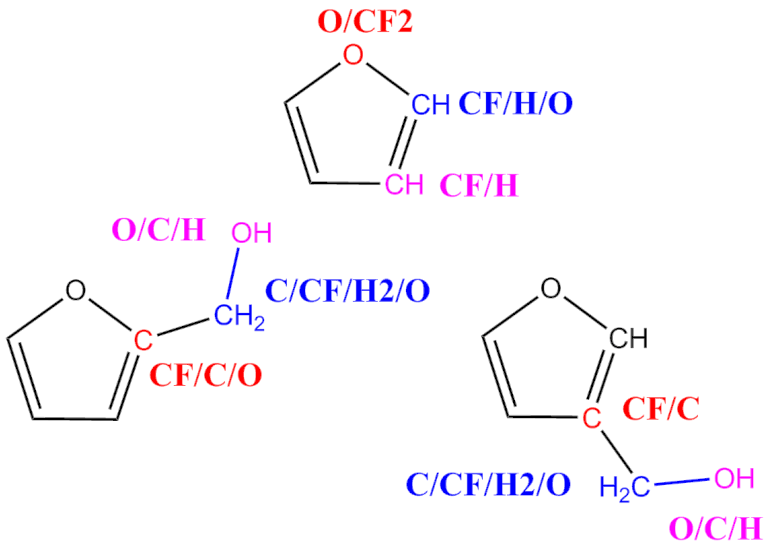

Figure 4: Functional groups assigned to furan and related hydroxymethyl derivatives.

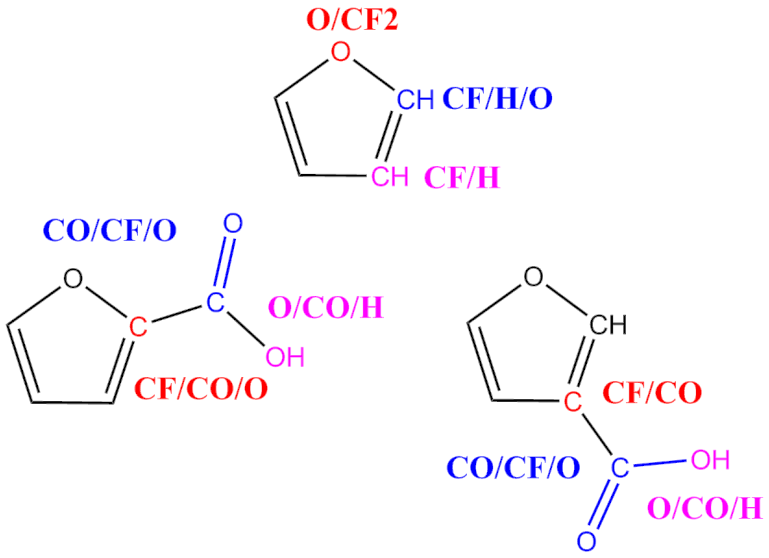

Figure 5: Functional groups assigned to furan and related furoic acid derivatives.

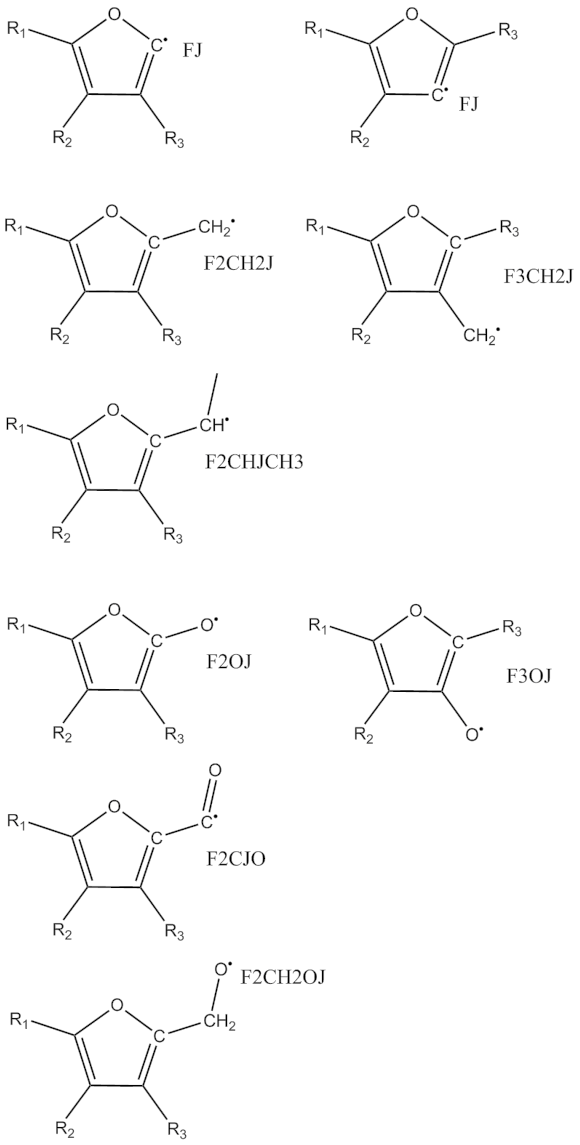

Figure 6: Bond dissociation groups optimized as part of *this work*. R_1, R_2 and R_3 can refer to a range of differing substituents (–H, $–CH_3$, C_2H_5, –OH, –CHO, etc.).

2 Comparison of Theoretical and Final Group Additivity Values

Table 1: Comparison of theoretical thermochemical functions (Detailed) with optimized group additivity values (GA) for stable and radical species. $\Delta_f H^\circ$ (kcal mol^{-1}), S$^\circ$ and C_p (cal mol^{-1} K^{-1}).

Species		$\Delta_f H^\circ$	S$^\circ$	C_p 300	400	500	600	800	1000	1500
Furan	Detailed	-8.32	63.68	15.45	20.87	25.42	29.00	34.11	37.58	42.68
	GA	-8.45	63.82	15.46	20.86	25.37	28.92	33.99	37.48	42.60
	% Difference	1.59	0.22	0.06	-0.05	-0.20	-0.28	-0.35	-0.27	-0.19
Furan-2-yl	Detailed	60.21	66.38	15.14	19.88	23.80	26.87	31.19	34.06	38.19
	GA	59.42	66.50	15.00	19.72	23.63	26.68	30.98	33.89	38.07
	% Difference	-1.31	0.18	-0.92	-0.80	-0.71	-0.71	-0.67	-0.50	-0.31
Furan-3-yl	Detailed	60.30	66.23	14.97	19.71	23.65	26.73	31.08	33.98	38.14
	GA	59.42	66.50	15.00	19.72	23.63	26.68	30.98	33.89	38.07
	% Difference	-1.46	0.41	0.20	0.05	-0.08	-0.19	-0.32	-0.26	-0.18
2-methylfuran	Detailed	-19.19	73.78	21.03	27.44	33.05	37.66	44.55	49.39	56.65
	GA	-19.43	73.62	21.02	27.44	33.06	37.67	44.54	49.40	56.65
	% Difference	1.24	-0.22	-0.05	0.00	0.03	0.03	-0.02	0.02	0.00
2-furanylmethyl	Detailed	14.84	72.39	21.22	27.77	33.07	37.21	43.13	47.18	53.22
	GA	13.57	72.34	21.12	27.70	33.03	37.18	43.10	47.18	53.22
	% Difference	-8.56	-0.07	-0.47	-0.25	-0.12	-0.08	-0.07	0.00	0.00
2-methylfuran-3-yl	Detailed	49.16	75.09	20.43	26.18	31.20	35.33	41.47	45.76	52.10
	GA	48.44	74.92	20.56	26.30	31.32	35.43	41.53	45.81	52.12
	% Difference	-1.46	-0.23	0.64	0.46	0.38	0.28	0.14	0.11	0.04

Table 1: Comparison of theoretical thermochemical functions (Detailed) with optimized group additivity values (GA) for stable and radical species. $\Delta_f H^\circ$ (kcal mol^{-1}), S$^\circ$ and C_p (cal mol^{-1} K^{-1}).

Species		$\Delta_f H^\circ$	S$^\circ$	C_p 300	400	500	600	800	1000	1500
	Detailed	48.97	74.99	20.47	26.24	31.26	35.39	41.52	45.78	52.11
2-methylfuran-4-yl	GA	48.44	74.92	20.56	26.30	31.32	35.43	41.53	45.81	52.12
	% Difference	-1.08	-0.09	0.44	0.23	0.19	0.11	0.02	0.07	0.02
	Detailed	48.97	75.13	20.79	26.48	31.46	35.55	41.62	45.87	52.16
2-methylfuran-5-yl	GA	48.44	74.92	20.56	26.30	31.32	35.43	41.53	45.81	52.12
	% Difference	-1.08	-0.28	-1.11	-0.68	-0.45	-0.34	-0.22	-0.13	-0.08
	Detailed	-16.50	73.80	21.04	27.41	33.00	37.61	44.50	49.35	56.63
3-methylfuran	GA	-16.68	73.88	21.03	27.40	32.99	37.58	44.45	49.32	56.59
	% Difference	1.09	0.11	-0.05	-0.04	-0.03	-0.08	-0.11	-0.06	-0.07
	Detailed	51.94	75.33	20.51	26.23	31.24	35.36	41.49	45.78	52.11
3-methylfuran-2-yl	GA	51.19	75.18	20.57	26.26	31.25	35.34	41.44	45.73	52.06
	% Difference	-1.44	-0.20	0.29	0.11	0.03	-0.06	-0.12	-0.11	-0.10
	Detailed	21.61	72.73	21.51	27.93	33.13	37.22	43.11	47.16	53.21
3-furanylmethyl	GA	20.43	72.81	21.50	27.93	33.13	37.20	43.07	47.13	53.17
	% Difference	-5.46	0.11	-0.05	0.00	0.00	-0.05	-0.09	-0.06	-0.08
	Detailed	51.70	74.99	20.54	26.22	31.20	35.32	41.45	45.73	52.07
3-methylfuran-4-yl	GA	51.19	75.18	20.57	26.26	31.25	35.34	41.44	45.73	52.06

Table 1: Comparison of theoretical thermochemical functions (Detailed) with optimized group additivity values (GA) for stable and radical species. $\Delta_f H^\circ$ (kcal mol^{-1}), S$^\circ$ and C_p (cal mol^{-1} K^{-1}).

Species		$\Delta_f H^\circ$	S$^\circ$	C_p 300	400	500	600	800	1000	1500
	% Difference	-0.99	0.25	0.15	0.15	0.16	0.06	-0.02	0.00	-0.02
	Detailed	51.36	75.07	20.81	26.50	31.45	35.53	41.61	45.85	52.14
3-methylfuran-5-yl	GA	51.19	75.18	20.57	26.26	31.25	35.34	41.44	45.73	52.06
	% Difference	-0.33	0.15	-1.15	-0.91	-0.64	-0.53	-0.41	-0.26	-0.15
	Detailed	-29.78	80.99	26.71	34.06	40.72	46.35	55.00	61.22	70.62
2,5-dimethylfuran	GA	-30.41	80.66	26.58	34.02	40.75	46.42	55.09	61.32	70.70
	% Difference	2.12	-0.41	-0.49	-0.12	0.07	0.15	0.16	0.16	0.11
	Detailed	2.77	81.04	26.82	34.32	40.69	45.86	53.55	59.00	67.19
2-methyl-5-furanylmethylfuran	GA	2.59	80.76	26.68	34.28	40.72	45.93	53.65	59.10	67.27
	% Difference	-6.50	-0.35	-0.52	-0.12	0.07	0.15	0.19	0.17	0.12
	Detailed	37.57	83.79	26.03	32.74	38.83	43.99	51.90	57.57	66.06
2,5-dimethylfuran-3-yl	GA	37.46	83.33	26.12	32.88	39.01	44.18	52.08	57.73	66.17
	% Difference	-0.29	-0.55	0.35	0.43	0.46	0.43	0.35	0.28	0.17
	Detailed	-27.02	82.51	26.19	33.66	40.42	46.12	54.84	61.11	70.56
2,3-dimethylfuran	GA	-27.66	82.29	26.59	33.98	40.68	46.33	55.00	61.24	70.64
	% Difference	2.35	-0.27	1.53	0.95	0.64	0.46	0.29	0.21	0.11
	Detailed	5.31	81.31	26.32	33.96	40.40	45.63	53.42	58.90	67.14
3-methyl-2-furanylmethylfuran										

Table 1: Comparison of theoretical thermochemical functions (Detailed) with optimized group additivity values (GA) for stable and radical species. $\Delta_f H^\circ$ (kcal mol^{-1}), S$^\circ$ and C_p (cal mol^{-1} K^{-1}).

Species		$\Delta_f H^\circ$	S$^\circ$	C_p 300	400	500	600	800	1000	1500
	GA	5.34	81.02	26.69	34.24	40.65	45.84	53.56	59.02	67.21
	% Difference	0.56	-0.36	1.41	0.82	0.62	0.46	0.26	0.20	0.10
	Detailed	9.63	81.65	26.55	34.10	40.49	45.68	53.42	58.90	67.14
2-methyl-3-furanylmethylfuran	GA	9.45	81.23	27.06	34.51	40.82	45.95	53.62	59.05	67.22
	% Difference	-1.87	-0.51	1.92	1.20	0.82	0.59	0.37	0.25	0.12
	Detailed	40.20	83.80	25.58	32.41	38.59	43.80	51.78	57.48	66.00
2,3-dimethylfuran-4-yl	GA	40.21	83.59	26.13	32.84	38.94	44.09	51.99	57.65	66.11
	% Difference	0.02	-0.25	2.15	1.33	0.91	0.66	0.41	0.30	0.17
	Detailed	40.06	83.94	25.99	32.73	38.85	44.01	51.93	57.59	66.07
2,3-dimethylfuran-5-yl	GA	40.21	83.59	26.13	32.84	38.94	44.09	51.99	57.65	66.11
	% Difference	0.37	-0.42	0.54	0.34	0.23	0.18	0.12	0.10	0.06
	Detailed	-27.26	82.40	26.66	34.00	40.65	46.28	54.93	61.18	70.59
2,4-dimethylfuran	GA	-27.66	82.29	26.59	33.98	40.68	46.33	55.00	61.24	70.64
	% Difference	1.48	-0.13	-0.26	-0.06	0.07	0.11	0.13	0.10	0.07
	Detailed	5.81	81.22	26.61	34.16	40.56	45.75	53.48	58.93	67.16
4-methyl-2-furanylmethylfuran	GA	5.34	81.02	26.69	34.24	40.65	45.84	53.56	59.02	67.21
	% Difference	-8.09	-0.25	0.30	0.23	0.22	0.20	0.15	0.15	0.07

Table 1: Comparison of theoretical thermochemical functions (Detailed) with optimized group additivity values (GA) for stable and radical species. $\Delta_f H^\circ$ (kcal mol^{-1}), S$^\circ$ and C_p (cal mol^{-1} K^{-1}).

Species		$\Delta_f H^\circ$	S$^\circ$	C_p 300	400	500	600	800	1000	1500
	Detailed	40.08	83.78	26.05	32.71	38.78	43.91	51.83	57.49	65.99
2,4-dimethylfuran-3-yl	GA	40.21	83.59	26.13	32.84	38.94	44.09	51.99	57.65	66.11
	% Difference	0.32	-0.23	0.31	0.40	0.41	0.41	0.31	0.28	0.18
	Detailed	9.56	81.26	27.21	34.58	40.84	45.94	53.58	59.00	67.18
2-methyl-4-furanylmethylfuran	GA	9.45	81.23	27.06	34.51	40.82	45.95	53.62	59.05	67.22
	% Difference	-1.15	-0.04	-0.55	-0.20	-0.05	0.02	0.07	0.08	0.06
	Detailed	40.27	84.05	26.19	32.83	38.89	44.02	51.93	57.59	66.08
2,4-dimethylfuran-5-yl	GA	40.21	83.59	26.13	32.84	38.94	44.09	51.99	57.65	66.11
	% Difference	-0.15	-0.55	-0.23	0.03	0.13	0.16	0.12	0.10	0.05
	Detailed	-24.87	80.79	26.93	34.15	40.75	46.33	54.96	61.18	70.59
3,4-dimethylfuran	GA	-24.91	81.18	26.60	33.94	40.61	46.24	54.91	61.16	70.58
	% Difference	0.15	0.48	-1.23	-0.61	-0.34	-0.19	-0.09	-0.03	-0.01
	Detailed	42.40	83.70	26.46	33.03	39.03	44.12	51.97	57.62	66.08
3,4-dimethylfuran-2-yl	GA	42.96	83.85	26.14	32.80	38.87	44.00	51.90	57.57	66.05
	% Difference	1.32	0.18	-1.21	-0.70	-0.41	-0.27	-0.13	-0.09	-0.05
	Detailed	12.00	80.96	27.44	34.72	40.91	45.99	53.59	59.00	67.18
3-methyl-4-furanylmethylfuran	GA	12.20	81.49	27.07	34.47	40.75	45.86	53.53	58.97	67.16
	% Difference	1.67	0.65	-1.35	-0.72	-0.39	-0.28	-0.11	-0.05	-0.03

Table 1: Comparison of theoretical thermochemical functions (Detailed) with optimized group additivity values (GA) for stable and radical species. $\Delta_f H^\circ$ (kcal mol^{-1}), S$^\circ$ and C_p (cal mol^{-1} K^{-1}).

Species		$\Delta_f H^\circ$	S$^\circ$	C_p 300	400	500	600	800	1000	1500
2-ethylfuran	Detailed	-24.23	83.85	26.72	34.65	41.55	47.22	55.74	61.80	70.94
	GA	-24.15	83.94	26.74	34.72	41.54	47.19	55.76	61.79	70.93
	% Difference	-0.33	0.11	0.07	0.20	-0.02	-0.06	0.04	-0.02	-0.01
2-ethylfuran-2-yl (Allylic)	Detailed	7.77	81.92	25.89	33.64	40.25	45.59	53.49	59.02	67.27
	GA	7.65	82.13	25.93	33.66	40.25	45.57	53.46	59.00	67.25
	% Difference	-1.54	0.26	0.15	0.06	0.00	-0.04	-0.06	-0.03	-0.03
2-methyl-5-ethylfuran	Detailed	-35.05	92.45	32.35	41.38	49.21	55.91	66.34	73.69	84.97
	GA	-35.13	92.35	32.30	41.30	49.23	55.94	66.31	73.71	84.98
	% Difference	0.23	-0.11	-0.15	-0.19	0.04	0.05	-0.05	0.03	0.01
2-methyl-5-ethylfuran-5-yl (Allylic)	Detailed	-3.44	90.76	31.56	40.26	47.94	54.31	63.99	70.89	81.28
	GA	-3.33	90.54	31.49	40.24	47.94	54.32	64.01	70.92	81.30
	% Difference	-3.20	-0.24	-0.22	-0.05	0.00	0.02	0.03	0.04	0.02
2-vinylfuran	Detailed	5.12	77.95	25.89	33.21	39.33	44.23	51.34	56.18	63.21
	GA	5.18	77.98	25.98	33.29	39.38	44.26	51.33	56.18	63.21
	% Difference	1.17	0.04	0.35	0.24	0.13	0.07	-0.02	0.00	0.00
2-methyl-5-vinylfuran	Detailed	-5.73	86.44	31.65	39.95	47.12	53.03	61.89	68.10	77.26
	GA	-5.80	86.40	31.54	39.87	47.07	53.01	61.88	68.10	77.26

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Species		$\Delta_f H^\circ$	S$^\circ$	C_p 300	400	500	600	800	1000	1500
	% Difference	1.22	-0.05	-0.35	-0.20	-0.11	-0.04	-0.02	0.00	0.00
	Detailed	-50.00	72.40	20.58	25.99	30.43	33.94	38.95	42.36	47.44
2-furanol	GA	-49.29	72.57	20.67	26.05	30.46	33.93	38.90	42.32	47.40
	% Difference	-1.42	0.23	0.43	0.24	0.08	-0.02	-0.13	-0.10	-0.07
	Detailed	-34.94	71.08	18.70	24.03	28.31	31.64	36.32	39.43	43.86
2-Furanyloxy	GA	-34.23	71.25	18.79	24.09	28.34	31.63	36.27	39.39	43.82
	% Difference	-2.04	0.24	0.48	0.25	0.11	-0.03	-0.14	-0.10	-0.09
	Detailed	-44.89	71.68	20.84	26.38	30.82	34.28	39.20	42.54	47.52
3-furanol	GA	-45.11	71.97	20.80	26.34	30.79	34.26	39.18	42.54	47.52
	% Difference	0.50	0.40	-0.20	-0.17	-0.11	-0.06	-0.04	0.00	0.00
	Detailed	-16.82	71.28	18.86	24.20	28.50	31.83	36.49	39.58	43.95
3-furanyloxy	GA	-17.04	71.57	18.82	24.16	28.47	31.81	36.47	39.58	43.95
	% Difference	1.31	0.41	-0.21	-0.17	-0.11	-0.06	-0.05	0.00	0.00
	Detailed	-60.28	81.25	26.28	32.59	38.10	42.63	49.43	54.22	61.44
5-methyl-2-furanol	GA	-60.27	80.99	26.23	32.63	38.15	42.68	49.45	54.24	61.45
	% Difference	-0.01	-0.32	-0.17	0.11	0.14	0.11	0.05	0.04	0.01
	Detailed	-55.59	80.60	26.41	32.97	38.51	43.01	49.70	54.41	61.53
5-methyl-3-furanol										

Table 1: Comparison of theoretical thermochemical functions (Detailed) with optimized group additivity values (GA) for stable and radical species. $\Delta_f H^\circ$ (kcal mol^{-1}), S$^\circ$ and C_p (cal mol^{-1} K^{-1}).

Species		$\Delta_f H^\circ$	S$^\circ$	C_p 300	400	500	600	800	1000	1500
	GA	-56.09	80.39	26.36	32.92	38.48	43.01	49.73	54.46	61.57
	% Difference	0.89	-0.26	-0.19	-0.15	-0.08	0.00	0.06	0.09	0.07
	Detailed	-44.62	81.52	25.57	32.57	38.43	43.13	50.00	54.78	61.88
2-methoxyfuran	GA	-44.74	81.62	25.48	32.47	38.38	43.11	50.01	54.82	61.91
	% Difference	0.26	0.13	-0.35	-0.30	-0.14	-0.04	0.01	0.08	0.05
	Detailed	-41.09	81.12	25.55	32.67	38.64	43.40	50.32	55.07	62.06
3-methoxyfuran	GA	-40.56	81.02	25.61	32.76	38.71	43.44	50.29	55.04	62.03
	% Difference	-1.28	-0.13	0.24	0.28	0.19	0.09	-0.05	-0.05	-0.05
	Detailed	-37.57	75.83	22.27	28.55	33.87	38.14	44.35	48.53	54.35
2-formylfuran	GA	-37.11	76.30	22.18	28.48	33.79	38.07	44.24	48.43	54.22
	% Difference	-1.23	0.61	-0.39	-0.24	-0.23	-0.19	-0.25	-0.22	-0.23
	Detailed	1.32	76.76	21.65	27.28	31.95	35.64	40.90	44.39	49.31
2-formylfuran-2-yl	GA	1.78	77.23	21.56	27.21	31.87	35.57	40.79	44.29	49.18
	% Difference	34.85	0.61	-0.42	-0.26	-0.25	-0.20	-0.27	-0.23	-0.26
	Detailed	-36.78	76.13	22.36	28.61	33.90	38.17	44.37	48.53	54.24
3-formylfuran	GA	-37.29	76.35	22.38	28.65	33.95	38.21	44.35	48.49	54.17
	% Difference	1.38	0.29	0.08	0.13	0.14	0.11	-0.04	-0.07	-0.14

Table 1: Comparison of theoretical thermochemical functions (Detailed) with optimized group additivity values (GA) for stable and radical species. $\Delta_f H^\circ$ (kcal mol^{-1}), S$^\circ$ and C_p (cal mol^{-1} K^{-1}).

Species		$\Delta_f H^\circ$	S$^\circ$	C_p 300	400	500	600	800	1000	1500
	Detailed	-48.80	84.67	27.80	35.10	41.52	46.84	54.83	60.39	68.35
5-methyl-2-formylfuran	GA	-48.09	84.72	27.74	35.06	41.48	46.82	54.79	60.35	68.27
	% Difference	-1.46	0.06	-0.21	-0.12	-0.10	-0.04	-0.06	-0.06	-0.11
	Detailed	-47.97	84.93	28.12	35.36	41.75	47.04	54.92	60.31	67.95
5-methyl-3-formylfuran	GA	-48.27	84.77	27.94	35.23	41.64	46.96	54.90	60.41	68.22
	% Difference	0.63	-0.18	-0.63	-0.38	-0.26	-0.17	-0.04	0.16	0.39
	Detailed	-56.96	93.70	32.83	41.30	48.90	55.33	65.17	72.15	82.29
4,5-dimethyl-2-formylfuran	GA	-56.32	93.39	33.31	41.60	49.10	55.48	65.25	72.19	82.26
	% Difference	-1.12	-0.33	1.45	0.73	0.40	0.28	0.12	0.06	-0.04
	Detailed	-65.20	86.73	29.15	36.25	42.33	47.29	54.58	59.43	65.83
2,5-diformylfuran	GA	-65.77	86.02	28.90	36.10	42.21	47.22	54.49	59.38	65.84
	% Difference	0.87	-0.81	-0.85	-0.42	-0.29	-0.16	-0.16	-0.09	0.01
	Detailed	-50.26	85.55	28.02	35.42	41.70	46.79	54.30	59.51	67.19
2-acetylfuran	GA	-49.46	86.00	27.97	35.41	41.72	46.83	54.36	59.61	67.31
	% Difference	-1.60	0.53	-0.19	-0.02	0.06	0.10	0.12	0.17	0.17
	Detailed	-48.88	87.10	28.10	35.51	41.79	46.86	54.35	59.54	67.21
3-acetylfuran	GA	-49.64	86.05	28.17	35.58	41.88	46.97	54.47	59.67	67.26
	% Difference	1.56	-1.21	0.26	0.20	0.22	0.23	0.23	0.21	0.08

Table 1: Comparison of theoretical thermochemical functions (Detailed) with optimized group additivity values (GA) for stable and radical species. $\Delta_f H^\circ$ (kcal mol^{-1}), S$^\circ$ and C_p (cal mol^{-1} K^{-1}).

Species		$\Delta_f H^\circ$	S$^\circ$	C_p 300	400	500	600	800	1000	1500
	Detailed	-61.42	94.38	33.55	41.99	49.38	55.52	64.81	71.39	81.20
5-methyl-2-acetylfuran	GA	-60.44	94.41	33.53	41.99	49.41	55.58	64.91	71.53	81.36
	% Difference	-1.60	0.03	-0.06	0.01	0.06	0.11	0.16	0.20	0.19
	Detailed	-60.04	94.59	33.72	42.07	49.40	55.51	64.77	71.35	81.18
5-methyl-3-acetylfuran	GA	-60.62	94.46	33.73	42.16	49.57	55.72	65.02	71.59	81.31
	% Difference	0.97	-0.14	0.03	0.21	0.34	0.38	0.39	0.33	0.16
	Detailed	-71.13	102.18	39.37	48.90	57.55	64.90	76.14	84.09	95.82
2,5-dimethyl-3-acetylfuran	GA	-71.60	102.88	39.29	48.74	57.26	64.47	75.57	83.51	95.36
	% Difference	0.66	0.68	-0.20	-0.32	-0.51	-0.66	-0.74	-0.69	-0.48
	Detailed	-52.58	83.03	25.03	31.75	37.56	42.29	49.26	54.11	61.37
2-hydroxymethylfuran	GA	-53.03	81.70	25.09	31.78	37.58	42.29	49.22	54.09	61.36
	% Difference	0.85	-1.60	0.25	0.10	0.04	0.00	-0.08	-0.04	-0.02
	Detailed	1.81	82.03	24.19	30.97	36.58	41.03	47.43	51.80	58.15
2-furylmethanoxy	GA	1.36	80.70	24.25	31.00	36.60	41.03	47.39	51.78	58.14
	% Difference	-24.86	-1.62	0.25	0.10	0.05	0.00	-0.08	-0.04	-0.02
	Detailed	-63.65	89.59	30.77	38.45	45.32	51.07	59.79	66.00	75.39
5-methyl-2-hydroxymethylfuran	GA	-64.01	90.12	30.65	38.36	45.27	51.04	59.77	66.01	75.41

Table 1: Comparison of theoretical thermochemical functions (Detailed) with optimized group additivity values (GA) for stable and radical species. $\Delta_f H^\circ$ (kcal mol^{-1}), S$^\circ$ and C_p (cal mol^{-1} K^{-1}).

Species		$\Delta_f H^\circ$	S$^\circ$	C_p 300	400	500	600	800	1000	1500
	% Difference	0.57	0.59	-0.40	-0.24	-0.12	-0.06	-0.03	0.01	0.03
	Detailed	-61.90	90.72	30.87	38.54	45.38	51.10	59.80	66.01	75.40
5-methyl-3-hydroxymethylfuran	GA	-61.26	90.38	30.66	38.32	45.20	50.95	59.68	65.93	75.35
	% Difference	-1.04	-0.37	-0.66	-0.56	-0.39	-0.30	-0.21	-0.12	-0.06
	Detailed	-81.86	91.68	31.59	39.15	45.76	51.22	59.32	64.92	72.93
5-hydroxymethyl-2-formylfuran	GA	-81.69	92.80	31.81	39.40	46.00	51.44	59.47	65.04	72.98
	% Difference	-0.21	1.22	0.71	0.65	0.52	0.44	0.25	0.19	0.07
	Detailed	-98.49	80.86	25.85	32.95	38.79	43.40	49.91	54.16	59.82
2-furoic acid	GA	-98.47	81.42	25.84	32.94	38.76	43.34	49.78	54.01	0.00
	% Difference	-0.02	0.70	-0.03	-0.04	-0.08	-0.13	-0.26	-0.27	-100.00
	Detailed	-99.31	81.15	25.98	33.07	38.89	43.47	49.91	54.08	59.66
3-furoic acid	GA	-98.65	81.47	26.04	33.11	38.92	43.48	49.89	54.07	0.00
	% Difference	-0.66	0.39	0.25	0.12	0.08	0.03	-0.04	-0.03	-100.00
	Detailed	-109.75	89.72	31.43	39.56	46.50	52.14	60.41	65.99	73.75
5-methyl-2-furoic acid	GA	-109.45	89.84	31.40	39.52	46.45	52.09	60.33	65.93	0.00
	% Difference	-0.27	0.13	-0.09	-0.09	-0.10	-0.09	-0.13	-0.10	-100.00
	Detailed	-110.37	89.85	31.63	39.70	46.59	52.19	60.36	65.87	73.61
5-methyl-3-furoic acid										

Table 1: Comparison of theoretical thermochemical functions (Detailed) with optimized group additivity values (GA) for stable and radical species. $\Delta_f H^\circ$ (kcal mol^{-1}), S$^\circ$ and C_p (cal mol^{-1} K^{-1}).

Species		$\Delta_f H^\circ$	S$^\circ$	C_p 300	400	500	600	800	1000	1500
	GA	-109.63	89.89	31.60	39.69	46.61	52.23	60.44	65.99	0.00
	% Difference	-0.67	0.04	-0.09	-0.02	0.03	0.08	0.14	0.17	-100.00
	Detailed	-121.80	98.29	37.15	46.23	54.23	60.88	70.86	77.77	87.65
2,5-dimethyl-3-furoic acid	GA	-120.61	98.30	37.16	46.27	54.30	60.98	70.99	77.91	0.00
	% Difference	-0.97	0.01	0.04	0.09	0.14	0.17	0.19	0.18	-100.00
	Detailed	-187.05	96.80	36.28	45.04	52.17	57.78	65.61	70.54	76.70
2,5-difuroic acid	GA	-188.49	96.26	36.22	45.02	52.15	57.76	65.57	70.54	0.00
	% Difference	0.77	-0.56	-0.16	-0.05	-0.04	-0.03	-0.06	0.00	-100.00

3 Optimized Group Contributions

Table 2: Optimized group contributions to the $\Delta_f H^\circ$ (kcal mol^{-1}), S$^\circ$ and C_p (cal mol^{-1} K^{-1}) of stable validation targets. Groups in italics were not optimized as part of *this work*.

			C_p						
Group	$\Delta_f H^\circ$	S	300	400	500	600	800	1000	1500
CF/H	6.19	12.19	2.50	3.39	4.16	4.78	5.70	6.31	7.23
CF/C	8.67	5.43	4.79	5.86	6.85	7.70	9.00	9.85	11.21
CF/H/O	5.59	12.85	1.36	2.20	2.89	3.42	4.17	4.72	5.34
CF/C/O	5.32	5.83	3.64	4.71	5.65	6.43	7.56	8.34	9.38
CF/CD/O	24.08	-0.98	3.39	4.16	4.73	5.17	5.76	6.11	6.39
CF/CO/O	-1.28	6.91	4.47	5.33	6.04	6.63	7.41	7.91	10.00
CF/O/O	11.30	5.63	2.62	2.97	3.22	3.39	3.61	3.76	3.80
CF/O	16.08	4.37	3.89	4.45	4.82	5.08	5.42	5.57	5.81
CF/CO	-0.86	6.30	5.81	6.69	7.47	8.13	9.05	9.56	11.84
C/CF/H3	-10.71	17.62	3.28	4.07	4.93	5.74	7.16	8.30	10.01
C/CF/C/H2	-5.40	-2.48	2.74	3.49	4.05	4.58	5.50	5.77	7.10
C/CF/C3	0.60	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
C/CF/H2/O	-6.24	-6.68	2.86	3.88	4.69	5.17	5.50	5.81	5.26
CD/CF/H	-11.14	-0.98	3.39	4.16	4.73	5.17	5.76	6.11	6.39
CO/CF/H	-21.79	17.04	3.61	4.49	5.27	5.94	7.01	7.76	6.96
CO/CF/C	-23.96	-1.49	3.21	3.58	3.80	3.91	4.11	4.17	2.47
CO/CF/O	-25.05	-2.34	3.47	3.95	4.44	4.91	5.35	5.54	12.41
O/CF2	-32.01	15.12	7.74	9.68	11.27	12.52	14.25	15.42	17.46
O/CF/H	-46.55	14.59	3.95	4.42	4.76	5.04	5.47	5.80	6.34
O/CF/C	-32.00	-4.59	2.57	3.00	3.28	3.43	3.55	3.53	3.27
C/CO/H3	-10.18	30.41	6.19	7.84	9.40	10.79	13.02	14.77	17.58
O/C/H	-38.07	30.20	4.49	4.53	4.76	5.19	6.34	7.18	9.46
C/H3/O	-10.00	30.41	6.19	7.84	9.40	10.79	13.03	14.77	17.58

Table 2: Optimized group contributions to the $\Delta_f H^\circ$ (kcal mol^{-1}), S$^\circ$ and C_p (cal mol^{-1} K^{-1}) of stable validation targets. Groups in italics were not optimized as part of *this work*.

			C_p						
Group	$\Delta_f H^\circ$	S	300	400	500	600	800	1000	1500
O/CO/H	-58.10	24.50	3.80	5.00	5.80	6.30	7.20	7.80	
C/C/H3	-10.03	30.42	6.26	7.86	9.36	10.68	12.88	14.92	17.19
CD/H2	6.28	27.59	5.10	6.31	7.44	8.42	9.99	11.20	13.17

Table 3: Optimized bond dissociation group contributions to the $\Delta_f H^\circ$ (kcal mol^{-1}), S$^\circ$ and C_p (cal mol^{-1} K^{-1}) of validation targets.

			C_p						
Group	$\Delta_f H^\circ$	S$^\circ$	300	400	500	600	800	1000	1500
FJ	119.97	1.36	-0.46	-1.14	-1.74	-2.24	-3.01	-3.59	-4.53
F2CH2J	85.10	-3.46	0.10	0.26	-0.03	-0.49	-1.44	-2.22	-3.43
F3CH2J	89.21	-3.25	0.47	0.53	0.14	-0.38	-1.38	-2.19	-3.42
F2CHJCH3	83.90	-1.81	-0.81	-1.06	-1.29	-1.62	-2.30	-2.79	-3.68
F2OJ	67.16	-1.32	-1.88	-1.96	-2.12	-2.30	-2.63	-2.93	-3.58
F3OJ	80.17	-0.40	-1.98	-2.18	-2.32	-2.45	-2.71	-2.96	-3.57
F2CJO	90.99	0.93	-0.62	-1.27	-1.92	-2.50	-3.45	-4.14	-5.04
F2CH2OJ	106.98	0.25	0.53	0.24	-0.27	-0.76	-1.54	-2.13	-3.15

4 S P I C
T P *via* G A

Table 4: Group contributions, symmetry numbers, number of rotors and unpaired electrons for molecules used to develop rules are provided below. Bond dissociation (BD) groups are emboldened.

Species	Molecular Formula	Group	Quantity	Symmetry	Rotors	Unpaired Electrons
Furan	C4H4O	O/CF2	1	2	0	0
		CF/H/O	2			
		CF/H	2			
Furan-2-yl	C4H3O	O/CF2	1	1	0	1
		CF/H/O	2			
		CF/H	2			
		FJ	1			
Furan-3-yl	C4H3O	O/CF2	1	1	0	1
		CF/H/O	2			
		CF/H	2			
		FJ	1			
2-methylfuran	C5H6O	O/CF2	1	3	1	0
		CF/H/O	1			
		CF/H	2			
		CF/C/O	1			
		C/CF/H3	1			
2-furanylmethyl	C5H5O	O/CF2	1	1	0	1
		CF/H/O	1			
		CF/H	2			
		CF/C/O	1			

Table 4: Group contributions, symmetry numbers, number of rotors and unpaired electrons for molecules used to develop rules are provided below. Bond dissociation (BD) groups are emboldened.

Species	Molecular Formula	Group	Quantity	Symmetry	Rotors	Unpaired Electrons
		C/CF/H3	1			
		F2CH2J	**1**			
		O/CF2	1	3	0	1
		CF/H/O	1			
2-methylfuran-3-yl	C5H5O	CF/H	2			
		CF/C/O	1			
		C/CF/H3	1			
		FJ	**1**			
		O/CF2	1	3	0	1
		CF/H/O	1			
2-methylfuran-4-yl	C5H5O	CF/H	2			
		CF/C/O	1			
		C/CF/H3	1			
		FJ	**1**			
		O/CF2	1	3	0	1
		CF/H/O	1			
2-methylfuran-5-yl	C5H5O	CF/H	2			
		CF/C/O	1			
		C/CF/H3	1			
		FJ	**1**			

Table 4: Group contributions, symmetry numbers, number of rotors and unpaired electrons for molecules used to develop rules are provided below. Bond dissociation (BD) groups are emboldened.

Species	Molecular Formula	Group	Quantity	Symmetry	Rotors	Unpaired Electrons
3-methylfuran	C5H6O	O/CF2	1	3	1	0
		CF/H/O	2			
		CF/C	1			
		C/CF/H3	1			
		CF/H	1			
3-methylfuran-2-yl	C5H5O	O/CF2	1	3	0	1
		CF/H/O	2			
		CF/C	1			
		C/CF/H3	1			
		CF/H	1			
		FJ	**1**			
3-furanylmethyl	C5H5O	O/CF2	1	1	0	1
		CF/H/O	2			
		CF/C	1			
		C/CF/H3	1			
		CF/H	1			
		F3CH2J	**1**			
3-methylfuran-4-yl	C5H5O	O/CF2	1	3	0	1
		CF/H/O	2			
		CF/C	1			
		C/CF/H3	1			

Table 4: Group contributions, symmetry numbers, number of rotors and unpaired electrons for molecules used to develop rules are provided below. Bond dissociation (BD) groups are emboldened.

Species	Molecular Formula	Group	Quantity	Symmetry	Rotors	Unpaired Electrons
		CF/H	1			
		FJ	**1**			
		O/CF2	1	3	0	1
		CF/H/O	2			
3-methylfuran-5-yl	C5H5O	CF/C	1			
		C/CF/H3	1			
		CF/H	1			
		FJ	**1**			
		O/CF2	1	18	2	0
		CF/C/O	2			
2,5-dimethylfuran	C6H8O	C/CF/H3	2			
		CF/H	2			
		O/CF2	1	3	1	1
		CF/C/O	2			
2-methyl-5-furanylmethylfuran	C6H7O	C/CF/H3	2			
		CF/H	2			
		F2CH2J	1			
		O/CF2	1	9	1	1
		CF/C/O	2			
2,5-dimethylfuran-3-yl	C6H7O	C/CF/H3	2			

Table 4: Group contributions, symmetry numbers, number of rotors and unpaired electrons for molecules used to develop rules are provided below. Bond dissociation (BD) groups are emboldened.

Species	Molecular Formula	Group	Quantity	Symmetry	Rotors	Unpaired Electrons
2,3-dimethylfuran	C6H8O	CF/H	2	9	2	0
		FJ	1			
		O/CF2	1			
		CF/C/O	1			
		CF/C	1			
		CF/H	2			
		CF/H/O	1			
		C/CF/H3	2			
3-methyl-2-furanylmethylfuran	C6H7O	O/CF2	1	3	1	1
		CF/C/O	1			
		CF/C	1			
		CF/H	2			
		CF/H/O	1			
		C/CF/H3	2			
		F2CH2J	1			
2-methyl-3-furanylmethylfuran	C6H7O	O/CF2	1	3	1	1
		CF/C/O	1			
		CF/C	1			
		CF/H	2			
		CF/H/O	1			
		C/CF/H3	2			

Table 4: Group contributions, symmetry numbers, number of rotors and unpaired electrons for molecules used to develop rules are provided below. Bond dissociation (BD) groups are emboldened.

Species	Molecular Formula	Group	Quantity	Symmetry	Rotors	Unpaired Electrons
		F3CH2J	1			
		O/CF2	1	9	2	1
		CF/C/O	1			
		CF/C	1			
2,3-dimethylfuran-4-yl	C6H7O	CF/H	2			
		CF/H/O	1			
		C/CF/H3	2			
		FJ	1			
		O/CF2	1	9	2	1
		CF/C/O	1			
		CF/C	1			
2,3-dimethylfuran-5-yl	C6H7O	CF/H	2			
		CF/H/O	1			
		C/CF/H3	2			
		FJ	1			
		O/CF2	1	9	2	0
		CF/C/O	1			
		CF/H	1			
2,4-dimethylfuran	C6H8O	CF/C	1			
		CF/H/O	1			
		C/CF/H3	2			

Table 4: Group contributions, symmetry numbers, number of rotors and unpaired electrons for molecules used to develop rules are provided below. Bond dissociation (BD) groups are emboldened.

Species	Molecular Formula	Group	Quantity	Symmetry	Rotors	Unpaired Electrons
4-methyl-2-furanylmethylfuran	C6H7O	O/CF2	1	3	1	1
		CF/C/O	1			
		CF/H	1			
		CF/C	1			
		CF/H/O	1			
		C/CF/H3	2			
		F2CH2J	**1**			
2,4-dimethylfuran-3-yl	C6H7O	O/CF2	1	9	1	1
		CF/C/O	1			
		CF/H	1			
		CF/C	1			
		CF/H/O	1			
		C/CF/H3	2			
		FJ	**1**			
2-methyl-4-furanylmethylfuran	C6H7O	O/CF2	1	3	1	1
		CF/C/O	1			
		CF/H	1			
		CF/C	1			
		CF/H/O	1			
		C/CF/H3	2			
		F3CH2J	**1**			

Table 4: Group contributions, symmetry numbers, number of rotors and unpaired electrons for molecules used to develop rules are provided below. Bond dissociation (BD) groups are emboldened.

Species	Molecular Formula	Group	Quantity	Symmetry	Rotors	Unpaired Electrons
2,4-dimethylfuran-5-yl	C6H7O	O/CF2	1	9	1	1
		CF/C/O	1			
		CF/H	1			
		CF/C	1			
		CF/H/O	1			
		C/CF/H3	2			
		FJ	**1**			
3,4-dimethylfuran	C6H8O	O/CF2	1	18	2	0
		CF/H/O	2			
		CF/C	2			
		C/CF/H3	2			
3,4-dimethylfuran-2-yl	C6H7O	O/CF2	1	9	2	1
		CF/H/O	2			
		CF/C	2			
		C/CF/H3	2			
		FJ				
3-methyl-4-furanylmethylfuran	C6H7O	O/CF2	1	3	1	1
		CF/H/O	2			
		CF/C	2			
		C/CF/H3	2			

Table 4: Group contributions, symmetry numbers, number of rotors and unpaired electrons for molecules used to develop rules are provided below. Bond dissociation (BD) groups are emboldened.

Species	Molecular Formula	Group	Quantity	Symmetry	Rotors	Unpaired Electrons
		F3CH2J				
2-ethylfuran	C6H8O	O/CF2	1	3	2	0
		CF/C/O	1			
		C/CF/C/H2	1			
		C/C/H3	1			
		CF/H	2			
		CF/H/O	1			
2-ethylfuran-2-yl (allylic)	C6H7O	O/CF2	1	3	1	1
		CF/C/O	1			
		C/CF/C/H2	1			
		C/C/H3	1			
		CF/H	2			
		CF/H/O	1			
		F2CHJCH3	1			
2-methyl-5-ethylfuran	C7H10O	O/CF2	1	9	3	0
		CF/C/O	2			
		C/CF/H3	1			
		CF/H	2			
		C/CF/C/H2	1			
		C/C/H3	1			

Table 4: Group contributions, symmetry numbers, number of rotors and unpaired electrons for molecules used to develop rules are provided below. Bond dissociation (BD) groups are emboldened.

Species	Molecular Formula	Group	Quantity	Symmetry	Rotors	Unpaired Electrons
2-methyl-5-ethylfuran-5-yl (secondary allylic)	C7H9O	O/CF2	1	9	2	1
		CF/C/O	2			
		C/CF/H3	1			
		CF/H	2			
		C/CF/C/H2	1			
		C/C/H3	1			
		F2CHJCH3	1			
2-vinylfuran	C6H6O	O/CF2	1	1	1	0
		CF/H/O	1			
		CF/H	2			
		CF/CD/O	1			
		CD/CF/H	1			
		CD/H2	1			
2-methyl-5-vinylfuran	C7H8O	O/CF2	1	3	2	0
		CF/C/O	1			
		C/CF/H3	1			
		CF/H	2			
		CF/CD/O	1			
		CD/CF/H	1			
		CD/H2	1			
2-furanol	C4H4O2	O/CF2	1	1	1	0

Table 4: Group contributions, symmetry numbers, number of rotors and unpaired electrons for molecules used to develop rules are provided below. Bond dissociation (BD) groups are emboldened.

Species	Molecular Formula	Group	Quantity	Symmetry	Rotors	Unpaired Electrons
2-furanyloxy	C4H3O2	CF/H/O	1	1	1	1
		CF/H	2			
		CF/O/O	1			
		O/CF/H	1			
		O/CF2	1			
		CF/H/O	1			
		CF/H	2			
		CF/O/O	1			
		O/CF/H	1			
		F2OJ	**1**			
3-furanol	C4H4O2	O/CF2	1	1	1	0
		CF/H/O	2			
		CF/H	1			
		CF/O	1			
		O/CF/H	1			
3-furanyloxy	C4H3O2	O/CF2	1	1	1	1
		CF/H/O	2			
		CF/H	1			
		CF/O	1			
		O/CF/H	1			
		F3OJ	**1**			

Table 4: Group contributions, symmetry numbers, number of rotors and unpaired electrons for molecules used to develop rules are provided below. Bond dissociation (BD) groups are emboldened.

Species	Molecular Formula	Group	Quantity	Symmetry	Rotors	Unpaired Electrons
5-methyl-2-furanol	C5H6O2	O/CF2	1	3	2	0
		CF/O/O	1			
		O/CF/H	1			
		CF/H	2			
		CF/C/O	1			
		C/CF/H3	1			
5-methyl-3-furanol	C5H6O2	O/CF2	1	3	2	0
		CF/H/O	1			
		CF/O	1			
		O/CF/H	1			
		CF/H	1			
		CF/C/O	1			
		C/CF/H3	1			
2-formylfuran	C5H4O2	O/CF2	1	1	1	0
		CF/CO/O	1			
		CO/CF/H	1			
		CF/H	2			
		CF/H/O	1			
2-formylfuran-2-yl	C5H4O2	O/CF2	1	1	1	1
		CF/CO/O	1			

Table 4: Group contributions, symmetry numbers, number of rotors and unpaired electrons for molecules used to develop rules are provided below. Bond dissociation (BD) groups are emboldened.

Species	Molecular Formula	Group	Quantity	Symmetry	Rotors	Unpaired Electrons
		CO/CF/H	1			
		CF/H	2			
		CF/H/O	1			
		F2CJO	**1**			
		O/CF2	1	1	1	0
		CF/H/O	2			
3-formylfuran	C5H4O2	CF/CO	1			
		CO/CF/H	1			
		CF/H	1			
		O/CF2	1	3	2	0
		CF/CO/O	1			
		CO/CF/H	1			
5-methyl-2-formylfuran	C6H6O2	CF/H	2			
		CF/C/O	1			
		C/CF/H3	1			
		O/CF2	1	3	2	0
		CF/H/O	1			
		CF/CO	1			
5-methyl-3-formylfuran	C6H6O2	CO/CF/H	1			
		CF/H	1			

Table 4: Group contributions, symmetry numbers, number of rotors and unpaired electrons for molecules used to develop rules are provided below. Bond dissociation (BD) groups are emboldened.

Species	Molecular Formula	Group	Quantity	Symmetry	Rotors	Unpaired Electrons
4,5-dimethyl-2-formylfuran	C7H8O2	CF/C/O	1	9	3	0
		C/CF/H3	1			
		O/CF2	1			
		CF/CO/O	1			
		CO/CF/H	1			
		CF/H	1			
		CF/C	1			
		C/CF/H3	1			
		CF/C/O	1			
		C/CF/H3	1			
2,5-diformylfuran	C6H4O2	O/CF2	1	18	2	0
		CF/CO/O	2			
		CO/CF/H	2			
		CF/H	2			
2-acetylfuran	C6H6O2	O/CF2	1	3	2	0
		CF/CO/O	1			
		CO/CF/C	1			
		C/CO/H3	1			
		CF/H	2			
		CF/H/O	1			

Table 4: Group contributions, symmetry numbers, number of rotors and unpaired electrons for molecules used to develop rules are provided below. Bond dissociation (BD) groups are emboldened.

Species	Molecular Formula	Group	Quantity	Symmetry	Rotors	Unpaired Electrons
3-acetylfuran	C6H6O2	O/CF2	1	3	2	0
		CF/H/O	2			
		CF/CO	1			
		CO/CF/C	1			
		C/CO/H3	1			
		CF/H/O	1			
5-methyl-2-acetylfuran	C7H8O2	O/CF2	1	9	3	0
		CF/CO/O	1			
		CO/CF/C	1			
		C/CO/H3	1			
		CF/H	2			
		CF/C/O	1			
		C/CF/H3	1			
5-methyl-3-acetylfuran	C7H8O2	O/CF2	1	9	3	0
		CF/H/O	1			
		CF/CO	1			
		CO/CF/C	1			
		C/CO/H3	1			
		CF/H	1			
		CF/C/O	1			
		C/CF/H3	1			

Table 4: Group contributions, symmetry numbers, number of rotors and unpaired electrons for molecules used to develop rules are provided below. Bond dissociation (BD) groups are emboldened.

Species	Molecular Formula	Group	Quantity	Symmetry	Rotors	Unpaired Electrons
2,5-dimethyl-3-acetylfuran	C8H10O2	O/CF2	1	27	4	0
		CF/C/O	2			
		C/CF/H3	2			
		CF/H	1			
		CF/CO	1			
		CO/CF/C	1			
		C/CO/H3	1			
2-hydroxymethylfuran	C5H6O2	O/CF2	1	1	2	0
		CF/C/O	1			
		C/CF/H2/O	1			
		O/C/H	1			
		CF/H	2			
		CF/H/O	1			
2-furylmethanoxy	C5H6O2	O/CF2	1	1	1	1
		CF/C/O	1			
		C/CF/H2/O	1			
		O/C/H	1			
		CF/H	2			
		CF/H/O	1			
		F2CH2OJ	**1**			
5-methyl-2-hydroxymethylfuran	C6H8O2	O/CF2	1	3	3	0

Table 4: Group contributions, symmetry numbers, number of rotors and unpaired electrons for molecules used to develop rules are provided below. Bond dissociation (BD) groups are emboldened.

Species	Molecular Formula	Group	Quantity	Symmetry	Rotors	Unpaired Electrons
5-methyl-3-hydroxymethylfuran	C6H8O2	CF/C/O	1	3	3	0
		C/CF/H2/O	1			
		O/C/H	1			
		CF/H	2			
		CF/C/O	1			
		C/CF/H3	1			
		O/CF2	1			
		CF/H/O	1			
		CF/C	1			
		C/CF/H2/O	1			
		O/C/H	1			
		CF/H	1			
		CF/C/O	1			
		C/CF/H3	1			
5-hydroxymethyl-2-formylfuran	C6H6O3	O/CF2	1	1	3	0
		CF/CO/O	1			
		CO/CF/H	1			
		CF/H	2			
		CF/C/O	1			
		C/CF/H2/O	1			
		O/C/H	1			

Table 4: Group contributions, symmetry numbers, number of rotors and unpaired electrons for molecules used to develop rules are provided below. Bond dissociation (BD) groups are emboldened.

Species	Molecular Formula	Group	Quantity	Symmetry	Rotors	Unpaired Electrons
2-methoxyfuran	C5H6O2	O/CF2	1	3	2	0
		CF/O/O	1			
		O/CF/C	1			
		C/H3/O	1			
		CF/H	2			
		CF/H/O	1			
3-methoxyfuran	C5H6O2	O/CF2	1	3	2	0
		CF/H/O	2			
		CF/O	1			
		O/CF/C	1			
		C/H3/O	1			
		CF/H/O	1			
2-furoic acid	C5H4O3	O/CF2	1	1	2	0
		CF/CO/O	1			
		CO/CF/O	1			
		O/CO/H	1			
		CF/H	2			
		CF/H/O	1			
3-furoic acid	C5H4O3	O/CF2	1	1	2	0
		CF/H/O	2			
		CF/CO	1			

Table 4: Group contributions, symmetry numbers, number of rotors and unpaired electrons for molecules used to develop rules are provided below. Bond dissociation (BD) groups are emboldened.

Species	Molecular Formula	Group	Quantity	Symmetry	Rotors	Unpaired Electrons
		CO/CF/O	1			
		O/CO/H	1			
		CF/H/O	1			
		O/CF2	1	3	3	0
		CF/CO/O	1			
		CO/CF/O	1			
5-methyl-2-furoic acid	C6H6O3	O/CO/H	1			
		CF/H	2			
		CF/C/O	1			
		C/CF/H3	1			
		O/CF2	1	3	3	0
		CF/H/O	1			
		CF/CO	1			
		CO/CF/O	1			
5-methyl-3-furoic acid	C6H6O3	O/CO/H	1			
		CF/H	1			
		CF/C/O	1			
		C/CF/H3	1			
		O/CF2	1	9	4	0
		CF/C/O	2			
		C/CF/H3	2			
2,5-dimethyl-3-furoic acid	C7H8O3					

Table 4: Group contributions, symmetry numbers, number of rotors and unpaired electrons for molecules used to develop rules are provided below. Bond dissociation (BD) groups are emboldened.

Species	Molecular Formula	Group	Quantity	Symmetry	Rotors	Unpaired Electrons
		CF/CO	1			
		CO/CF/O	1			
		O/CO/H	1			
		CF/H	1			
		O/CF2	1	18	4	0
		CF/CO/O	2			
2,5-difuroic acid	C6H4O5	CO/CF/O	2			
		O/CO/H	2			
		CF/H	2			