APPENDIX B.

EVALUATION TABULATIONS AND FIGURES

This Appendix contains the table and figures giving the results of the evaluation of the mechanism against the individual environmental chamber experiments. Table B-1 lists all the environmental chamber experiments that were simulated in this study, and summarizes their major characteristics and selected experimental and calculated $\Delta(O_3\text{-NO})$ results. Percentage differences between experimental and calculated data are also shown. Figure B-1 through Figure B-90 contain plots of the experimental and calculated data, or distribution plots of the errors in the simulations of the $\Delta(O_3\text{-NO})$ data, for the various types of experiments that were modeled. The methods of procedure and the results of this evaluation are discussed in Section V of this report.

Table B-1. Summary of environmental chamber experiments used for mechanism evaluation.

Run	Run Type or VOC [a]	Rct'y Type [a]	Char Set [b]	NOx (ppm)	Pr.Eq. (ppm) [c]	k1 (min^{-1}) [d]	T (K) [e]	Ref [f]	Δ (O3-NO) Results (pphm) 2 Hour Expt	2 Hour Calc	2 Hour Δ%	4 Hour Expt	4 Hour Calc	4 Hour Δ%	6 Hour Expt	6 Hour Calc	6 Hour Δ%
Characterization Runs																	
ETC458	Pure Air		3			0.35	301	1	1	2	55	3	4	44	4	6	38
ETC485	Pure Air		3		0.00	0.35	300	1	1	2	51	3	5	46	3	7	49
DTC049A	Pure Air		1			0.39	301	1	1	1	37	2	3	28	4	4	20
ITC1009	Acetald - Air		11		0.42	0.35	302	1	1	2	34	4	4	2	7	7	-11
ITC627	Acetald - Air		5		0.23	0.35	300	1	1	2	41	3	4	23	6	7	9
ITC892	Acetald - Air		9		0.19	0.35	299	1	1	2	41	4	4	1	-		
ITC957	Acetald - Air		10		0.46	0.35	301	1	2	2	12	5	4	-7	8	7	-15
ETC319	Acetald - Air		2		0.30	0.35	298	1	0	1	69	1	3	49	3	5	49
ETC382	Acetald - Air		3		0.21	0.35	301	1	1	2	48	2	4	50	4	8	48
CTC019	Acetald - Air		1		0.34	0.20	304	2	1	0	-23	1	2	16	2	3	35
EC253	Acetald - Air		1		0.33	0.29	303	1	4	3	-20	9	9	-2	13	14	2
CTC031	CO - NOx		1	0.26	0.03	0.20	300	2	5	4	-26	10	8	-18	14	12	-17
CTC061	CO - NOx		2	0.23	0.03	0.19	300	2	4	4	13	7	9	15	-	12	
CTC090A	CO - NOx		4	0.26	0.03	0.19	294	2	-	4		8	8	1	-	11	
CTC090B	CO - NOx		4	0.26	0.03	0.19	294	2	-	4		9	8	-22	12	11	-12
ITC507	n-C4 - NOx		2	0.09	0.37	0.37	301	1	10	9	-6	16	16	3	23	25	10
ITC533	n-C4 - NOx		3	0.10	0.29	0.36	303	1	8	8	-3	14	14	-4	21	21	1
ITC939	n-C4 - NOx		10	0.53	0.48	0.35	301	1	5	4	-19	7	7	-2	10	10	0
ITC948	n-C4 - NOx		10	0.26	0.46	0.35	301	1	7	6	-12	12	11	-7	17	16	-6
ETC214	n-C4 - NOx		2	0.49	0.39	0.35	299	1	1	4	83	3	8	61	7	13	47
ETC318	n-C4 - NOx		2	0.52	0.42	0.35	298	1	1	3	61	3	6	48	6	9	35
DTC058A	n-C4 - NOx		1	0.24	0.38	0.39	301	1	4	4	-7	9	9	-7	14	13	-8
DTC058B	n-C4 - NOx		1	0.24	0.39	0.39	301	1	4	4	6	8	9	11	12	13	7
DTC145A	n-C4 - NOx		3	0.65	0.43	0.26	298	2	8	5	-39	13	11	-22	19	16	-18
DTC145B	n-C4 - NOx		3	0.66	0.43	0.26	298	2	6	7	16	13	14	7	20	20	2
DTC171A	n-C4 - NOx		3	0.59	0.51	0.24	298	2	9	7	-27	18	16	-17	-	23	
DTC171B	n-C4 - NOx		3	0.58	0.49	0.24	298	2	10	9	-11	21	18	-12	-	27	
DTC215A	n-C4 - NOx		3	0.54	0.44	0.23	299	2	4	6	28	-	13		-	19	
DTC215B	n-C4 - NOx		3	0.56	0.45	0.23	299	2	6	8	20	14	17	14	22	24	8
DTC228A	n-C4 - NOx		10	0.28	0.19	0.23	297	3	2	2	3	4	4	12	6	6	13
DTC228B	n-C4 - NOx		10	0.28	0.20	0.23	297	3	2	2	14	4	4	17	5	6	18
DTC236A	n-C4 - NOx		10	0.26	0.38	0.23	296	3	4	3	-23	7	6	-22	11	8	-28
DTC253A	n-C4 - NOx		10	0.27	0.41	0.23	297	3	3	3	-9	6	6	-1	10	10	-4
DTC253B	n-C4 - NOx		10	0.27	0.41	0.23	297	3	3	3	3	6	6	5	9	10	5
DTC285A	n-C4 - NOx		10	0.25	0.42	0.22	298	4	4	3	-21	8	6	-22	12	10	-23
DTC285B	n-C4 - NOx		10	0.25	0.41	0.22	298	4	3	3	-9	7	6	-8	11	10	-12
DTC299A	n-C4 - NOx		10	0.26	0.43	0.22	297	4	3	3	6	6	7	7	10	10	3
DTC299B	n-C4 - NOx		10	0.26	0.42	0.22	297	4	3	3	18	5	6	22	7	9	23
XTC085	n-C4 - NOx		1	0.55	0.39	0.26	302	1	4	4	-5	8	7	-10	11	11	-4
XTC098	n-C4 - NOx		1	0.57	0.42	0.25	303	1	4	4	4	8	8	0	-	12	
CTC013	n-C4 - NOx		1	0.45	0.30	0.20	303	2	2	2	40	3	5	39	-	8	
CTC020	n-C4 - NOx		1	0.26	0.40	0.20	304	2	2	3	32	4	6	32	7	9	28
CTC028	n-C4 - NOx		1	0.27	0.38	0.20	304	2	2	3	19	5	6	22	-	10	
CTC042	n-C4 - NOx		2	0.26	0.38	0.20	301	2	5	3	-61	9	6	-50	-	10	
CTC045	n-C4 - NOx		2	0.46	0.37	0.20	301	2	-	3		6	6	-10	8	8	0
CTC058	n-C4 - NOx		2	0.26	0.37	0.19	299	2	4	3	-34	8	6	-37	-	9	
CTC074	n-C4 - NOx		3	0.25	0.38	0.19	297	2	2	3	17	6	6	-3	-	10	
CTC084A	n-C4 - NOx		4	0.25	0.41	0.19	299	2	2	3	19	5	6	20	-	9	
CTC084B	n-C4 - NOx		4	0.25	0.41	0.19	299	2	2	3	12	5	6	22	8	9	10
CTC099A	n-C4 - NOx		4	0.27	0.36	0.19	295	2	3	2	-19	5	5	-6	-	8	
CTC099B	n-C4 - NOx		4	0.27	0.37	0.19	295	2	4	2	-65	8	5	-53	-	8	
CTC114A	n-C4 - NOx		5	0.24	0.38	0.19	296	2	3	2	-19	5	5	-6	-	8	
CTC114B	n-C4 - NOx		5	0.24	0.38	0.19	296	2	3	2	-19	5	5	-5	-	8	
CTC120A	n-C4 - NOx		5	0.26	0.37	0.19	294	2	2	2	26	4	5	27	-	8	
CTC120B	n-C4 - NOx		5	0.25	0.37	0.19	294	2	3	2	-2	5	5	11	-	8	
CTC135A	n-C4 - NOx		6	0.26	0.35	0.18	294	2	3	2	-15	5	5	-4	-	8	
CTC135B	n-C4 - NOx		6	0.26	0.35	0.18	294	2	3	2	-20	6	5	-11	-	8	
CTC241A	n-C4 - NOx		9	0.27	0.53	0.13	302	5	3	3	-3	8	7	-3	-	12	
CTC241B	n-C4 - NOx		9	0.27	0.53	0.13	302	5	3	3	7	7	7	1	12	12	-5

Table B-1 (continued)

Run	Run Type or VOC [a]	Rct'y Type [a]	Char Set [b]	NOx (ppm)	Pr.Eq. (ppm) [c]	k1 (min^{-1}) [d]	T (K) [e]	Ref [f]	Δ (O3-NO) Results (pphm) 2 Hour Expt	2 Hour Calc	2 Hour Δ%	4 Hour Expt	4 Hour Calc	4 Hour Δ%	6 Hour Expt	6 Hour Calc	6 Hour Δ%
CTC244A	n-C4 - NOx		9	0.26	0.60	0.13	293	6	4	3	-29	8	7	-16	15	12	-23
CTC244B	n-C4 - NOx		9	0.26	0.59	0.13	293	6	4	3	-18	8	7	-8	13	12	-11
CTC252A	n-C4 - NOx		9	0.25	0.61	0.13	293	6	3	3	18	6	8	20	11	12	15
CTC252B	n-C4 - NOx		9	0.25	0.58	0.13	293	6	3	3	6	6	7	18	9	11	17
EC162	n-C4 - NOx		1	0.54	0.20	0.34	301	1	21	16	-35	36	27	-31	44	37	-18
EC178	n-C4 - NOx		1	0.10	0.19	0.34	304	1	20	18	-10	36	36	1	45	50	10
EC304	n-C4 - NOx		1	0.51	0.42	0.40	302	1	29	30	1	49	51	4	63	71	11
EC305	n-C4 - NOx		1	0.11	0.42	0.41	302	1	28	30	6	43	52	18	48	64	26
EC307	n-C4 - NOx		1	0.11	0.63	0.41	302	1	30	35	14	46	60	24	50	71	29
EC355	n-C4 - NOx		1	0.50	0.41	0.35	302	1	20	26	25	33	43	22	46	59	22
EC356	n-C4 - NOx		1	0.50	0.43	0.35	302	1	20	27	27	33	44	24	45	60	25
OTC296A	n-C4 - NOx		11	0.53	0.46	0.00	310	7	8	7	-12	23	20	-13	-	31	
OTC296B	n-C4 - NOx		11	0.52	0.51	0.00	310	7	6	7	17	19	22	16	31	35	11
OTC303A	n-C4 - NOx		12	0.54	0.40	0.00	313	7	-	6		27	19	-40	-	28	
OTC303B	n-C4 - NOx		12	0.52	0.39	0.00	313	7	7	6	-23	20	19	-2	-	29	
OTC307A	n-C4 - NOx		12	0.46	0.38	0.00	319	7	14	12	-21	35	32	-9	-	43	
OTC307B	n-C4 - NOx		12	0.48	0.38	0.00	319	7	13	12	-4	32	33	4	44	44	0
Single VOC - NOx Runs																	
ITC1555	ETHENE		12	0.45	0.68	0.35	301	1	33	41	18	94	111	15	132	126	-5
ITC926	ETHENE		10	0.53	1.28	0.35	301	1	94	114	17	130	134	3	112	111	-1
ITC936	ETHENE		10	0.52	0.63	0.35	301	1	29	33	13	70	93	25	119	134	11
ETC220	ETHENE		2	0.51	0.20	0.35	299	1	5	5	8	12	13	14	20	23	11
ETC221	ETHENE		2	0.51	1.31	0.35	299	1	98	104	5	151	154	2	-	140	
ETC381	ETHENE		3	0.52	0.67	0.35	301	1	33	35	7	95	99	4	151	149	-1
ETC439	ETHENE		3	0.66	0.63	0.35	300	1	26	23	-17	66	61	-8	130	115	-13
ETC464	ETHENE		3	0.38	0.48	0.35	301	1	23	25	9	63	71	11	116	117	0
ETC466	ETHENE		3	0.41	0.48	0.35	300	1	22	23	4	55	63	12	108	112	3
ETC467	ETHENE		3	0.52	0.48	0.35	300	1	17	19	12	41	50	18	73	90	19
ETC469	ETHENE		3	0.46	0.58	0.35	301	1	22	29	25	58	82	30	114	133	14
ETC471	ETHENE		3	0.45	0.58	0.35	302	1	25	30	18	70	86	19	127	135	6
ETC473	ETHENE		3	0.46	0.61	0.35	301	1	25	31	21	66	89	26	123	137	10
ETC476	ETHENE		3	0.43	0.55	0.35	300	1	20	26	26	52	77	32	104	126	17
ETC479	ETHENE		3	0.42	0.57	0.35	301	1	22	30	26	59	86	31	115	131	12
ETC482	ETHENE		3	0.41	0.51	0.35	301	1	25	26	5	61	73	15	114	121	6
ETC486	ETHENE		3	0.44	0.51	0.35	301	1	20	24	17	54	66	19	108	118	9
ETC497	ETHENE		3	0.45	0.57	0.35	301	1	22	27	20	61	80	23	118	131	9
ETC505	ETHENE		3	0.40	0.53	0.35	300	1	23	25	10	59	75	21	108	122	11
DTC041B	ETHENE		1	0.17	0.57	0.39	300	1	30	47	36	79	88	10	88	92	4
DTC043A	ETHENE		1	0.47	0.55	0.39	300	1	17	23	23	49	65	25	101	122	18
DTC044B	ETHENE		1	0.16	0.59	0.39	300	1	33	50	35	81	88	7	89	91	2
DTC045A	ETHENE		1	0.48	0.57	0.39	301	1	19	24	22	54	70	24	113	130	13
DTC046B	ETHENE		1	0.17	0.57	0.19	300	1	10	14	33	36	48	24	58	64	10
DTC047A	ETHENE		1	0.48	0.59	0.39	301	1	20	24	16	55	70	22	113	131	14
DTC048B	ETHENE		1	0.17	0.59	0.39	301	1	35	49	28	82	88	7	89	92	3
DTC050A	ETHENE		1	0.16	0.59	0.39	301	1	34	50	33	80	87	9	86	90	4
DTC051A	ETHENE		1	0.48	0.59	0.39	301	1	20	25	20	56	73	23	117	134	13
DTC072B	ETHENE		1	0.47	0.56	0.39	302	1	18	24	24	49	64	24	102	117	13
XTC105	ETHENE		1	0.24	0.60	0.25	301	1	20	17	-17	71	57	-24	99	85	-16
XTC112	ETHENE		1	0.52	0.87	0.25	302	1	24	23	-3	74	71	-4	134	125	-7
EC142	ETHENE		1	0.49	0.31	0.31	301	1	40	32	-24	80	61	-31	109	91	-21
EC143	ETHENE		1	0.50	0.66	0.31	300	1	109	73	-49	145	124	-17	123	120	-2
EC156	ETHENE		1	0.47	0.65	0.33	301	1	110	75	-48	139	124	-12	117	121	3
EC285	ETHENE		1	1.01	0.63	0.38	302	1	66	77	14	115	151	24	165	193	15
EC286	ETHENE		1	0.97	1.22	0.38	302	1	144	172	17	169	192	12	141	163	14
EC287	ETHENE		1	0.54	1.30	0.37	302	1	137	148	7	116	133	13	97	110	13
OTC278B	ETHENE		11	0.46	0.25	0.00	313	8	12	8	-52	38	30	-27	62	48	-29
OTC279A	ETHENE		11	0.53	0.37	0.00	313	8	23	15	-49	87	56	-56	-	94	
OTC280B	ETHENE		11	0.54	0.39	0.00	312	8	23	19	-18	82	57	-44	-	85	
OTC297A	ETHENE		11	0.63	0.37	0.00	309	7	17	9	-96	60	39	-55	-	69	
OTC297B	ETHENE		11	0.28	0.37	0.00	309	7	24	18	-34	-	82		111	110	-1
OTC304A	ETHENE		12	0.60	0.36	0.00	316	7	18	14	-29	63	51	-23	-	79	
OTC304B	ETHENE		12	0.23	0.36	0.00	316	7	-	32		91	93	3	-	104	

Table B-1 (continued)

Run	Run Type or VOC [a]	Rct'y Type [a]	Char Set [b]	NOx (ppm)	Pr.Eq. (ppm) [c]	k1 (min^{-1}) [d]	T (K) [e]	Ref [f]	Δ (O3-NO) Results (pphm) 2 Hour Expt	2 Hour Calc	2 Hour Δ%	4 Hour Expt	4 Hour Calc	4 Hour Δ%	6 Hour Expt	6 Hour Calc	6 Hour Δ%
ITC1550	PROPENE		12	0.49	0.98	0.35	301	1	70	71	1	106	106	0	-		
ITC1556	PROPENE		12	0.49	0.99	0.35	301	1	53	67	21	104	109	5	114	111	-3
ITC484	PROPENE		2	0.45	0.46	0.39	300	1	14	21	36	32	45	30	40	67	41
ITC510	PROPENE		2	0.59	0.95	0.53	302	1	57	69	17	107	134	20	127	157	19
ITC532	PROPENE		3	0.56	0.91	0.36	302	1	32	45	28	76	104	27	100	125	20
ITC569	PROPENE		4	0.48	0.94	0.36	299	1	44	53	17	96	109	12	-	117	
ITC693	PROPENE		6	0.48	1.07	0.35	301	1	62	73	16	110	117	6	115	118	2
ITC716	PROPENE		6	0.53	1.01	0.35	300	1	59	54	-8	101	115	13	108	124	13
ITC728	PROPENE		6	0.49	1.02	0.35	299	1	51	62	18	94	114	17	101	116	13
ITC736	PROPENE		7	0.49	0.50	0.35	299	1	21	19	-14	40	40	2	58	61	6
ITC754	PROPENE		7	0.57	0.95	0.35	299	1	56	43	-30	-	102		-	124	
ITC791	PROPENE		7	0.53	0.92	0.35	299	1	58	44	-32	103	102	-1	117	120	2
ITC792	PROPENE		8	0.50	0.95	0.35	296	1	50	50	-1	95	104	8	110	113	2
ITC810	PROPENE		8	0.52	0.90	0.35	298	1	52	43	-21	104	98	-6	122	117	-4
ITC860	PROPENE		9	0.52	0.98	0.35	298	1	42	50	17	86	109	21	99	120	18
ITC925	PROPENE		10	0.56	1.06	0.35	302	1	45	64	30	90	118	23	109	123	11
ITC938	PROPENE		10	0.54	0.81	0.35	301	1	43	36	-18	90	87	-3	105	109	4
ITC947	PROPENE		10	0.54	0.60	0.35	301	1	40	20	-98	81	49	-65	99	75	-31
ETC321	PROPENE		2	0.44	1.02	0.35	299	1	48	51	6	114	112	-2	117	116	0
ETC440	PROPENE		3	0.60	1.16	0.35	300	1	51	48	-6	123	123	0	133	138	4
ETC449	PROPENE		3	0.25	0.91	0.35	300	1	71	73	3	76	81	6	75	80	6
ETC475	PROPENE		3	0.26	0.89	0.35	300	1	79	73	-8	73	84	14	71	83	15
DTC026A	PROPENE		1	0.49	1.15	0.39	302	1	100	77	-29	126	128	1	125	128	3
DTC026B	PROPENE		1	0.49	1.16	0.39	302	1	98	78	-25	127	129	1	125	129	4
DTC052A	PROPENE		1	0.30	0.94	0.39	301	1	84	82	-2	83	92	10	82	92	10
DTC054A	PROPENE		1	0.29	0.98	0.39	301	1	80	82	3	80	88	10	79	88	10
DTC060A	PROPENE		1	0.24	0.93	0.39	301	1	75	76	2	73	84	13	-		
DTC060B	PROPENE		1	0.51	0.97	0.39	301	1	52	41	-27	118	111	-6	-		
DTC128A	PROPENE		3	0.48	0.89	0.29	299	2	45	36	-26	100	88	-13	110	106	-4
DTC128B	PROPENE		3	0.49	0.87	0.29	299	2	47	35	-34	101	82	-24	110	99	-11
DTC129A	PROPENE		3	0.47	0.96	0.29	299	2	51	42	-20	103	98	-5	-	109	
DTC129B	PROPENE		3	0.47	0.94	0.29	299	2	51	41	-25	102	91	-12	-	101	
DTC146A	PROPENE		3	0.51	1.06	0.26	298	2	36	36	0	95	98	2	110	113	3
DTC146B	PROPENE		3	0.52	1.05	0.26	298	2	38	36	-4	95	92	-3	108	107	0
DTC153A	PROPENE		3	0.51	1.12	0.25	297	2	41	36	-15	104	101	-3	110	112	2
DTC155B	PROPENE		3	0.10	0.43	0.25	298	2	18	23	24	37	40	7	38	42	9
DTC158B	PROPENE		3	0.51	0.78	0.25	298	2	48	21	-129	108	50	-117	109	77	-42
DTC159A	PROPENE		3	0.51	0.73	0.25	298	2	50	18	-172	109	45	-140	109	74	-48
DTC168A	PROPENE		3	0.52	1.20	0.24	299	2	49	39	-26	109	107	-2	110	113	2
DTC169A	PROPENE		3	0.55	1.20	0.24	299	2	44	37	-20	110	106	-3	114	117	2
DTC170B	PROPENE		3	0.51	1.13	0.24	299	2	53	34	-55	-	95		107	108	0
DTC179B	PROPENE		3	0.50	1.22	0.24	299	2	50	41	-23	106	104	-3	106	105	0
DTC187A	PROPENE		3	0.57	1.13	0.23	299	2	35	32	-12	101	94	-7	119	117	-2
DTC187B	PROPENE		3	0.59	1.08	0.23	299	2	38	30	-29	102	79	-29	117	107	-9
DTC190A	PROPENE		3	0.57	1.20	0.23	299	2	47	35	-33	113	103	-9	115	116	1
DTC205A	PROPENE		3	0.57	1.10	0.23	299	2	41	30	-38	105	88	-19	-	114	
DTC205B	PROPENE		3	0.60	1.15	0.23	299	2	45	32	-43	107	88	-21	116	111	-4
DTC246A	PROPENE		10	0.48	0.95	0.23	297	3	20	22	10	58	71	18	87	101	14
DTC288A	PROPENE		10	0.54	1.04	0.22	298	4	28	31	11	76	86	12	91	99	8
DTC288B	PROPENE		10	0.54	1.02	0.22	298	4	28	29	4	78	85	9	95	102	6
DTC301A	PROPENE		11	0.52	1.04	0.21	296	4	23	28	19	69	84	17	96	100	4
DTC301B	PROPENE		11	0.51	1.03	0.21	296	4	22	28	21	69	84	17	99	100	1
DTC331A	PROPENE		11	0.55	1.07	0.21	296	9	24	27	13	72	83	14	97	100	3
DTC331B	PROPENE		11	0.54	1.06	0.21	296	9	23	27	13	71	82	14	100	101	2
DTC346A	PROPENE		11	0.58	1.01	0.20	299	10	29	24	-24	82	72	-14	98	100	2
DTC346B	PROPENE		11	0.59	1.02	0.20	299	10	30	23	-30	83	71	-17	99	100	1
DTC371A	PROPENE		11	0.57	0.64	0.20	299	10	28	11	-156	82	26	-214	100	44	-127
DTC371B	PROPENE		11	0.57	0.64	0.20	299	10	28	11	-153	82	26	-214	101	44	-128
DTC393A	PROPENE		11	0.57	0.92	0.19	296	11	23	18	-27	62	49	-27	94	84	-11
DTC393B	PROPENE		11	0.56	0.91	0.19	296	11	23	18	-29	62	49	-26	91	84	-9
DTC405A	PROPENE		11	0.56	0.99	0.19	299	10	29	20	-43	83	65	-28	103	98	-5
DTC405B	PROPENE		11	0.56	0.98	0.19	299	10	30	20	-46	82	63	-31	102	96	-6
DTC417A	PROPENE		11	0.53	1.19	0.19	297	10	27	29	7	83	92	10	105	100	-4

Table B-1 (continued)

Run	Run Type or VOC [a]	Rct'y Type [a]	Char Set [b]	NOx (ppm)	Pr.Eq. (ppm) [c]	k1 (min^{-1}) [d]	T (K) [e]	Ref [f]	Δ (O3-NO) Results (pphm) 2 Hour Expt	2 Hour Calc	2 Hour Δ%	4 Hour Expt	4 Hour Calc	4 Hour Δ%	6 Hour Expt	6 Hour Calc	6 Hour Δ%
DTC417B	PROPENE		11	0.53	1.23	0.19	297	10	28	32	12	84	93	10	105	98	-7
DTC431A	PROPENE		11	0.56	1.11	0.18	297	12	31	25	-25	90	78	-15	104	98	-6
DTC431B	PROPENE		11	0.56	1.11	0.18	297	12	32	25	-28	91	78	-17	108	98	-10
DTC443A	PROPENE		11	0.53	1.20	0.17	297	13	26	29	8	83	90	7	103	96	-7
DTC443B	PROPENE		11	0.53	1.21	0.17	297	13	27	29	7	84	89	6	103	95	-9
DTC458A	PROPENE		12	0.53	1.19	0.16	298	14	34	32	-5	87	90	3	-	95	
DTC458B	PROPENE		11	0.53	1.23	0.16	298	14	26	27	4	80	86	8	-	93	
DTC472A	PROPENE		14	0.51	1.05	0.23	298	13	38	31	-21	99	90	-9	109	104	-5
DTC472B	PROPENE		15	0.51	1.05	0.23	298	13	37	30	-21	99	89	-11	110	104	-6
DTC483A	PROPENE		14	0.49	1.17	0.22	298	13	43	44	1	103	99	-4	108	99	-10
DTC483B	PROPENE		15	0.49	1.17	0.22	298	13	41	44	6	102	99	-2	108	100	-8
DTC503A	PROPENE		14	0.52	1.09	0.22	299	15	38	31	-23	102	93	-10	114	105	-8
DTC503B	PROPENE		15	0.51	1.09	0.22	299	15	36	30	-19	101	93	-8	113	105	-7
DTC526A	PROPENE		14	0.51	1.10	0.21	300	10	42	31	-32	104	94	-11	112	102	-9
DTC526B	PROPENE		15	0.51	1.11	0.21	300	10	41	31	-35	104	94	-11	112	103	-8
DTC578A	PROPENE		14	0.49	1.19	0.20	298	16	29	34	14	91	94	3	105	96	-9
DTC578B	PROPENE		15	0.49	1.19	0.20	298	16	27	33	18	89	96	7	104	98	-6
DTC597A	PROPENE		14	0.49	1.16	0.19	298	16	23	29	22	74	92	20	99	99	0
DTC597B	PROPENE		15	0.49	1.15	0.19	298	16	21	28	27	69	91	25	98	99	1
XTC081	PROPENE		1	0.56	1.10	0.26	302	1	43	27	-55	122	94	-31	134	121	-11
XTC082	PROPENE		1	0.54	1.06	0.26	302	1	45	27	-69	122	89	-37	131	116	-13
XTC097	PROPENE		1	0.56	1.20	0.25	302	1	42	29	-45	122	105	-16	131	125	-5
XTC113	PROPENE		1	0.53	1.19	0.25	302	1	44	27	-64	118	92	-28	123	113	-9
CTC012	PROPENE		1	0.42	0.79	0.20	302	2	18	15	-17	57	48	-20	-	80	
CTC018	PROPENE		1	0.47	1.00	0.20	303	2	25	20	-25	86	76	-13	105	99	-6
CTC023	PROPENE		1	0.50	1.14	0.20	301	2	32	24	-31	100	89	-13	110	102	-8
CTC049	PROPENE		2	0.50	1.18	0.20	301	2	38	25	-54	99	91	-8	-	102	
CTC059	PROPENE		2	0.49	1.07	0.19	300	2	26	21	-25	86	75	-15	-	99	
CTC078	PROPENE		3	0.47	1.16	0.19	298	2	30	22	-36	92	83	-11	-	98	
CTC083A	PROPENE		4	0.51	1.25	0.19	298	2	26	23	-12	83	79	-5	106	99	-7
CTC083B	PROPENE		4	0.51	1.23	0.19	298	2	28	22	-26	87	73	-19	-	98	
CTC086A	PROPENE		4	0.44	1.22	0.19	295	2	28	25	-10	88	83	-7	105	91	-15
CTC086B	PROPENE		4	0.44	1.23	0.19	295	2	30	26	-16	92	87	-6	105	93	-13
CTC102A	PROPENE		5	0.49	1.13	0.19	295	2	25	19	-32	77	66	-16	-	98	
CTC102B	PROPENE		5	0.49	1.14	0.19	295	2	27	19	-38	78	69	-13	-	98	
CTC115A	PROPENE		5	0.47	1.15	0.19	295	2	23	20	-16	73	71	-3	-	96	
CTC115B	PROPENE		5	0.47	1.14	0.19	295	2	24	20	-21	75	71	-5	-	96	
CTC132A	PROPENE		6	0.49	1.16	0.18	293	2	26	19	-41	80	61	-30	-	95	
CTC132B	PROPENE		6	0.49	1.15	0.18	293	2	27	19	-45	80	63	-27	-	96	
CTC147A	PROPENE		6	0.53	1.32	0.18	299	4	37	29	-27	102	95	-8	-	98	
CTC147B	PROPENE		6	0.53	1.32	0.18	299	4	36	29	-24	102	94	-9	107	97	-11
CTC153A	PROPENE		6	0.54	1.28	0.18	301	4	42	25	-69	107	94	-13	-	102	
CTC153B	PROPENE		6	0.54	1.26	0.18	301	4	43	24	-75	107	92	-16	-	102	
CTC163A	PROPENE		7	0.50		0.18	299	0	32	23	-41	99	87	-14	-	99	
CTC163B	PROPENE		7	0.50	1.25	0.18	299	0	33	23	-45	100	88	-14	-	98	
CTC170A	PROPENE		7	0.54		0.17	299	5	35	22	-59	105	85	-22	-	99	
CTC170B	PROPENE		7	0.53	1.32	0.17	299	5	36	23	-56	104	89	-17	-	98	
CTC191A	PROPENE		7	0.48	1.26	0.16	298	17	29	21	-41	95	80	-20	-	91	
CTC191B	PROPENE		7	0.47	1.25	0.16	298	17	29	20	-42	96	80	-19	105	90	-17
CTC203A	PROPENE		8	0.48	1.35	0.15	298	18	30	22	-35	96	83	-16	-	89	
CTC203B	PROPENE		8	0.47	1.39	0.15	298	18	30	24	-26	96	84	-15	100	87	-16
CTC219A	PROPENE		8	0.49	1.23	0.14	297	19	31	17	-76	94	65	-44	-	90	
CTC219B	PROPENE		8	0.48	1.22	0.14	297	19	28	18	-54	93	72	-28	100	89	-12
CTC234A	PROPENE		9	0.51	1.53	0.14	302	5	25	27	8	90	90	0	-	86	
CTC234B	PROPENE		9	0.51	1.54	0.14	302	5	25	28	14	90	89	-1	96	85	-13
CTC245A	PROPENE		9	0.49	1.52	0.13	295	6	25	19	-32	90	82	-10	108	91	-19
CTC245B	PROPENE		9	0.49	1.51	0.13	295	6	25	19	-29	89	76	-16	109	91	-19
CTC264A	PROPENE		10	0.50	1.39	0.12	294	20	21	13	-54	78	48	-62	100	92	-9
CTC264B	PROPENE		10	0.50	1.42	0.12	294	20	20	14	-40	74	49	-52	99	90	-11
EC121	PROPENE		1	0.51	0.48	0.27	302	1	64	37	-71	86	64	-33	90	80	-13
EC177	PROPENE		1	0.50	0.49	0.33	305	1	47	46	-2	74	84	12	89	105	15
EC216	PROPENE		1	0.52	0.50	0.43	301	1	50	54	8	77	86	11	93	102	9
EC230	PROPENE		1	0.50	0.55	0.29	302	1	35	43	20	55	73	25	67	87	23

Table B-1 (continued)

Run	Run Type or VOC [a]	Rct'y Type [a]	Char Set [b]	NOx (ppm)	Pr.Eq. (ppm) [c]	k1 (min^{-1}) [d]	T (K) [e]	Ref [f]	Δ (O3-NO) Results (pphm) 2 Hour Expt	2 Hour Calc	2 Hour Δ%	4 Hour Expt	4 Hour Calc	4 Hour Δ%	6 Hour Expt	6 Hour Calc	6 Hour Δ%
EC256	PROPENE		1	0.53	0.11	0.29	303	1	11	10	-11	21	21	0	28	28	1
EC276	PROPENE		1	0.52	0.54	0.35	302	1	40	49	20	63	80	22	78	96	19
EC277	PROPENE		1	0.11	0.56	0.36	302	1	40	49	19	39	49	20	39	49	20
EC278	PROPENE		1	0.50	1.02	0.36	302	1	86	103	17	97	110	12	93	105	12
EC279	PROPENE		1	0.98	1.15	0.36	302	1	77	96	19	123	146	15	141	159	12
EC314	PROPENE		1	0.98	1.06	0.46	302	1	87	102	15	127	151	16	144	168	15
EC317	PROPENE		1	0.57	0.49	0.53	303	1	49	57	14	74	85	13	87	101	14
EC665	PROPENE		1	0.44	0.48	0.38	303	1	37	34	-7	50	55	9	57	67	15
EC684	PROPENE		1	0.44	1.13	0.38	303	1	66	92	28	72	107	33	69	105	35
EC687	PROPENE		1	0.47	1.04	0.37	303	1	64	82	22	95	107	12	89	110	19
EC691	PROPENE		1	0.49	1.08	0.37	304	1	63	87	27	90	111	19	86	113	24
EC863	PROPENE		1	0.57	0.52	0.22	302	1	33	25	-33	49	41	-20	56	52	-7
EC870	PROPENE		1	0.54	1.04	0.33	302	1	78	68	-14	91	101	10	84	107	21
EC885	PROPENE		1	0.52	0.93	0.29	301	1	61	53	-15	88	86	-2	87	93	7
EC899	PROPENE		1	0.48	1.06	0.27	302	1	60	63	6	83	95	12	77	96	20
OTC272A	PROPENE		11	0.54	1.08	0.00	311	7	134	88	-52	158	149	-6	158	153	-3
OTC272B	PROPENE		11	0.53	1.07	0.00	311	7	125	90	-39	152	149	-2	-	155	
OTC295A	PROPENE		11	0.54	1.51	0.00	313	7	135	129	-5	154	150	-3	-	153	
OTC295B	PROPENE		11	0.52	1.49	0.00	313	7	124	127	3	145	149	3	-	153	
OTC298A	PROPENE		11	0.58	1.29	0.00	311	7	136	92	-48	156	156	0	153	160	4
OTC298B	PROPENE		11	0.57	1.35	0.00	311	7	121	102	-18	151	155	3	-	159	
ITC927	1-BUTENE		10	0.54	1.27	0.35	301	1	38	41	7	81	84	3	98	105	7
ITC928	1-BUTENE		10	1.05	0.01	0.35	301	1	-2			13	16	18	42	54	23
ITC930	1-BUTENE		10	0.53	3.33	0.35	302	1	103	99	-4	88	76	-15	85	76	-11
ITC935	1-BUTENE		10	1.09	3.42	0.35	301	1	66	99	34	142	162	12	154	154	0
EC122	1-BUTENE		1	0.51	0.26	0.27	301	1	29	21	-40	45	37	-22	56	47	-18
EC123	1-BUTENE		1	0.51	0.48	0.27	300	1	48	35	-39	70	56	-27	86	68	-26
EC124	1-BUTENE		1	1.00	0.51	0.27	301	1	26	32	20	46	53	14	60	67	10
ITC929	1-HEXENE		10	0.52	1.19	0.35	302	1	13	14	10	34	38	9	60	65	8
ITC931	1-HEXENE		10	0.51	2.40	0.35	301	1	28	32	13	89	96	7	80	103	22
ITC934	1-HEXENE		10	1.07	2.27	0.35	303	1	20	15	-34	46	47	2	79	85	7
ITC937	1-HEXENE		10	1.08	0.01	0.35	301	1	-3			7	9	24	19	25	26
ITC694	ISOBUTEN		6	0.50	1.98	0.35	301	1	109	102	-6	126	142	11	126	144	12
DTC052B	ISOBUTEN		1	0.30	1.06	0.39	301	1	64	67	5	85	96	11	92	103	11
EC146	T-2-BUTE		1	0.51	0.56	0.32	301	1	41	43	5	52	53	2	60	60	-1
EC147	T-2-BUTE		1	0.96	1.01	0.32	301	1	66	72	9	79	86	8	89	95	7
EC157	T-2-BUTE		1	0.56	0.52	0.33	301	1	41	41	-1	50	51	1	58	57	-2
ITC511	ISOPRENE		2	0.60	3.83	0.53	300	1	135	146	8	125	135	7	-		
ITC811	ISOPRENE		8	0.46	2.42	0.35	297	1	121	90	-34	130	109	-19	-		
ITC812	ISOPRENE		8	0.53	1.28	0.35	297	1	59	32	-84	96	58	-65	114	75	-51
DTC053A	ISOPRENE		1	0.15	1.16	0.39	301	1	37	41	10	55	53	-4	56	52	-8
DTC053B	ISOPRENE		1	0.24	1.17	0.39	301	1	29	32	8	64	69	7	79	79	1
DTC056A	ISOPRENE		1	0.47	2.73	0.39	301	1	102	112	9	125	114	-10	122	110	-11
DTC056B	ISOPRENE		1	0.47	1.48	0.39	301	1	38	40	5	77	81	5	97	104	7
XTC093	ISOPRENE		1	0.16	1.07	0.25	301	1	20	16	-26	46	42	-8	-	45	
XTC101	ISOPRENE		1	0.53	1.55	0.25	302	1	28	27	-4	65	60	-8	89	89	1
EC520	ISOPRENE		1	0.49	1.69	0.31	302	1	63	67	6	86	93	7	89	99	11
EC522	ISOPRENE		1	0.96	1.72	0.32	304	1	66	69	3	89	94	5	102	110	7
EC524	ISOPRENE		1	1.00	3.34	0.33	302	1	133	144	8	157	168	7	148	164	10
EC527	ISOPRENE		1	0.53	1.61	0.34	301	1	65	62	-4	89	90	1	91	101	10
EC669	ISOPRENE		1	0.47	1.82	0.38	303	1	56	69	19	66	98	33	70	106	34
OTC309A	ISOPRENE		12	0.21	0.99	0.00	318	0	45	49	8	79	88	10	-	96	
OTC309B	ISOPRENE		12	0.37	0.99	0.00	318	0	40	39	-1	90	95	5	-	112	
OTC316A	ISOPRENE		12	0.42	0.86	0.00	310	0	31	25	-25	65	55	-20	77	66	-17
OTC316B	ISOPRENE		12	0.42	1.70	0.00	310	0	74	73	-1	120	115	-5	124	115	-8
ETC420	A-PINENE		3	0.29	0.54	0.35	299	1	36	39	6	51	50	-2	57	56	-1
ETC443	A-PINENE		3	0.26	0.57	0.35	300	1	41	46	10	54	55	2	61	62	2
ETC444	A-PINENE		3	0.30	0.56	0.35	300	1	40	44	9	51	52	2	58	59	2
ETC446	A-PINENE		3	0.53	0.56	0.35	300	1	19	20	4	43	44	2	55	54	-1
ETC447	A-PINENE		3	0.13	0.56	0.35	300	1	36	38	5	39	41	5	41	45	8
XTC095	A-PINENE		1	0.24	0.59	0.25	302	1	39	39	0	45	45	0	-	47	
OTC318A	A-PINENE		12	0.26	0.43	0.00	310	0	20	20	3	48	48	1	-	55	
ETC421	B-PINENE		3	0.25	0.82	0.35	299	1	7	5	-48	13	14	12	24	41	42

Table B-1 (continued)

Run	Run Type or VOC [a]	Rct'y Type [a]	Char Set [b]	NOx (ppm)	Pr.Eq. (ppm) [c]	k1 (min^{-1}) [d]	T (K) [e]	Ref [f]	Δ (O3-NO) Results (pphm) 2 Hour Expt	2 Hour Calc	2 Hour Δ%	4 Hour Expt	4 Hour Calc	4 Hour Δ%	6 Hour Expt	6 Hour Calc	6 Hour Δ%
ETC433	B-PINENE		3	0.27	0.80	0.35	300	1	4	5	15	11	13	21	21	32	35
ETC434	B-PINENE		3	0.29	2.92	0.35	300	1	16	11	-44	52	71	27	44	64	31
ETC435	B-PINENE		3	0.14	0.84	0.35	301	1	5	6	22	19	37	49	37	48	24
ETC442	B-PINENE		3	0.29	0.82	0.35	301	1	4	5	14	11	13	15	22	29	24
XTC099	B-PINENE		1	0.23	1.59	0.25	304	1	9	4	-101	33	17	-97	46	59	22
OTC318B	B-PINENE		12	0.26	0.53	0.00	310	0	17	5	-234	49	15	-223	-	26	
ETC424	3-CARENE		3	0.25	0.99	0.35	299	1	19	19	4	52	42	-24	57	49	-15
ETC456	3-CARENE		3	0.23	0.83	0.35	300	1	17	15	-7	48	36	-32	54	44	-24
ETC457	3-CARENE		3	0.16	0.88	0.35	301	1	29	24	-22	41	41	2	42	48	13
ETC459	3-CARENE		3	0.50	0.76	0.35	301	1	11	8	-37	30	19	-55	51	30	-72
ETC423	SABINENE		3	0.25	1.15	0.35	299	1	16	22	29	47	49	4	53	55	4
ETC436	SABINENE		3	0.29	1.14	0.35	300	1	12	18	36	43	47	8	51	53	4
ETC437	SABINENE		3	0.58	1.14	0.35	300	1	13	12	-13	34	28	-20	46	38	-19
ETC438	SABINENE		3	0.14	0.59	0.35	300	1	7	12	40	25	27	7	31	31	2
ETC425	D-LIMONE		3	0.25	1.97	0.35	299	1	48	49	1	56	57	1	62	63	3
ETC450	D-LIMONE		3	0.24	1.77	0.35	301	1	49	45	-8	57	54	-6	63	61	-4
ETC451	D-LIMONE		3	0.57	1.69	0.35	301	1	34	40	16	52	48	-8	58	51	-13
ETC452	D-LIMONE		3	0.16	1.76	0.35	301	1	45	43	-4	50	51	3	51	57	10
ITC560	BENZENE		3	0.11	2.84	0.36	301	1	38	46	17	-			-		
ITC561	BENZENE		3	0.11	0.34	0.36	301	1	35	33	-4	-			-		
ITC562	BENZENE		3	0.57	0.36	0.36	301	1	35	8	-340	75	19	-297	80	32	-150
ITC698	BENZENE		6	0.49	0.70	0.35	301	1	34	23	-44	76	61	-25	-		
ITC710	BENZENE		6	0.53	0.70	0.35	300	1	32	20	-58	71	50	-41	73	99	26
ITC831	BENZENE		8	1.01	0.01	0.35	298	1	-1	2		4	5	21	8	8	-5
CTC159A	BENZENE		6	0.26	1.74	0.18	303	0	31	31	-1	56	53	-5	-	49	
CTC159B	BENZENE		6	0.26	0.86	0.18	303	0	13	11	-20	50	38	-33	-	51	
CTC160A	BENZENE		6	0.49	0.96	0.18	302	0	4	8	50	16	22	30	-	45	
CTC160B	BENZENE		6	0.49	1.74	0.18	302	0	8	19	60	38	66	42	-	73	
ITC534	TOLUENE		3	0.53	0.49	0.36	302	1	61	58	-6	87	101	14	-		
ITC699	TOLUENE		6	0.49	0.37	0.35	300	1	59	41	-44	83	85	2	-		
ITC828	TOLUENE		8	1.01	0.01	0.35	297	1	-1	2		5	7	25	13	12	-2
DTC042A	TOLUENE		1	0.99	0.24	0.39	300	1	4	5	25	19	20	7	45	41	-10
DTC042B	TOLUENE		1	0.10	0.13	0.39	300	1	32	27	-19	35	37	7	34	38	9
DTC151A	TOLUENE		3	0.32	0.43	0.25	298	2	36	39	8	65	67	2	59	65	9
DTC155A	TOLUENE		3	0.10	0.16	0.25	298	2	25	21	-22	28	32	13	27	33	18
DTC158A	TOLUENE		3	0.50	0.57	0.25	298	2	41	45	10	87	86	-1	79	89	12
DTC170A	TOLUENE		3	0.49	0.58	0.24	299	2	42	45	8	89	86	-4	81	89	9
XTC106	TOLUENE		1	0.25	0.47	0.25	301	1	57	56	-2	58	61	5	-	60	
CTC026	TOLUENE		1	0.27	0.50	0.20	302	2	45	47	4	54	58	7	-	58	
CTC034	TOLUENE		1	0.52	0.50	0.20	305	2	36	41	14	83	88	6	-	92	
CTC048	TOLUENE		2	0.25	0.22	0.20	301	2	17	18	8	49	46	-7	48	53	9
CTC065	TOLUENE		2	0.66	0.23	0.19	300	2	5	6	6	22	23	4	-	46	
CTC079	TOLUENE		3	0.26	0.12	0.19	298	2	4	5	16	19	20	4	-	32	
EC264	TOLUENE		1	0.44	0.26	0.34	303	1	53	68	22	79	87	9	-		
EC266	TOLUENE		1	0.44	0.27	0.34	302	1	52	68	23	78	86	9	73	81	10
EC269	TOLUENE		1	0.48	0.13	0.34	302	1	32	34	6	51	60	15	69	83	17
EC270	TOLUENE		1	0.47	0.20	0.35	302	1	44	52	15	67	83	19	78	89	13
EC271	TOLUENE		1	0.21	0.26	0.35	302	1	47	57	18	42	54	21	40	50	21
EC273	TOLUENE		1	0.11	0.13	0.40	303	1	30	40	25	29	39	26	28	38	26
EC293	TOLUENE		1	0.49	0.24	0.40	302	1	74	69	-7	77	93	17	72	87	17
EC327	TOLUENE		1	0.49	0.13	0.41	302	1	33	39	17	57	69	17	76	89	15
EC340	TOLUENE		1	0.49	0.12	0.36	302	1	35	33	-4	57	59	3	-		
OTC299A	TOLUENE		11	0.51	0.28	0.00	312	7	56	50	-12	98	111	11	-	114	
OTC299B	TOLUENE		11	0.50	0.12	0.00	312	7	-	9		37	41	11	-	62	
OTC300A	TOLUENE		11	0.52	0.12	0.00	312	7	14	12	-13	54	48	-12	-	71	
OTC300B	TOLUENE		11	0.22	0.12	0.00	312	7	27	30	10	61	64	4	-	67	
DTC223A	C2-BENZ		3	0.26	0.43	0.22	299	2	19	24	24	49	51	3	-	58	
DTC223B	C2-BENZ		3	0.27	0.22	0.22	299	2	9	12	25	26	25	-7	42	35	-19
DTC224A	C2-BENZ		3	0.53	0.45	0.22	298	2	15	15	-3	41	37	-10	-	55	
DTC224B	C2-BENZ		3	0.55	0.20	0.22	298	2	7	7	2	20	17	-12	-	27	
CTC057	C2-BENZ		2	0.27	0.55	0.20	300	2	16	17	7	48	47	-1	50	57	11
CTC092A	C2-BENZ		4	0.27	0.29	0.19	295	2	7	5	-24	23	18	-28	-	29	
CTC092B	C2-BENZ		4	0.27	0.54	0.19	295	2	16	14	-10	43	39	-10	51	57	10

Table B-1 (continued)

Run	Run Type or VOC [a]	Rct'y Type [a]	Char Set [b]	NOx (ppm)	Pr.Eq. (ppm) [c]	k1 (min^{-1}) [d]	T (K) [e]	Ref [f]	Δ (O3-NO) Results (pphm) 2 Hour Expt	2 Hour Calc	2 Hour Δ%	4 Hour Expt	4 Hour Calc	4 Hour Δ%	6 Hour Expt	6 Hour Calc	6 Hour Δ%
CTC098B	C2-BENZ		4	0.49	0.51	0.19	295	2	5	8	29	20	25	21	-	43	
DTC073A	M-XYLENE		1	0.48	0.11	0.39	302	1	10	9	-12	31	27	-14	43	39	-10
DTC188A	M-XYLENE		3	0.55	0.12	0.23	299	2	7	7	0	22	21	-7	35	32	-8
DTC188B	M-XYLENE		3	0.57	0.22	0.23	299	2	24	18	-31	53	42	-26	67	55	-21
DTC189A	M-XYLENE		3	0.25	0.24	0.23	299	2	34	30	-11	56	51	-10	58	57	-3
DTC189B	M-XYLENE		3	0.26	0.11	0.23	299	2	16	13	-26	31	25	-24	40	33	-22
DTC191A	M-XYLENE		3	0.57	0.49	0.23	298	2	57	50	-13	96	87	-11	98	104	5
DTC191B	M-XYLENE		3	0.59	1.01	0.23	298	2	97	94	-4	97	99	3	85	94	9
DTC192A	M-XYLENE		3	0.30	0.49	0.23	298	2	61	56	-9	63	63	0	-	62	
DTC192B	M-XYLENE		3	0.15	0.49	0.23	298	2	40	43	8	37	42	12	35	40	13
DTC193A	M-XYLENE		3	0.13	0.27	0.23	299	2	36	35	-1	37	38	3	35	38	7
DTC193B	M-XYLENE		3	0.13	0.15	0.23	299	2	27	22	-20	39	34	-14	40	35	-13
CTC029	M-XYLENE		1	0.27	0.33	0.20	300	2	38	46	17	62	64	3	63	65	3
CTC035	M-XYLENE		1	0.28	0.15	0.20	301	2	20	18	-10	43	39	-9	57	54	-6
CTC036	M-XYLENE		1	0.51	0.15	0.20	302	2	7	8	15	30	29	-1	45	43	-3
CTC066	M-XYLENE		2	0.56	0.30	0.19	300	2	19	32	41	57	65	13	77	87	12
CTC080	M-XYLENE		3	0.51	0.48	0.19	298	2	52	64	18	93	97	4	92	98	6
CTC094A	M-XYLENE		4	0.49	0.51	0.19	294	2	41	62	33	77	93	18	-	93	
CTC094B	M-XYLENE		4	0.49	0.52	0.19	294	2	44	62	30	78	93	16	-	92	
DTC207A	O-XYLENE		3	0.28	0.17	0.23	299	2	21	24	12	47	43	-9	62	59	-4
DTC207B	O-XYLENE		3	0.30	0.36	0.23	299	2	48	54	11	65	67	4	-	65	
DTC208A	O-XYLENE		3	0.52	0.31	0.23	300	2	35	41	15	76	71	-7	-	98	
DTC208B	O-XYLENE		3	0.56	0.16	0.23	300	2	13	13	3	39	34	-14	53	47	-13
DTC209A	O-XYLENE		3	0.12	0.15	0.23	299	2	27	28	2	-	37		-	38	
DTC209B	O-XYLENE		3	0.13	0.09	0.23	299	2	15	16	11	-	28		-	35	
CTC038	O-XYLENE		1	0.25	0.16	0.20	301	2	16	16	0	47	40	-18	59	57	-4
CTC039	O-XYLENE		1	0.48	0.08	0.20	301	2	3	3	-20	11	10	-10	-	20	
CTC046	O-XYLENE		2	0.50	0.16	0.20	303	2	3	6	48	18	24	26	-	43	
CTC068	O-XYLENE		2	0.26	0.34	0.19	302	2	39	44	12	58	62	6	57	63	9
CTC081	O-XYLENE		3	0.26	0.29	0.19	298	2	35	34	-4	57	60	5	-	62	
CTC091A	O-XYLENE		4	0.28	0.25	0.19	295	2	23	25	7	54	52	-4	-	64	
EC288	O-XYLENE		1	0.50	0.10	0.38	302	1	42	33	-26	59	55	-8	69	68	-1
EC291	O-XYLENE		1	0.49	0.32	0.39	302	1	84	100	16	91	109	17	91	105	13
DTC198A	P-XYLENE		3	0.26	0.24	0.23	299	2	7	10	25	23	23	2	-	36	
DTC198B	P-XYLENE		3	0.27	0.47	0.23	299	2	15	20	26	-	46		-	57	
DTC199A	P-XYLENE		3	0.55	0.47	0.23	299	2	10	12	18	34	32	-6	-	50	
DTC199B	P-XYLENE		3	0.55	0.25	0.23	299	2	8	8	1	23	18	-26	41	29	-40
DTC200A	P-XYLENE		3	0.13	0.22	0.23	299	2	12	14	14	-	30		-	36	
DTC200B	P-XYLENE		3	0.13	0.12	0.23	299	2	8	8	7	19	16	-15	30	24	-26
CTC041	P-XYLENE		1	0.26	0.21	0.20	300	2	5	4	-35	17	13	-32	32	23	-41
CTC043	P-XYLENE		2	0.25	0.11	0.20	301	2	2	2	-17	7	5	-26	14	10	-40
CTC044	P-XYLENE		2	0.51	0.22	0.20	301	2	1	3	50	6	7	21	13	13	3
CTC047	P-XYLENE		2	0.28	0.54	0.20	301	2	9	12	26	37	39	5	-	59	
CTC069	P-XYLENE		2	0.24	1.11	0.19	302	2	17	35	52	57	56	-1	57	53	-8
CTC070	P-XYLENE		2	0.50	1.12	0.19	301	2	10	22	53	50	70	29	93	94	1
DTC201A	124-TMB		3	0.25	0.23	0.23	299	2	13	14	11	31	29	-6	-	41	
DTC203A	124-TMB		3	0.51	0.44	0.23	298	2	15	18	21	44	45	2	-	63	
DTC203B	124-TMB		3	0.54	0.23	0.23	298	2	10	9	-9	29	24	-18	44	36	-22
DTC204A	124-TMB		3	0.12	0.22	0.23	298	2	14	18	21	31	32	5	39	34	-13
DTC204B	124-TMB		3	0.12	0.13	0.23	298	2	9	11	15	20	20	-1	-	27	
CTC056	124-TMB		2	0.25	0.28	0.20	300	2	8	10	18	32	29	-9	50	45	-13
CTC091B	124-TMB		4	0.28	0.58	0.19	295	2	19	23	19	47	52	9	-	59	
CTC093A	124-TMB		4	0.48	0.60	0.19	294	2	13	15	11	43	42	-2	-	64	
CTC093B	124-TMB		4	0.49	1.42	0.19	294	2	35	48	27	74	86	15	-	83	
ITC703	135-TMB		6	0.49	1.23	0.35	301	1	107	105	-3	106	103	-3	-		
ITC706	135-TMB		6	0.47	0.61	0.35	300	1	70	78	10	94	102	7	101	104	3
ITC709	135-TMB		6	0.97	1.10	0.35	301	1	108	123	13	139	170	18	154	173	11
ITC742	135-TMB		7	0.52	1.09	0.35	300	1	-	107		-	106		-		
ITC826	135-TMB		8	0.90	0.01	0.35	297	1	-2	1		19	17	-13	35	34	-5
DTC194A	135-TMB		3	0.26	0.38	0.23	299	2	38	37	-4	57	54	-6	62	59	-5
DTC194B	135-TMB		3	0.28	0.76	0.23	299	2	58	58	1	57	57	-1	-	54	
DTC195A	135-TMB		3	0.55	0.77	0.23	300	2	60	59	-2	91	91	1	93	97	4
DTC195B	135-TMB		3	0.56	0.38	0.23	300	2	33	25	-30	53	43	-21	63	54	-16

Table B-1 (continued)

Run	Run Type or VOC [a]	Rct'y Type [a]	Char Set [b]	NOx (ppm)	Pr.Eq. (ppm) [c]	k1 (min^{-1}) [d]	T (K) [e]	Ref [f]	Δ (O3-NO) Results (pphm) 2 Hour Expt	2 Hour Calc	2 Hour Δ%	4 Hour Expt	4 Hour Calc	4 Hour Δ%	6 Hour Expt	6 Hour Calc	6 Hour Δ%
DTC196A	135-TMB		3	0.13	0.38	0.23	300	2	36	37	3	38	38	0	39	38	-1
DTC196B	135-TMB		3	0.14	0.19	0.23	300	2	27	23	-16	37	32	-14	-	37	
DTC206A	135-TMB		3	0.27	0.32	0.23	299	2	38	33	-18	58	48	-20	63	58	-7
XTC103	135-TMB		1	0.50	0.67	0.25	301	1	77	73	-5	107	102	-4	109	108	-1
CTC030	135-TMB		1	0.52	0.71	0.20	300	2	-	62		-	95		-	103	
CTC050	135-TMB		2	0.27	0.43	0.20	303	2	44	41	-7	56	60	7	-	66	
CTC071	135-TMB		2	0.52	0.73	0.19	300	2	64	62	-3	96	95	-1	-	102	
CTC073	135-TMB		3	0.26	0.39	0.19	297	2	32	36	10	52	55	5	56	60	6
CTC098A	135-TMB		4	0.48	0.44	0.19	295	2	32	32	0	58	55	-6	-	69	
EC901	135-TMB		1	0.49	0.68	0.27	303	1	67	82	19	74	93	21	63	92	32
EC903	135-TMB		1	1.01	1.21	0.27	302	1	111	131	16	127	153	17	124	148	16
DTC211A	123-TMB		3	0.25	0.17	0.23	299	2	28	26	-8	47	41	-15	-	52	
DTC211B	123-TMB		3	0.26	0.39	0.23	299	2	52	52	-1	63	55	-15	-	53	
DTC212A	123-TMB		3	0.51	0.40	0.23	299	2	49	50	1	-	77		-	94	
DTC212B	123-TMB		3	0.54	0.22	0.23	299	2	24	23	-4	49	45	-8	59	56	-5
DTC213A	123-TMB		3	0.11	0.19	0.23	299	2	31	30	-2	-	33		-	34	
DTC213B	123-TMB		3	0.11	0.12	0.23	299	2	18	21	15	30	31	3	35	32	-10
CTC054	123-TMB		2	0.23	0.27	0.20	302	2	35	37	6	53	53	1	54	56	3
CTC075	123-TMB		3	0.52	0.29	0.19	298	2	22	24	10	53	55	3	68	72	6
CTC076	123-TMB		3	0.26	0.23	0.19	297	2	29	27	-7	49	48	-3	58	56	-3
ITC751	NAPHTHAL		7	0.54	0.62	0.35	299	1	15	17	7	32	34	5	44	47	5
ITC755	NAPHTHAL		7	0.27	1.18	0.35	299	1	18	24	24	40	40	0	-	53	
ITC756	NAPHTHAL		7	0.25	2.28	0.35	299	1	28	26	-10	45	42	-5	-		
ITC798	NAPHTHAL		8	0.60	1.62	0.35	298	1	20	30	34	46	53	13	65	69	6
ITC802	NAPHTHAL		8	0.59	0.71	0.35	296	1	18	17	-6	39	35	-11	54	48	-12
ITC739	TETRALIN		7	0.54	0.36	0.35	299	1	8	6	-44	14	13	-10	18	19	6
ITC747	TETRALIN		7	0.54	15.10	0.35	299	1	29	37	22	63	72	13	90	82	-9
ITC748	TETRALIN		7	0.23	13.61	0.35	299	1	31	25	-23	52	47	-11	-		
ITC750	TETRALIN		7	0.54	7.12	0.35	299	1	25	32	22	50	65	23	88	79	-10
ITC832	TETRALIN		8	0.99	0.01	0.35	298	1	10	2	-333	29	49	40	65	98	34
ITC771	23-DMN		7	0.25	1.18	0.35	299	1	31	33	6	48	49	2	-		
ITC774	23-DMN		7	0.56	0.99	0.35	299	1	33	45	26	60	64	6	77	81	5
ITC775	23-DMN		7	0.26	0.42	0.35	299	1	21	22	7	38	34	-11	49	44	-10
ITC806	23-DMN		8	0.38	1.45	0.35	297	1	36	39	7	60	59	-1	63	64	1
ITC1000	ACETYLEN		11	0.10	0.01	0.35	302	1	2	2	-26	42	49	14	54	58	7
ITC1006	ACETYLEN		11	0.27	1.78	0.35	302	1	111	114	3	105	107	1	-		
ITC1007	ACETYLEN		11	0.23	1.92	0.35	301	1	104	106	2	96	99	3	-		
CTC188A	ACETYLEN		7	0.13	0.36	0.16	298	17	4	6	27	20	27	28	46	47	2
CTC188B	ACETYLEN		7	0.13	0.65	0.16	298	17	17	19	12	55	50	-10	-	59	
ITC1549	FORMALD		12	0.37	0.02	0.35	301	1	-1			12	18	33	19	26	26
ITC1554	FORMALD		12	0.44	0.38	0.35	300	1	26	42	39	37	56	34	-		
ITC864	FORMALD		9	0.54	0.01	0.35	299	1	1	1	38	18	25	28	-		
ETC378	FORMALD		3	0.24	0.08	0.35	301	1	5	9	39	9	12	28	11	13	21
ETC441	FORMALD		3	0.27	0.17	0.35	301	1	17	20	15	24	26	9	27	29	6
DTC149A	FORMALD		3	0.32	0.20	0.25	298	2	22	21	-6	32	30	-6	37	35	-6
DTC149B	FORMALD		3	0.34	0.21	0.25	298	2	23	22	-6	33	30	-8	38	35	-8
DTC218A	FORMALD		3	0.28	0.17	0.23	299	2	17	16	-7	26	23	-11	30	27	-12
DTC218B	FORMALD		3	0.29	0.19	0.23	299	2	18	18	-3	-	25		32	29	-10
DTC270A	FORMALD		10	0.28	0.14	0.22	298	3	14	11	-21	20	17	-18	24	21	-16
DTC270B	FORMALD		10	0.27	0.14	0.22	298	3	14	12	-16	20	18	-12	24	22	-11
DTC387A	FORMALD		11	0.26	0.20	0.19	299	11	19	18	-7	28	26	-6	34	32	-7
XTC086	FORMALD		1	0.16	0.21	0.26	302	1	23	23	0	36	36	0	45	45	-1
CTC016	FORMALD		1	0.24	0.34	0.20	303	2	26	29	10	40	44	9	51	54	6
CTC024	FORMALD		1	0.17	0.17	0.20	302	2	13	13	3	21	21	2	26	26	0
CTC077	FORMALD		3	0.16	0.15	0.19	299	2	12	10	-15	19	17	-13	24	21	-14
CTC095A	FORMALD		4	0.26	0.19	0.19	294	2	12	13	9	20	21	7	-	26	
CTC095B	FORMALD		4	0.26	0.19	0.19	294	2	12	13	5	20	21	4	-	26	
CTC116A	FORMALD		5	0.24	0.16	0.19	296	2	12	10	-10	18	17	-7	-	21	
CTC116B	FORMALD		5	0.26	0.16	0.19	296	2	12	10	-18	18	16	-12	-	21	
CTC133A	FORMALD		6	0.26	0.18	0.18	296	2	13	11	-13	20	18	-10	-	23	
CTC133B	FORMALD		6	0.25	0.18	0.18	296	2	13	11	-18	21	18	-12	-	23	
CTC176A	FORMALD		7	0.25	0.18	0.16	299	10	11	10	-12	18	17	-9	-	22	
CTC176B	FORMALD		7	0.25	0.18	0.16	299	10	11	10	-13	19	17	-11	-	22	

Table B-1 (continued)

Run	Run Type or VOC [a]	Rct'y Type [a]	Char Set [b]	NOx (ppm)	Pr.Eq. (ppm) [c]	k1 (min^{-1}) [d]	T (K) [e]	Ref [f]	Δ (O3-NO) Results (pphm) 2 Hour Expt	2 Hour Calc	2 Hour Δ%	4 Hour Expt	4 Hour Calc	4 Hour Δ%	6 Hour Expt	6 Hour Calc	6 Hour Δ%
DTC055B	ACETALD		1	0.14	0.79	0.39	301	1	18	23	19	32	39	18	43	52	17
DTC150A	ACETALD		3	0.14	1.05	0.25	298	2	15	18	14	25	29	13	33	38	14
DTC150B	ACETALD		3	0.15	1.03	0.25	298	2	16	18	9	26	28	7	34	36	6
DTC152B	ACETALD		3	0.20	0.99	0.25	301	2	28	21	-34	49	33	-48	60	42	-42
DTC387B	ACETALD		11	0.26	0.30	0.19	299	11	8	10	15	15	17	10	21	23	8
XTC083	ACETALD		1	0.25	0.62	0.26	302	1	24	26	7	37	39	5	49	51	4
XTC092	ACETALD		1	0.25	0.69	0.25	301	1	20	22	8	31	34	9	41	46	10
CTC014	ACETALD		1	0.23	0.58	0.20	303	2	13	18	29	22	29	23	-	37	
CTC015	ACETALD		1	0.24	0.57	0.20	303	2	12	17	30	20	27	26	-	36	
CTC032	ACETALD		1	0.28	0.70	0.20	301	2	16	19	14	26	29	12	33	37	12
CTC072	ACETALD		3	0.26	0.66	0.19	298	2	15	17	14	24	27	12	-	34	
EC164	ACETALD		1	0.54	0.21	0.35	305	1	23	23	-1	35	36	5	41	46	11
EC254	ACETALD		1	0.11	0.28	0.29	303	1	16	17	7	26	28	6	34	37	8
OTC273B	ACETALD		11	0.30	0.72	0.00	315	8	50	53	6	100	109	8	113	126	10
OTC274A	ACETALD		11	0.28	0.69	0.00	308	8	49	40	-22	86	75	-15	-	95	
OTC305A	ACETALD		12	0.28	0.90	0.00	316	7	58	58	0	104	107	3	-	115	
OTC317B	ACETALD		12	0.26	0.78	0.00	305	0	27	28	4	47	46	-1	-	49	
ITC941	ACROLEIN		10	0.55	0.51	0.35	301	1	15	16	5	28	31	11	37	42	12
ITC944	ACROLEIN		10	0.27	1.24	0.35	301	1	25	23	-8	45	40	-12	65	58	-14
ITC945	ACROLEIN		10	0.52	0.01	0.35	301	1	1	3	61	17	20	16	-		
ITC946	ACROLEIN		10	0.54	1.20	0.35	302	1	68	36	-86	110	78	-42	107	105	-2
ITC513	METHACRO		2	0.57	3.22	0.53	301	1	68	82	17	111	116	4	105	110	5
ITC819	METHACRO		8	0.48	2.21	0.35	298	1	44	45	2	78	74	-6	110	95	-16
ITC823	METHACRO		8	0.51	41.39	0.35	298	1	64	60	-7	108	91	-19	98	80	-22
ETC386	METHACRO		3	0.56	2.83	0.35	301	1	56	57	2	105	97	-8	100	106	6
DTC075A	METHACRO		1	0.50	5.69	0.39	302	1	64	79	19	97	79	-23	85	73	-16
DTC075B	METHACRO		1	0.26	3.09	0.39	302	1	32	51	37	64	58	-9	63	56	-14
XTC094	METHACRO		1	0.49	5.06	0.25	302	1	51	46	-11	85	70	-21	-	70	
XTC102	METHACRO		1	0.24	2.00	0.25	301	1	31	24	-27	55	41	-32	-	57	
EC530	METHACRO		1	0.43	0.96	0.34	301	1	37	40	7	56	60	7	69	77	10
EC651	METHACRO		1	0.45	1.85	0.34	302	1	48	48	1	59	76	23	59	91	35
EC652	METHACRO		1	0.45	1.01	0.34	302	1	44	43	-2	55	64	14	62	83	26
EC655	METHACRO		1	0.80	1.88	0.34	302	1	67	72	7	88	99	10	104	125	16
OTC317A	METHACRO		12	0.25	0.64	0.00	305	0	24	17	-46	44	31	-41	51	36	-42
ETC445	ACETONE		3	0.14	0.08	0.35	300	1	13	15	15	23	28	18	33	41	21
DTC054B	ACETONE		1	0.29	0.13	0.39	301	1	15	20	22	27	35	23	39	51	24
DTC055A	ACETONE		1	0.15	0.17	0.39	301	1	20	25	19	36	46	21	50	61	18
XTC084	ACETONE		1	0.24	0.12	0.26	302	1	24	18	-34	40	31	-29	-	44	
XTC090	ACETONE		1	0.19	0.13	0.25	302	1	20	18	-8	34	31	-10	-	44	
OTC273A	ACETONE		11	0.30	0.14	0.00	315	8	51	42	-21	107	95	-12	-	120	
OTC274B	ACETONE		11	0.27	0.12	0.00	308	8	34	30	-11	71	64	-12	90	89	-2
DTC337A	MEK		11	0.29	0.39	0.21	296	10	26	27	5	39	42	6	51	56	8
DTC337B	MEK		11	0.11	0.39	0.21	296	10	19	20	8	-	33		-	38	
DTC361A	MEK		11	0.10	0.45	0.20	298	10	21	22	4	33	34	3	36	38	5
DTC361B	MEK		11	0.23	0.47	0.20	298	10	27	29	7	43	45	4	59	59	1
CTC178A	MEK		7	0.24	0.44	0.16	298	10	24	23	-5	36	34	-6	-	44	
CTC178B	MEK		7	0.09	0.44	0.16	298	10	17	16	-7	28	26	-7	-	33	
CTC256A	MPK		10	0.20		0.13	296	20	11	12	12	19	19	5	-	25	
CTC256B	C7-KET-2		10	0.20		0.13	296	20	4	4	8	8	8	6	13	13	-1
ITC512	MVK		2	0.60	1.44	0.53	301	1	69	82	16	-	106		100	105	5
ITC815	MVK		8	0.52	1.33	0.35	298	1	53	52	-2	100	93	-7	-		
ITC816	MVK		8	0.51	0.63	0.35	297	1	37	31	-19	64	58	-10	97	88	-10
EC529	MVK		1	0.48	0.70	0.34	301	1	44	52	16	77	87	12	91	97	6
EC644	MVK		1	0.49	0.42	0.34	303	1	54	44	-23	72	71	-2	-		
EC648	MVK		1	0.83	0.65	0.34	303	1	73	66	-11	103	102	-1	104	132	21
EC649	MVK		1	0.46	0.01	0.34	302	1	6	3	-89	51	58	12	62	90	31
EC281	O-CRESOL		1	0.49	0.64	0.37	302	1	18	15	-20	35	37	5	46	49	7
EC289	M-CRESOL		1	0.47	0.48	0.40	302	1	39	16	-137	49	34	-46	51	42	-21
EC290	P-CRESOL		1	0.50	0.59	0.39	302	1	17	18	5	32	37	14	41	46	11
Incremental Reactivity Runs -- VOC Added to Base Case Surrogate																	
ETC483	CO	MRE	3	0.42	1.95	0.35	300	1	45	42	-7	120	116	-3	148	152	3
ETC487	CO	MRE	3	0.46	1.52	0.35	301	1	41	38	-9	112	109	-2	143	152	6

Table B-1 (continued)

Run	Run Type or VOC [a]	Rct'y Type [a]	Char Set [b]	NOx (ppm)	Pr.Eq. (ppm) [c]	k1 (min^{-1}) [d]	T (K) [e]	Ref [f]	Δ (O3-NO) Results (pphm) 2 Hour Expt	2 Hour Calc	2 Hour Δ%	4 Hour Expt	4 Hour Calc	4 Hour Δ%	6 Hour Expt	6 Hour Calc	6 Hour Δ%
ETC416	CO	MR3	3	0.62	1.82	0.35	299	1	31	27	-15	68	65	-4	115	115	0
ETC418	CO	MR3	3	0.52	1.39	0.35	299	1	29	28	-3	66	68	3	114	121	6
DTC014A	CO	MR8	1	0.48	1.83	0.39	301	1	91	79	-14	130	120	-8	146	147	0
DTC015B	CO	MR8	1	0.50	1.89	0.39	301	1	102	80	-28	142	121	-17	153	148	-3
DTC016A	CO	MR8	1	0.48	1.08	0.39	300	1	65	56	-18	99	85	-17	122	111	-10
DTC020B	CO	MR8	1	0.50	1.33	0.39	300	1	66	49	-33	100	81	-23	125	111	-13
DTC029A	CO	R8	1	0.17	1.21	0.39	301	1	74	73	0	84	86	2	84	88	5
CTC105B	CO	MR3	5	0.30	0.45	0.19	296	2	18	21	13	44	53	17	69	80	14
CTC123A	CO	MR8	5	0.40	0.54	0.18	293	2	53	52	0	76	83	8	91	99	8
ETC506	ETHANE	MRE	3	0.41	1.03	0.35	300	1	32	37	13	83	92	10	121	128	5
ETC092	ETHANE	MR3	2	0.51	0.54	0.36	301	1	13	18	27	34	45	23	58	72	20
ETC099	ETHANE	MR3	2	0.50	0.53	0.36	300	1	14	17	17	35	43	19	56	69	18
ETC235	ETHANE	MR3	2	0.49	0.87	0.35	301	1	24	27	11	58	63	8	98	106	7
DTC242A	ETHANE	MR3	10	0.32	0.59	0.23	296	3	15	18	19	36	44	20	59	75	21
ETC226	PROPANE	MR3	2	0.48	0.92	0.35	299	1	14	20	29	40	54	27	71	100	29
ETC230	PROPANE	MR3	2	0.51	1.67	0.35	300	1	25	25	0	63	66	5	114	123	7
ETC305	PROPANE	MR3	2	0.54	1.27	0.35	301	1	19	19	-2	53	50	-5	100	92	-8
ETC484	N-C4	MRE	3	0.46	2.04	0.35	300	1	45	27	-65	121	89	-36	139	142	2
ETC488	N-C4	MRE	3	0.42	1.53	0.35	300	1	32	26	-24	95	78	-21	132	131	-1
ETC094	N-C4	MR3	2	0.48	1.02	0.36	301	1	13	16	23	33	42	21	57	72	21
ETC097	N-C4	MR3	2	0.50	0.94	0.36	301	1	14	16	10	35	42	17	62	72	14
ETC135	N-C4	MR3	2	0.52	0.89	0.35	301	1	11	13	16	31	35	12	53	60	11
ETC224	N-C4	MR3	2	0.50	1.41	0.35	300	1	20	18	-8	52	51	-3	93	93	0
ETC389	N-C4	R3	3	0.16	0.72	0.35	301	1	20	22	13	55	58	6	72	76	5
ETC393	N-C4	R3	3	0.16	0.69	0.35	300	1	19	21	11	56	56	0	74	75	2
DTC019B	N-C4	MR8	1	0.46	1.00	0.39	300	1	72	67	-7	107	103	-4	130	132	2
DTC031A	N-C4	R8	1	0.17	0.93	0.39	301	1	70	72	2	80	83	3	79	83	5
ETC201	N-C6	MR3	2	0.50		0.35	300	1	11	10	-9	30	29	-5	55	52	-5
ETC209	N-C6	MR3	2	0.51	0.74	0.35	299	1	-	9		25	27	7	47	49	3
DTC072A	N-C6	MRE	1	0.47	1.16	0.39	302	1	14	11	-23	41	33	-22	91	73	-26
ETC237	N-C8	MR3	2	0.48	0.95	0.35	301	1	6	5	-12	18	14	-25	34	26	-29
ETC239	N-C8	MR3	2	0.53	0.92	0.35	301	1	6	6	-6	18	15	-16	34	28	-21
DTC024B	N-C8	MR8	1	0.50	0.75	0.39	301	1	41	35	-16	72	63	-14	100	85	-17
DTC070A	N-C8	MR8	1	0.49	0.63	0.39	301	1	38	36	-6	66	63	-4	87	86	-1
DTC037B	N-C8	R8	1	0.18	0.77	0.39	301	1	54	55	1	66	73	9	67	76	12
DTC071B	N-C8	R8	1	0.18	0.56	0.39	302	1	52	49	-7	65	69	7	65	74	12
CTC110B	N-C8	MR3	5	0.30	0.57	0.19	296	2	8	9	11	26	30	13	-	55	
CTC131A	N-C8	MR8	5	0.39	0.87	0.18	293	2	32	26	-23	56	58	5	70	76	8
DTC271B	N-C12	MR3	10	0.30	0.57	0.22	298	4	7	7	2	23	23	2	38	43	13
DTC273A	N-C12	MR3	10	0.31	0.52	0.22	298	4	9	9	-5	28	26	-6	49	48	-1
DTC283B	N-C12	MR3	10	0.32	0.61	0.22	297	4	6	7	19	18	22	17	34	41	18
DTC272A	N-C12	MR8	10	0.14	0.42	0.22	298	4	24	28	16	36	42	14	26	48	45
DTC274B	N-C12	MR8	10	0.16	0.40	0.22	298	4	28	29	5	42	44	5	47	51	7
DTC284A	N-C12	MR8	10	0.15	0.48	0.22	298	4	28	32	13	42	45	8	47	49	6
DTC293A	N-C12	R8	10	0.08	0.50	0.22	297	4	26	29	9	31	31	0	31	30	-2
CTC150B	N-C12	MR8	6	0.42	0.68	0.18	299	4	30	24	-24	58	55	-5	74	73	-2
CTC154A	N-C12	MR8	6	0.42	0.87	0.18	301	4	32	22	-49	61	56	-9	77	74	-3
DTC275A	N-C14	MR3	10	0.32	0.58	0.22	298	4	6	6	-7	19	18	-7	35	34	-3
DTC277B	N-C14	MR3	10	0.31	0.57	0.22	298	4	7	12	40	23	35	35	42	64	34
DTC289B	N-C14	MR3	10	0.35	0.67	0.22	297	4	5	5	13	14	15	9	26	29	10
DTC276B	N-C14	MR8	10	0.17	0.48	0.22	298	4	29	29	0	44	45	3	50	53	5
DTC278A	N-C14	MR8	10	0.16	0.44	0.22	298	4	29	35	18	43	48	10	49	51	4
DTC290A	N-C14	MR8	10	0.17	0.48	0.22	298	4	24	31	20	39	46	15	45	52	14
CTC151A	N-C14	MR8	6	0.50	0.71	0.18	303	4	34	27	-22	55	54	-2	68	68	1
CTC158A	N-C14	MR8	6	0.36	0.92	0.18	304	4	22	18	-22	52	53	1	68	72	4
DTC279B	N-C15	MR3	10	0.32	0.64	0.22	298	4	4	6	30	15	19	20	31	36	16
DTC280A	N-C15	MR8	10	0.16	0.43	0.22	298	4	26	32	20	40	47	14	46	51	11
DTC282A	N-C16	MR3	10	0.33	0.56	0.22	299	4	8	10	21	23	29	22	40	52	23
DTC291B	N-C16	MR3	10	0.33	0.70	0.22	297	4	5	5	-4	14	14	-5	28	27	-4
DTC281B	N-C16	MR8	10	0.16	0.49	0.22	298	4	26	28	7	41	45	9	48	52	8
CTC152B	N-C16	MR8	6	0.37	0.65	0.18	301	4	22	17	-29	43	43	0	-	55	
CTC156B	N-C16	MR8	6	0.41	0.88	0.18	303	4	25	16	-52	52	49	-6	65	67	3
ETC228	2-ME-C3	MR3	2	0.51	0.67	0.35	300	1	14	18	23	41	49	18	72	90	20

Table B-1 (continued)

Run	Run Type or VOC [a]	Rct'y Type [a]	Char Set [b]	NOx (ppm)	Pr.Eq. (ppm) [c]	k1 (min^{-1}) [d]	T (K) [e]	Ref [f]	Δ (O3-NO) Results (pphm) 2 Hour Expt	2 Hour Calc	2 Hour Δ%	4 Hour Expt	4 Hour Calc	4 Hour Δ%	6 Hour Expt	6 Hour Calc	6 Hour Δ%
ETC232	2-ME-C3	MR3	2	0.51	2.31	0.35	299	1	21	19	-7	63	53	-19	133	116	-16
ETC241	2-ME-C3	MR3	2	0.48	1.32	0.35	301	1	17	20	13	54	54	0	119	115	-3
ETC303	2-ME-C3	MR3	2	0.45	0.96	0.35	300	1	13	18	29	41	49	17	88	100	11
ETC291	224TM-C5	MR3	2	0.50	1.81	0.35	303	1	13	13	2	43	41	-6	102	94	-8
ETC293	224TM-C5	MR3	2	0.49	1.92	0.35	302	1	12	12	-4	42	39	-8	99	90	-10
DTC733A	26DM-C8	MR4	18	0.30	0.53	0.16	296	21	4	3	-37	12	7	-76	23	12	-82
DTC749A	26DM-C8	MR4	18	0.38	0.55	0.16	298	21	6	5	-39	20	12	-72	36	22	-69
DTC738B	26DM-C8	MR8	18	0.31	0.41	0.16	293	21	18	13	-41	42	36	-19	55	49	-12
DTC747A	26DM-C8	MR8	18	0.29	0.42	0.16	299	21	16	13	-22	44	43	-4	59	58	-3
DTC739A	26DM-C8	R8	18	0.10	0.39	0.16	295	21	27	29	7	31	34	10	30	35	12
DTC734B	2-ME-C9	MR3	18	0.40	0.50	0.16	295	21	5	3	-70	13	6	-116	24	10	-133
DTC741A	2-ME-C9	MR3	18	0.38	0.48	0.16	295	21	5	4	-27	14	9	-52	27	17	-63
DTC737A	2-ME-C9	MR8	18	0.32	0.43	0.16	294	21	17	12	-37	42	36	-16	55	51	-7
DTC746B	2-ME-C9	MR8	18	0.30	0.44	0.16	298	21	13	12	-8	39	39	-1	53	54	3
DTC740B	2-ME-C9	R8	18	0.10	0.39	0.16	295	21	24	27	10	28	33	14	28	34	19
DTC725A	34-DE-C6	MR4	18		0.51	0.16	295	21	9	8	-14	29	22	-29	47	37	-28
DTC730A	34-DE-C6	MR4	18	0.30	0.51	0.16	296	21	6	4	-50	18	11	-69	32	20	-56
DTC726B	34-DE-C6	MR8	18	0.29	0.43	0.16	294	21	22	22	1	42	42	0	54	53	-2
DTC729B	34-DE-C6	MR8	18	0.24	0.40	0.16	294	21	15	15	-3	39	43	8	52	55	6
DTC732B	34-DE-C6	R8	18	0.08	0.41	0.16	296	21	-	26		30	30	2	29	30	5
DTC748B	34-DE-C6	R8	18	0.09	0.41	0.16	297	21	25	28	12	28	33	16	27	34	20
DTC541A	CYCC6	MR3	14	0.38	0.76	0.21	299	10	8	9	13	24	25	5	45	45	2
DTC551A	CYCC6	MR3	14	0.38	0.93	0.20	300	10	8	7	-10	21	18	-13	37	32	-14
DTC543B	CYCC6	MR8	15	0.30	0.96	0.21	299	10	42	38	-8	65	61	-6	81	77	-5
DTC552B	CYCC6	MR8	15	0.31	0.73	0.20	300	10	36	26	-39	64	52	-21	81	69	-18
DTC544A	CYCC6	R8	14	0.13	0.63	0.21	299	10	40	38	-5	49	48	-3	52	50	-3
DTC553A	CYCC6	R8	14	0.13	0.78	0.20	300	10	41	40	-4	51	50	-3	54	53	-3
DTC315B	C6-CYCC6	MR3	11	0.33	0.62	0.21	298	5	8	6	-19	21	18	-12	36	34	-5
DTC318B	C6-CYCC6	MR3	11	0.33	0.57	0.21	297	5	7	8	12	21	24	13	37	43	14
DTC317A	C6-CYCC6	MR8	11	0.17	0.54	0.21	297	5	27	28	3	41	44	6	46	52	11
DTC319B	C6-CYCC6	MR8	11	0.18	0.57	0.21	297	5	20	21	2	37	39	5	45	50	10
CTC167A	C6-CYCC6	MR8	7	0.41	0.95	0.18	300	5	28	22	-28	58	58	0	-	76	
CTC233A	C6-CYCC6	R8	9	0.17	0.85	0.14	299	5	37	40	7	44	47	7	-	48	
DTC324A	C8-CYCC6	MR3	11	0.32	0.59	0.21	298	5	9	10	18	25	30	16	44	55	20
DTC325B	C8-CYCC6	R8	11	0.18	0.68	0.21	299	5	25	29	12	40	46	14	46	55	16
CTC231A	C8-CYCC6	MR3	9	0.27	0.70	0.14	303	5	4	5	30	12	14	17	24	26	8
CTC168B	C8-CYCC6	MR8	7	0.41	0.96	0.18	300	5	27	22	-24	55	58	6	-	77	
CTC232B	C8-CYCC6	MR8	9	0.46	0.81	0.14	301	5	14	16	12	38	46	18	54	64	16
CTC239B	C8-CYCC6	MR8	9	0.44	1.01	0.13	301	5	18	17	-4	48	51	6	61	69	11
CTC240A	C8-CYCC6	R8	9	0.17	1.01	0.13	300	5	33	37	11	41	45	10	43	47	9
ETC199	ETHENE	MR3	2		0.52	0.35	301	1	23	22	-3	65	61	-7	120	108	-11
ETC203	ETHENE	MR3	2	0.52	0.46	0.35	301	1	20	19	-2	54	52	-2	96	90	-6
DTC017A	ETHENE	MR8	1	0.48	0.56	0.39	300	1	56	53	-5	94	88	-6	119	118	-1
DTC038A	ETHENE	R8	1	0.17	0.57	0.39	301	1	63	65	3	65	69	5	62	66	6
ETC496	PROPENE	MRE	3	0.38	0.82	0.35	301	1	45	57	22	111	117	5	123	121	-2
ETC500	PROPENE	MRE	3	0.42	0.76	0.35	300	1	35	43	19	100	113	12	127	131	3
ETC106	PROPENE	MR3	2	0.52	0.44	0.36	300	1	14	17	15	39	45	13	65	73	11
ETC108	PROPENE	MR3	2	0.52	0.45	0.36	300	1	14	16	12	37	43	16	59	71	17
ETC110	PROPENE	MR3	2	0.52	0.42	0.36	300	1	13	15	11	36	41	11	62	67	7
ETC118	PROPENE	MR3	2	0.50	0.49	0.36	302	1	14	20	28	39	53	26	70	90	23
DTC018A	PROPENE	MR8	1	0.48	0.71	0.39	301	1	73	65	-13	109	104	-6	117	124	6
DTC032B	PROPENE	R8	1	0.17	0.66	0.39	300	1	61	63	3	59	64	7	59	64	8
CTC142B	PROPENE	MR3	6	0.37	0.49	0.18	295	2	9	10	10	26	31	16	-	55	
CTC130B	PROPENE	MR8	5	0.39	0.86	0.18	293	2	52	53	3	79	83	5	84	87	4
ETC253	ISOBUTEN	MR3	2	0.48	0.81	0.35	301	1	29	26	-14	81	81	0	122	125	2
ETC255	ISOBUTEN	MR3	2	0.48	0.79	0.35	302	1	29	27	-10	80	83	4	121	127	5
ETC257	ISOBUTEN	MR3	2	0.48	0.62	0.35	301	1	22	20	-10	57	57	1	97	101	4
ETC493	T-2-BUTE	MRE	3	0.42	0.93	0.35	301	1	93	95	2	122	127	4	123	127	3
ETC501	T-2-BUTE	MRE	3	0.42	0.72	0.35	300	1	64	67	5	110	118	7	127	133	4
ETC307	T-2-BUTE	MR3	2	0.54	0.60	0.35	300	1	52	46	-12	81	73	-10	109	102	-7
ETC309	T-2-BUTE	MR3	2	0.52	0.53	0.35	301	1	44	37	-18	75	66	-14	105	93	-14
DTC043B	T-2-BUTE	MRE	1	0.47	0.79	0.39	300	1	72	73	2	122	125	2	141	146	3
DTC021B	T-2-BUTE	MR8	1	0.49	1.06	0.39	300	1	90	87	-3	107	110	3	112	124	10

Table B-1 (continued)

Run	Run Type or VOC [a]	Rct'y Type [a]	Char Set [b]	NOx (ppm)	Pr.Eq. (ppm) [c]	k1 (min^{-1}) [d]	T (K) [e]	Ref [f]	Δ (O3-NO) Results (pphm) 2 Hour Expt	2 Hour Calc	2 Hour Δ%	4 Hour Expt	4 Hour Calc	4 Hour Δ%	6 Hour Expt	6 Hour Calc	6 Hour Δ%
DTC069A	T-2-BUTE	MR8	1	0.48	0.72	0.39	302	1	69	66	-5	89	90	1	106	112	5
DTC041A	T-2-BUTE	RE	1	0.17	0.79	0.39	300	1	71	75	5	76	82	7	70	76	8
DTC033A	T-2-BUTE	R8	1	0.17	0.65	0.39	300	1	55	58	4	58	61	5	59	63	6
ETC495	ISOPRENE	MRE	3	0.42	1.28	0.35	300	1	42	55	24	106	119	11	131	126	-4
ETC503	ISOPRENE	MRE	3	0.42	1.61	0.35	301	1	65	80	20	119	119	0	126	113	-11
ETC510	ISOPRENE	MRE	3	0.41	1.43	0.35	300	1	45	64	30	109	118	8	127	118	-7
ETC271	ISOPRENE	MR3	2	0.49	0.98	0.35	299	1	31	31	2	78	73	-7	118	115	-3
ETC273	ISOPRENE	MR3	2	0.49	0.92	0.35	301	1	31	32	1	80	74	-8	121	115	-4
ETC275	ISOPRENE	MR3	2	0.49	0.79	0.35	302	1	29	27	-4	73	64	-14	117	106	-11
ETC277	ISOPRENE	MR3	2	0.50	0.67	0.35	302	1	26	25	-7	68	59	-16	113	97	-16
DTC047B	ISOPRENE	MRE	1	0.48	1.02	0.39	301	1	36	39	8	102	106	4	145	146	1
DTC046A	ISOPRENE	RE	1	0.17	1.04	0.19	300	1	14	18	22	48	53	9	55	55	-1
DTC050B	ISOPRENE	RE	1	0.16	0.99	0.39	301	1	50	55	11	78	76	-2	76	71	-7
ETC508	A-PINENE	MRE	3	0.41	0.82	0.35	301	1	54	66	19	103	111	8	121	124	2
DTC045B	A-PINENE	MRE	1	0.48	0.79	0.39	301	1	40	48	17	105	111	5	140	145	4
DTC044A	A-PINENE	RE	1	0.16	0.79	0.39	300	1	58	64	9	73	77	5	70	73	5
DTC034B	A-PINENE	R8	1	0.16	0.93	0.39	301	1	49	49	1	48	49	3	46	50	8
DTC051B	B-PINENE	MRE	1	0.48	0.92	0.39	301	1	16	18	9	52	73	28	118	134	12
DTC048A	B-PINENE	RE	1	0.17	0.91	0.39	301	1	18	36	50	66	78	15	70	80	12
ETC263	BENZENE	MR3	2	0.48	0.73	0.35	303	1	24	30	19	82	92	11	91	110	17
ETC265	BENZENE	MR3	2	0.49	0.69	0.35	300	1	23	26	11	67	76	12	96	114	16
DTC039B	BENZENE	R8	1	0.18	0.76	0.39	301	1	53	60	13	50	57	13	47	54	13
ETC101	TOLUENE	MR3	2	0.50	0.38	0.36	300	1	13	16	19	39	43	8	65	71	9
ETC103	TOLUENE	MR3	2	0.52	0.38	0.36	301	1	14	14	5	40	42	6	68	70	4
DTC023A	TOLUENE	MR8	1	0.47	0.52	0.39	301	1	60	57	-6	100	94	-7	108	114	6
DTC030B	TOLUENE	R8	1	0.17	0.64	0.39	300	1	50	55	9	48	54	10	47	53	11
CTC108B	TOLUENE	MR3	5	0.31	0.54	0.19	295	2	19	24	20	53	60	11	-	76	
CTC127B	TOLUENE	MR8	5	0.39	0.65	0.18	293	2	46	49	7	68	77	12	-	83	
ETC311	C2-BENZ	MR3	2	0.52	0.42	0.35	297	1	11	12	9	36	38	4	61	62	2
ETC313	C2-BENZ	MR3	2	0.53	0.40	0.35	298	1	13	12	-8	38	35	-7	64	58	-10
ETC315	C2-BENZ	MR3	2	0.53	0.44	0.35	298	1	14	14	3	45	42	-7	78	70	-12
ETC196	M-XYLENE	MR3	2	0.48		0.35	300	1	19	24	23	54	61	11	92	101	9
ETC207	M-XYLENE	MR3	2	0.51		0.35	299	1	21	23	10	59	58	0	98	96	-2
ETC301	M-XYLENE	MR3	2	0.46	0.43	0.35	300	1	19	23	17	56	58	4	97	98	1
DTC025A	M-XYLENE	MR8	1	0.47	0.50	0.39	302	1	57	56	-2	91	90	0	114	116	2
DTC068B	M-XYLENE	MR8	1	0.48	0.43	0.39	301	1	47	47	0	75	74	-1	100	101	2
DTC035A	M-XYLENE	R8	1	0.17	0.49	0.39	301	1	54	55	2	55	56	2	56	57	2
DTC067B	M-XYLENE	R8	1	0.17	0.52	0.39	301	1	54	55	4	54	56	4	53	56	5
CTC109A	M-XYLENE	MR3	5	0.31	0.51	0.19	295	2	37	25	-44	49	61	19	-	78	
CTC128A	M-XYLENE	MR8	5	0.41	0.64	0.18	294	2	43	49	11	66	76	12	-	87	
ETC259	O-XYLENE	MR3	2	0.49	0.44	0.35	300	1	22	20	-6	56	54	-3	95	93	-1
ETC261	O-XYLENE	MR3	2	0.48	0.44	0.35	301	1	21	22	1	57	57	0	100	100	0
ETC348	P-XYLENE	MR3	2	0.52	0.49	0.35	303	1	23	23	0	63	61	-4	107	104	-3
ETC267	124-TMB	MR3	2	0.49	0.45	0.35	300	1	21	18	-16	54	49	-9	93	85	-9
ETC269	124-TMB	MR3	2	0.48	0.45	0.35	302	1	23	20	-11	59	54	-9	102	93	-10
ETC249	135-TMB	MR3	2	0.49	0.57	0.35	301	1	35	35	1	85	83	-2	126	126	0
ETC297	123-TMB	MR3	2	0.46	0.45	0.35	301	1	34	32	-9	86	73	-17	122	113	-8
ETC299	123-TMB	MR3	2	0.48	0.44	0.35	301	1	29	27	-8	76	65	-17	117	105	-11
CTC246A	STYRENE	MR3	9	0.25	1.60	0.13	295	6	5	4	-9	15	13	-15	30	25	-19
CTC250B	STYRENE	MR3	9	0.23	0.96	0.13	296	6	4	6	27	15	18	13	29	32	8
CTC248B	STYRENE	MR8	9	0.31	1.72	0.13	292	6	37	45	18	54	61	12	61	62	1
CTC251A	STYRENE	MR8	9	0.35	2.22	0.13	294	6	37	46	20	52	64	19	58	62	7
CTC249A	STYRENE	R8	9	0.16	1.74	0.13	295	6	32	33	5	31	31	0	28	28	-2
CTC253B	STYRENE	R8	9	0.16	1.30	0.13	295	6	35	37	3	38	36	-3	36	34	-6
CTC184B	ACETYLEN	MR3	7	0.23	0.91	0.16	298	17	34	28	-22	74	66	-13	81	73	-11
CTC185A	ACETYLEN	MR3	7	0.27	0.95	0.16	301	17	42	31	-33	85	74	-15	92	82	-12
CTC192A	ACETYLEN	MR3	7	0.22	0.67	0.16	298	17	20	18	-16	61	52	-16	77	67	-14
CTC186B	ACETYLEN	MR8	7	0.37	0.77	0.16	298	17	41	42	3	74	74	0	89	86	-4
CTC193B	ACETYLEN	MR8	7	0.37	0.92	0.16	298	17	51	49	-3	85	82	-3	93	89	-4
CTC187A	ACETYLEN	R8	7	0.15	0.85	0.16	298	17	43	41	-4	47	44	-6	46	42	-8
CTC194A	ACETYLEN	R8	8	0.15	1.06	0.16	297	17	44	43	-3	48	46	-6	47	43	-9
ETC285	MEOH	MR3	2	0.52	0.66	0.35	303	1	24	24	-1	71	66	-7	127	120	-6
ETC287	MEOH	MR3	2	0.51	0.41	0.35	303	1	17	17	2	48	46	-5	85	77	-11

Table B-1 (continued)

Run	Run Type or VOC [a]	Rct'y Type [a]	Char Set [b]	NOx (ppm)	Pr.Eq. (ppm) [c]	k1 (min^{-1}) [d]	T (K) [e]	Ref [f]	Δ (O3-NO) Results (pphm) 2 Hour Expt	2 Hour Calc	2 Hour Δ%	4 Hour Expt	4 Hour Calc	4 Hour Δ%	6 Hour Expt	6 Hour Calc	6 Hour Δ%
ETC289	MEOH	MR3	2	0.50	0.47	0.35	304	1	20	20	0	58	53	-10	105	93	-14
ETC131	ETOH	MR3	2	0.54	0.70	0.35	302	1	14	15	8	37	41	9	60	64	7
ETC133	ETOH	MR3	2	0.53	0.66	0.35	302	1	13	15	12	38	39	5	60	62	3
ETC138	ETOH	MR3	2	0.54	0.70	0.35	300	1	13	14	10	35	38	9	56	60	8
ETC148	I-C3-OH	MR3	2	0.51	1.19	0.35	302	1	19	20	8	47	49	2	82	81	-1
ETC155	I-C3-OH	MR3	2	0.50	0.67	0.35	300	1	22	19	-12	55	50	-9	93	85	-10
ETC157	I-C3-OH	MR3	2	0.51	0.60	0.35	300	1	19	17	-7	46	47	1	78	79	2
ETC159	I-C3-OH	MR3	2	0.50	0.65	0.35	301	1	18	19	2	47	50	5	81	85	4
DTC395A	I-C3-OH	MR3	11	0.40	2.39	0.19	299	10	25	25	-3	64	57	-12	96	93	-3
DTC398B	I-C3-OH	MR3	11	0.43	0.98	0.19	297	10	19	15	-31	47	36	-30	80	61	-32
DTC396B	I-C3-OH	MR8	11	0.29	2.52	0.19	299	10	63	70	10	81	91	11	77	100	23
DTC399A	I-C3-OH	MR8	11	0.27	0.75	0.19	298	10	40	37	-10	62	55	-11	72	68	-6
DTC397A	I-C3-OH	R8	11	0.13	1.36	0.19	298	10	45	45	1	50	55	10	47	59	20
DTC400B	I-C3-OH	R8	11	0.11	0.79	0.19	298	10	39	37	-5	44	44	0	43	46	7
DTC233A	T-C4-OH	MR3	10	0.30	0.75	0.23	296	3	15	18	15	40	48	18	69	82	16
DTC241B	T-C4-OH	MR3	10	0.32	0.95	0.23	295	3	16	15	-8	39	41	6	68	78	14
DTC249A	T-C4-OH	MR8	10	0.25	0.82	0.23	297	3	40	54	26	61	80	24	72	91	20
DTC256A	T-C4-OH	MR8	10	0.26	0.62	0.23	297	3	33	42	21	51	67	25	54	82	34
DTC259A	T-C4-OH	R8	10	0.16	0.70	0.23	297	3	39	48	19	51	62	19	54	67	19
DTC268A	T-C4-OH	R8	10	0.16	0.59	0.22	299	3	39	46	14	52	60	13	54	64	15
DTC269A	T-C4-OH	R8	10	0.17	0.75	0.22	299	3	45	51	12	57	66	13	59	70	15
DTC508B	1-C8-OH	MR3	15	0.37	0.93	0.22	299	10	5	6	6	15	15	-1	30	28	-7
DTC529A	1-C8-OH	MR3	14	0.36	0.54	0.21	299	10	9	10	5	27	26	-2	49	46	-7
DTC509A	1-C8-OH	MR8	14	0.30	0.50	0.22	299	10	32	26	-23	55	49	-13	70	64	-10
DTC519B	1-C8-OH	R8	15	0.12	0.60	0.21	298	10	35	36	3	43	45	4	45	47	5
DTC517A	2-C8-OH	MR3	14	0.37		0.21	299	10	10	11	6	32	30	-6	60	54	-12
DTC521B	2-C8-OH	MR8	15	0.30		0.21	299	10	34	31	-11	59	57	-4	74	72	-2
DTC524B	2-C8-OH	R8	15	0.13		0.21	299	10	38	37	-1	45	46	1	46	48	4
DTC514B	3-C8-OH	MR3	15	0.38		0.21	299	10	9	10	9	28	27	-3	52	48	-7
DTC516B	3-C8-OH	MR8	15	0.32		0.21	299	10	34	33	-3	55	53	-3	70	68	-3
DTC520A	3-C8-OH	R8	14	0.13		0.21	299	10	38	38	0	46	47	3	46	49	7
DTC385A	PR-GLYCL	MR3	11	0.39	2.50	0.19	298	11	27	28	1	64	58	-10	94	87	-8
DTC389B	PR-GLYCL	MR3	11	0.36	1.31	0.19	299	11	20	20	3	48	46	-5	78	74	-5
DTC386B	PR-GLYCL	MR8	11	0.29	1.17	0.19	298	11	49	45	-8	69	63	-9	76	74	-3
DTC390A	PR-GLYCL	MR8	11	0.28	1.01	0.19	297	11	43	42	-2	64	60	-6	75	72	-3
DTC388A	PR-GLYCL	R8	11	0.11	1.26	0.19	298	11	39	38	-2	45	44	0	43	45	4
DTC391B	PR-GLYCL	R8	11	0.11	0.80	0.19	297	11	37	34	-8	42	40	-6	41	40	-3
ETC279	ME-O-ME	MR3	2	0.50	0.85	0.35	303	1	28	27	-5	75	67	-11	132	121	-9
ETC281	ME-O-ME	MR3	2	0.51	0.77	0.35	303	1	25	25	2	66	63	-5	121	114	-6
ETC283	ME-O-ME	MR3	2	0.51	0.63	0.35	303	1	24	23	-3	65	59	-11	117	103	-13
ETC295	ME-O-ME	MR3	2	0.48	0.62	0.35	301	1	21	24	11	56	59	4	102	103	1
DTC510B	ET-O-ET	MR3	15	0.39	0.84	0.22	299	10	19	21	11	53	56	4	99	97	-2
DTC522A	ET-O-ET	MR3	14	0.37	1.34	0.21	299	10	23	28	18	73	79	8	116	115	-1
DTC511A	ET-O-ET	MR8	14	0.31	1.30	0.21	299	10	78	88	11	107	114	6	109	120	10
DTC515A	ET-O-ET	MR8	14	0.31	0.65	0.21	299	10	57	49	-16	87	76	-15	101	93	-9
DTC513A	ET-O-ET	R8	14	0.13	0.72	0.21	298	10	49	50	2	57	59	3	57	60	5
DTC525A	ET-O-ET	R8	14	0.13	0.56	0.21	299	10	46	44	-3	53	53	-1	54	54	0
ETC120	MTBE	MR3	2	0.53		0.35	301	1	12	14	12	33	38	15	56	66	15
ETC123	MTBE	MR3	2	0.52		0.35	305	1	16	17	6	44	46	5	81	85	4
ETC125	MTBE	MR3	2	0.51		0.35	302	1	10	14	27	31	40	21	55	70	21
ETC127	MTBE	MR3	2	0.53		0.35	302	1	12	13	7	34	37	8	58	64	9
DTC489A	MEOC3OH	MR3	14	0.38	2.05	0.22	298	15	31	28	-11	71	63	-14	104	95	-10
DTC495A	MEOC3OH	MR3	14	0.38	1.33	0.22	299	15	25	25	-1	59	56	-5	94	88	-6
DTC492A	MEOC3OH	MR8	14	0.31	1.39	0.22	298	15	58	61	4	80	81	2	91	92	1
DTC500A	MEOC3OH	MR8	14	0.30	0.93	0.22	298	15	49	52	5	70	71	2	82	83	2
DTC496B	MEOC3OH	R8	15	0.12	1.13	0.22	299	15	47	45	-3	53	53	0	52	54	3
DTC501B	MEOC3OH	R8	15	0.13	0.85	0.22	299	15	45	43	-3	51	50	0	51	52	2
ETC163	ETO-ETOH	MR3	2	0.49		0.35	302	1	27	35	22	80	91	12	143	142	-1
ETC171	ETO-ETOH	MR3	2	0.49	1.03	0.35	301	1	21	27	20	62	71	13	122	122	0
ETC175	ETO-ETOH	MR3	2	0.50		0.35	298	1	18	21	15	49	57	14	91	99	8
DTC491B	BUO-ETOH	MR3	15	0.38	1.44	0.22	298	15	15	11	-34	42	34	-23	85	73	-17
DTC498B	BUO-ETOH	MR3	15	0.38	0.93	0.22	299	15	9	8	-14	24	22	-8	42	42	-1
DTC505B	BUO-ETOH	MR3	15	0.38	1.07	0.22	298	15	12	11	-1	35	34	-1	69	69	-1

Table B-1 (continued)

Run	Run Type or VOC [a]	Rct'y Type [a]	Char Set [b]	NOx (ppm)	Pr.Eq. (ppm) [c]	k1 (min^{-1}) [d]	T (K) [e]	Ref [f]	Δ (O3-NO) Results (pphm) 2 Hour Expt	2 Hour Calc	2 Hour Δ%	4 Hour Expt	4 Hour Calc	4 Hour Δ%	6 Hour Expt	6 Hour Calc	6 Hour Δ%
DTC493B	BUO-ETOH	MR8	15	0.30	0.99	0.22	297	15	57	59	5	85	87	2	97	98	2
DTC502A	BUO-ETOH	MR8	14	0.30	0.67	0.22	299	15	52	47	-11	78	73	-7	91	88	-4
DTC497A	BUO-ETOH	R8	14	0.13	0.87	0.22	299	15	48	48	-2	57	57	0	57	59	3
DTC506A	BUO-ETOH	R8	14	0.12	0.70	0.22	298	15	44	43	-3	52	51	-2	53	52	-1
ETC166	CARBITOL	MR3	2	0.51	1.43	0.35	304	1	19	19	-1	56	56	0	112	109	-2
ETC169	CARBITOL	MR3	2	0.51	1.21	0.35	300	1	16	15	-11	44	44	-1	82	81	-1
ETC173	CARBITOL	MR3	2	0.51	2.29	0.35	300	1	15	14	-4	42	45	6	87	97	10
DTC327A	ME-ACET	MR3	11	0.34	0.64	0.21	297	9	15	18	18	40	44	11	67	76	11
DTC328B	ME-ACET	MR3	11	0.32	0.72	0.21	297	9	13	19	30	37	47	21	66	79	16
DTC336A	ME-ACET	MR3	11	0.32	0.77	0.21	296	9	17	18	9	42	46	9	69	77	11
DTC332A	ME-ACET	MR8	11	0.57	0.52	0.21	297	9	19	20	3	37	37	2	46	48	4
DTC335B	ME-ACET	MR8	11	0.42	0.55	0.21	297	9	26	30	12	45	50	11	57	65	13
DTC329A	ME-ACET	R8	11	0.17	0.64	0.21	296	9	41	47	13	55	59	6	59	63	6
DTC330B	ME-ACET	R8	11	0.17	0.55	0.21	296	9	38	43	12	53	56	5	58	60	4
DTC358A	ET-ACET	MR3	11	0.33	0.88	0.20	298	10	13	13	-1	28	28	3	40	42	5
DTC362B	ET-ACET	MR3	11	0.30	0.79	0.20	298	10	11	13	14	25	29	12	39	45	12
DTC364B	ET-ACET	MR3	11	0.32	0.78	0.20	298	10	12	13	2	28	28	2	41	42	4
DTC359B	ET-ACET	MR8	11	0.27	0.78	0.20	298	10	28	30	6	42	46	8	51	58	11
DTC408B	ET-ACET	MR8	11	0.28	1.03	0.19	298	10	32	28	-12	45	43	-4	55	54	-2
DTC415B	ET-ACET	R3	11	0.20	0.76	0.19	297	10	12	11	-11	26	23	-13	42	37	-13
DTC394A	ET-ACET	R8	11	0.11	0.75	0.19	296	10	25	24	-2	31	33	5	33	36	8
DTC409A	ET-ACET	R8	11	0.11	0.94	0.19	298	10	25	23	-6	31	32	3	33	36	7
CTC195B	ET-ACET	R8	8	0.14	0.85	0.15	297	10	34	31	-8	40	37	-9	42	38	-8
DTC688B	IPR-ACET	MR3	18	0.43	1.40	0.17	294	20	19	16	-19	51	42	-19	95	78	-23
DTC689A	IPR-ACET	MR8	18	0.32	1.06	0.16	294	20	70	65	-8	101	94	-8	114	104	-10
DTC697A	IPR-ACET	MR8	18	0.32	0.66	0.16	296	20	46	41	-12	75	67	-11	91	83	-9
DTC528B	ME-IBUAT	MR3	15	0.38	0.88	0.21	299	10	10	13	23	29	30	5	49	46	-5
DTC533A	ME-IBUAT	MR3	14	0.36	0.74	0.21	299	10	10	14	30	31	34	9	53	53	0
DTC530B	ME-IBUAT	MR8	15	0.31	0.76	0.21	299	10	33	33	-2	54	50	-9	71	64	-11
DTC534B	ME-IBUAT	MR8	15	0.29	0.94	0.21	299	10	32	35	8	56	53	-4	73	68	-9
DTC531A	ME-IBUAT	R8	14	0.12	0.77	0.21	299	10	34	33	-5	44	40	-9	47	42	-11
DTC539A	ME-IBUAT	R8	14	0.13	0.92	0.21	299	10	34	33	-1	44	42	-5	47	44	-6
DTC548A	ME-IBUAT	R8	14	0.13	1.09	0.20	299	10	34	32	-7	44	42	-5	48	46	-4
CTC216B	TBU-ACET	MR3	8	0.23		0.14	298	19	9	8	-13	30	29	-3	56	56	-1
CTC221A	TBU-ACET	MR3	8	0.24	0.80	0.14	299	19	8	7	-8	27	26	-4	54	53	-1
CTC217A	TBU-ACET	MR8	8	0.42	0.86	0.14	297	19	44	42	-4	77	85	9	96	102	6
CTC222B	TBU-ACET	MR8	8	0.43	0.71	0.14	299	19	39	34	-16	70	71	2	89	90	2
CTC220B	TBU-ACET	R8	8	0.16	0.82	0.14	298	19	46	47	1	54	55	1	55	55	1
CTC223A	TBU-ACET	R8	8	0.16	0.90	0.14	298	19	49	49	1	57	58	1	59	59	0
DTC365A	BU-ACET	MR3	11		1.45	0.20	298	22	9	9	2	20	21	5	33	35	7
DTC368B	BU-ACET	MR3	11		1.53	0.20	299	22	8	9	8	19	21	9	32	35	9
DTC402B	BU-ACET	MR3	11		1.10	0.19	299	22	9	10	5	24	24	0	39	39	0
DTC403A	BU-ACET	MR8	11	0.29	1.25	0.19	299	22	37	40	7	58	62	7	70	76	8
DTC410B	BU-ACET	MR8	11	0.26	1.63	0.19	298	22	41	39	-5	61	60	-1	71	73	2
DTC406A	BU-ACET	R8	11	0.12	1.00	0.19	299	22	35	36	3	42	44	3	44	46	4
DTC411A	BU-ACET	R8	11	0.11	1.63	0.19	297	10	34	34	1	41	43	4	43	46	7
DTC235B	PC	MR3	10	0.30	0.51	0.23	297	10	13	17	25	33	41	20	57	70	18
DTC239B	PC	MR3	10	0.31	0.68	0.23	297	10	14	17	22	32	37	13	56	60	7
DTC243A	PC	MR3	10	0.32	1.09	0.23	296	10	20	16	-29	37	33	-9	59	58	-1
DTC264B	PC	MR3	10	0.30	0.68	0.22	298	10	13	17	22	32	38	17	54	67	19
DTC250B	PC	MR8	10	0.26	0.70	0.23	297	10	39	44	12	56	66	15	67	82	18
DTC260B	PC	R8	10	0.17	0.55	0.22	297	10	37	42	13	49	58	16	53	65	18
DTC266A	PC	R8	10	0.16	0.65	0.22	298	22	36	44	19	47	60	23	51	67	25
DTC532B	PGME-ACT	MR3	15	0.36	0.98	0.21	299	22	10	10	4	25	24	-2	40	39	-4
DTC537A	PGME-ACT	MR3	14	0.35	0.73	0.21	299	22	11	11	2	29	27	-8	48	43	-11
DTC549B	PGME-ACT	MR3	15	0.37	1.06	0.20	300	22	12	10	-18	28	23	-20	45	37	-23
DTC538B	PGME-ACT	MR8	15	0.29	0.94	0.21	299	22	36	35	-4	54	53	-1	68	68	1
DTC547B	PGME-ACT	MR8	15	0.30	1.24	0.20	300	22	39	35	-12	58	55	-5	72	70	-3
CTC197B	DBE-4	MR3	8	0.25		0.15	297	22	9	9	0	27	27	-3	51	50	-2
CTC211B	DBE-4	MR3	8	0.22	0.96	0.15	298	22	8	10	19	26	30	12	50	52	3
CTC198A	DBE-4	MR8	8	0.39	1.52	0.15	298	22	57	62	7	93	89	-4	109	98	-11
CTC208A	DBE-4	MR8	8	0.43	1.14	0.15	298	22	47	54	14	80	84	5	99	96	-3
CTC199B	DBE-4	R8	8	0.15	1.07	0.15	298	22	48	44	-8	56	50	-10	56	51	-9

Table B-1 (continued)

Run	Run Type or VOC [a]	Rct'y Type [a]	Char Set [b]	NOx (ppm)	Pr.Eq. (ppm) [c]	k1 (min^{-1}) [d]	T (K) [e]	Ref [f]	Δ (O3-NO) Results (pphm) 2 Hour Expt	2 Hour Calc	2 Hour Δ%	4 Hour Expt	4 Hour Calc	4 Hour Δ%	6 Hour Expt	6 Hour Calc	6 Hour Δ%
CTC210A	DBE-4	R8	8	0.16	1.36	0.15	298	22	50	46	-9	59	53	-11	59	54	-9
CTC201A	DBE-5	MR3	8	0.25	1.60	0.15	298	3	4	4	-2	11	12	3	22	22	3
CTC209B	DBE-5	MR3	8	0.25	1.03	0.15	298	3	6	5	-5	18	17	-3	33	33	2
CTC204A	DBE-5	MR8	8	0.44	1.21	0.15	298	3	37	38	3	70	78	11	88	93	6
CTC212B	DBE-5	MR8	8			0.15	298	3	33	32	-4	64	74	13	81	90	10
CTC205B	DBE-5	R8	8	0.16	1.20	0.15	298	3	45	44	-1	53	52	-3	54	53	-2
CTC215A	DBE-5	R8	8	0.18	1.46	0.15	297	3	48	46	-3	57	55	-4	58	57	-3
ETC470	FORMALD	MRE	3	0.39	0.63	0.35	301	3	56	81	30	119	130	8	137	137	0
ETC489	FORMALD	MRE	3	0.42	0.64	0.35	301	10	51	81	37	118	133	11	138	142	3
ETC352	FORMALD	MR3	2	0.53	0.46	0.35	303	10	35	39	10	71	74	4	111	113	2
ETC357	FORMALD	MR3	2	0.53	0.52	0.35	303	10	46	56	18	86	102	16	120	136	12
DTC022B	FORMALD	MR8	1	0.51	0.56	0.39	300	10	62	66	6	89	96	7	108	118	8
DTC036A	FORMALD	R8	1	0.18	0.53	0.39	300	10	60	63	5	64	68	5	64	68	7
CTC138B	FORMALD	MR8	6	0.40	0.60	0.18	293	18	42	42	1	61	65	6	75	81	7
CTC140A	FORMALD	MR8	6	0.36	0.62	0.18	294	18	39	46	15	58	68	14	73	81	10
ETC335	ACETALD	MR3	2	0.54	0.80	0.35	303	18	41	41	-1	71	70	-2	103	101	-2
ETC338	ACETALD	MR3	2	0.52	1.14	0.35	303	18	46	46	0	74	75	2	102	105	2
DTC065A	ACETALD	MR8	1	0.45	1.31	0.39	301	18	54	58	6	79	87	10	98	109	10
DTC066B	ACETALD	R8	1	0.18	1.37	0.39	302	18	43	47	8	51	57	11	55	62	13
CTC107A	ACETALD	MR3	5	0.31	0.78	0.19	295	18	18	20	10	31	33	5	-	44	
CTC266A	BENZALD	MR4	10	0.23	0.53	0.12	299	18	4	2	-61	16	8	-100	30	16	-82
CTC267B	BENZALD	R8	10	0.16	0.65	0.12	300	18	31	31	2	35	36	4	35	36	5
ETC480	ACETONE	MRE	3	0.42	0.58	0.35	301	18	28	42	33	72	100	29	120	133	10
ETC481	ACETONE	MRE	3	0.42	0.57	0.35	301	18	31	45	31	72	101	28	119	132	10
ETC490	ACETONE	MRE	3	0.42	0.58	0.35	301	18	37	48	22	89	103	13	125	131	4
ETC243	ACETONE	MR3	2	0.49	0.38	0.35	301	1	17	18	1	47	45	-3	78	73	-6
ETC245	ACETONE	MR3	2	0.50	0.40	0.35	302	1	22	23	5	51	53	3	86	85	-1
ETC247	ACETONE	MR3	2	0.49	0.40	0.35	301	1	25	27	4	56	57	2	92	90	-2
DTC028A	ACETONE	MR8	1	0.48	0.49	0.39	301	1	51	55	8	78	86	9	103	113	9
DTC064B	ACETONE	MR8	1	0.49	0.52	0.39	302	1	59	63	5	90	100	10	115	130	11
OTC275A	ACETONE	R8	11	0.56	0.53	0.00	319	1	133	122	-9	170	175	3	159	178	11
OTC276B	ACETONE	R8	11	0.57	0.47	0.00	315	2	95	91	-5	150	151	1	-	166	
DTC338A	MEK	MR8	11	0.29	0.57	0.21	297	2	38	40	7	54	58	7	64	70	8
DTC345B	MEK	MRX	11	0.34	0.56	0.20	300	1	26	27	2	52	52	1	75	76	2
DTC363A	MEK	MRX	11	0.32	0.60	0.20	298	1	30	30	-1	54	54	1	75	75	1
CTC181A	MEK	MR3	7	0.23	0.56	0.16	298	1	24	22	-11	47	40	-16	62	55	-12
CTC180B	MEK	MR8	7	0.39	0.75	0.16	298	1	47	46	-1	67	66	-2	82	79	-4
CTC255A	MPK	MR3	9	0.22	0.44	0.13	296	2	11	14	21	25	26	7	39	38	-2
CTC260B	MPK	MR8	10	0.38	0.66	0.12	295	6	38	43	12	57	63	9	71	74	4
CTC263B	MPK	MR8	10	0.16	0.60	0.12	294	6	36	35	-4	41	40	-1	40	40	-2
CTC258B	MPK	R8	10	0.17		0.13	296	1	38	36	-4	43	43	-2	-	43	
DTC554B	CC6-KET	MR3	15	0.37		0.20	299	1	9	8	-21	22	19	-13	33	31	-7
DTC558A	CC6-KET	MR3	14	0.34		0.20	300	1	10	9	-7	23	23	-3	38	37	-3
DTC556A	CC6-KET	MR8	14	0.28		0.20	300	1	26	32	17	44	50	12	56	63	11
DTC559A	CC6-KET	MR8	14	0.29	0.42	0.20	299	1	28	32	13	46	49	6	60	62	3
DTC557B	CC6-KET	R8	15	0.12		0.20	300	1	28	31	12	37	39	6	39	41	6
CTC235A	CC6-KET	R8	9	0.16		0.14	301	1	31	35	12	38	41	8	-	42	
CTC238A	CC6-KET	R8	9	0.17		0.13	301	1	36	37	5	43	44	1	-	45	
DTC366B	MIBK	MR3	11	0.32		0.20	298	8	17	19	9	32	33	2	47	45	-3
DTC369A	MIBK	MR3	11	0.35		0.20	298	8	19	21	7	35	35	2	50	49	-4
DTC370B	MIBK	MR8	11	0.29		0.20	298	10	32	34	5	50	52	4	63	67	6
DTC414A	MIBK	MR8	11	0.27		0.19	298	10	37	36	-3	56	54	-4	67	68	1
DTC412B	MIBK	R8	11	0.11		0.19	297	10	27	26	-1	29	34	15	30	36	18
DTC418A	MIBK	R8	11	0.11		0.19	298	10	27	27	-1	32	34	5	33	36	6
CTC183A	MIBK	MR3	7	0.23		0.16	298	10	11	10	-9	22	19	-13	32	27	-20
CTC182B	MIBK	MR8	7	0.38		0.16	298	20	42	39	-9	63	60	-4	78	75	-3
CTC257A	C7-KET-2	MR3	10	0.24	0.45	0.13	297	20	4	4	11	11	11	0	20	19	-9
CTC262A	C7-KET-2	MR8	10	0.38	0.60	0.12	294	20	29	29	0	58	64	8	73	76	4
CTC259A	C7-KET-2	R8	10	0.17	0.64	0.12	295	20	38	40	4	45	47	4	44	48	8
DTC447A	TDI	MR3	12	0.42	0.99	0.17	297	10	2	4	46	7	9	17	15	15	0
DTC450A	TDI	MR3	12	0.37	0.64	0.17	297	10	8	8	4	25	21	-17	42	34	-25
DTC456A	TDI	MR8	12	0.28	0.53	0.17	297	10	15	14	-7	31	28	-9	39	35	-12
DTC459A	TDI	MR8	12	0.30	0.43	0.16	298	10	19	21	6	37	36	-2	46	45	-1

Table B-1 (continued)

Run	Run Type or VOC [a]	Rct'y Type [a]	Char Set [b]	NOx (ppm)	Pr.Eq. (ppm) [c]	k1 (min^{-1}) [d]	T (K) [e]	Ref [f]	Δ (O3-NO) Results (pphm) 2 Hour Expt	2 Hour Calc	2 Hour Δ%	4 Hour Expt	4 Hour Calc	4 Hour Δ%	6 Hour Expt	6 Hour Calc	6 Hour Δ%
DTC453A	TDI	R8	12	0.16	0.86	0.17	295	10	9	8	-7	18	15	-17	21	20	-8
DTC454A	TDI	R8	12	0.13	0.51	0.17	297	10	20	22	8	26	26	0	26	25	-2
DTC462B	TDI	R8	13	0.14	0.54	0.16	299	10	19	23	15	28	27	-2	29	26	-9
DTC467A	TDI2	MR3	12	0.37	0.61	0.16	294	10	5	6	19	15	16	9	28	27	-5
DTC466A	TDI2	R8	12	0.15	0.46	0.16	297	10	21	21	0	-	27		27	27	-2
DTC601A	P-TI	MR3	16	0.39	0.58	0.19	298	10	11	16	27	33	37	11	57	57	1
DTC602A	P-TI	MR3	16	0.45	1.37	0.19	298	10	8	11	25	27	29	7	50	47	-6
DTC618A	P-TI	MR3	16	0.56	2.81	0.18	297	10	7	9	18	22	23	3	41	38	-8
DTC610A	P-TI	MR8	16	0.31	2.80	0.19	297	10	25	33	24	47	51	8	53	49	-8
DTC604B	P-TI	R8	17	0.20	1.24	0.19	298	10	31	31	1	33	33	0	32	32	1
DTC608A	P-TI	R8	16	0.15	2.05	0.19	297	10	29	34	14	32	33	3	30	32	5
DTC240A	NMP	MR3	10	0.31		0.23	296	20	9	8	-18	23	26	10	63	71	10
DTC244B	NMP	MR3	10	0.38		0.23	295	20	9	9	-8	24	30	20	-	76	
DTC252A	NMP	MR8	10	0.26		0.23	297	20	48	56	13	53	63	16	50	60	17
DTC255B	NMP	MR8	10	0.27		0.23	297	14	30	30	-1	55	60	8	54	61	11
DTC261A	NMP	R8	10	0.16		0.22	296	14	33	37	10	40	46	12	39	45	13
DTC267B	NMP	R8	10	0.16		0.22	299	14	39	42	7	43	47	7	41	45	9
DTC421A	C3-BR	MR3	11	0.38	0.81	0.19	297	14	18	17	-2	65	43	-50	66	73	10
DTC433A	C3-BR	MR3	11	0.39	0.60	0.18	297	14	17	13	-23	55	35	-55	82	59	-39
DTC423B	C3-BR	MR8	11	0.29	0.65	0.19	297	14	32	48	33	53	68	22	57	76	25
DTC427A	C3-BR	MR8	11	0.26	0.72	0.18	298	14	36	51	30	58	71	18	50	78	36
DTC424A	C3-BR	R8	11	0.10	0.55	0.18	297	14	31	32	5	30	34	13	28	34	18
DTC428B	C3-BR	R8	11	0.11	0.73	0.18	298	14	31	38	20	29	43	34	26	43	39
DTC401A	C4-BR	MR3	11	0.35	1.65	0.19	298	23	17	34	51	68	77	12	52	100	48
DTC426B	C4-BR	MR3	11	0.34	1.15	0.18	297	23	15	27	45	63	64	2	68	90	25
DTC419B	C4-BR	MR8	11	0.28	1.14	0.19	297	23	43	67	35	61	85	28	49	90	46
DTC430A	C4-BR	MR8	11	0.24	0.94	0.18	297	23	39	58	34	60	75	20	49	81	40
DTC420B	C4-BR	R8	11	0.11	1.16	0.19	297	23	32	42	22	29	48	39	26	48	47
DTC432B	C4-BR	R8	11	0.12	1.54	0.18	297	23	33	45	27	29	53	45	26	55	53
DTC303B	CL3-ETHE	MR3	11	0.33		0.21	298	3	24	35	31	91	79	-15	87	101	13
DTC305A	CL3-ETHE	MR3	11	0.33		0.21	299	3	12	20	42	39	51	23	76	81	6
DTC308B	CL3-ETHE	MR8	11	0.17		0.21	301	3	37	39	5	47	53	12	46	58	20
DTC311B	CL3-ETHE	MR8	11	0.29		0.21	298	3	33	35	8	60	55	-8	66	70	5
DTC320A	CL3-ETHE	MR8	11	0.30		0.21	297	3	28	32	11	48	49	3	59	64	8
DTC309A	CL3-ETHE	R8	11	0.17		0.21	299	3	46	50	8	45	57	21	43	57	26
DTC321B	CL3-ETHE	R8	11	0.11		0.21	298	12	33	37	9	34	42	19	33	43	23
DTC312A	CL3-ETHE	RX	11	0.32		0.21	299	12	18	17	-4	48	44	-9	76	74	-3
DTC692B	DMC	MR3	18	0.44	0.82	0.16	298	12	18	14	-30	46	34	-34	77	57	-36
DTC703B	DMC	MR3	18	0.42	1.04	0.16	296	12	18	16	-8	46	39	-16	79	68	-16
DTC693A	DMC	MR8	18	0.31	0.71	0.16	298	12	46	48	3	71	69	-2	86	82	-5
DTC705A	DMC	MR8	18	0.29	0.64	0.16	296	12	37	41	10	-	62		78	74	-5
DTC698B	DMC	R8	18	0.10	0.69	0.16	295	10	36	34	-4	41	40	-4	42	41	-1
DTC763B	DMC	R8	18	0.09		0.16	299	12	28	32	10	32	35	9	32	36	10
DTC750B	MIPR-CB	MR3	18	0.35		0.16	300	12	17	16	-12	44	41	-7	74	73	-1
DTC759A	MIPR-CB	MR3	18	0.37		0.16	299	12	12	14	12	37	36	-2	70	67	-5
DTC755A	MIPR-CB	MR8	18	0.29		0.16	299	12	50	51	2	77	74	-4	88	84	-4
DTC762A	MIPR-CB	MR8	18	0.30		0.16	299	12	39	37	-6	65	61	-6	78	75	-3
DTC758B	MIPR-CB	R8	18	0.09		0.16	299	24	35	35	0	40	40	0	40	40	1
DTC763B	MIPR-CB	R8	18	0.09		0.16	299	24	28	32	10	32	35	9	32	36	10
DTC694A	ME-PVAT	MR3	18	0.40	0.81	0.16	298	24	8	8	2	22	19	-14	38	32	-20
DTC701B	ME-PVAT	MR3	18	0.39	0.95	0.16	296	24	7	7	-2	18	16	-15	31	26	-21
DTC695B	ME-PVAT	MR8	18	0.31	0.81	0.16	299	24	28	31	8	54	56	5	69	71	2
DTC702A	ME-PVAT	MR8	18	0.32	1.01	0.16	297	24	27	27	-1	54	53	-1	71	67	-5
DTC700A	ME-PVAT	R8	18	0.11	0.96	0.16	296	24	30	29	-1	36	35	-5	39	35	-9
DTC707B	ME-PVAT	R8	18	0.11	1.21	0.16	297	24	27	28	5	35	36	2	38	38	1
DTC442A	MS-A	MR3	11	0.34		0.17	294	13	5	7	22	16	21	22	31	37	15
DTC486A	MS-A	MR8	14	0.30		0.22	298	13	33	27	-22	57	51	-11	72	68	-6
DTC487B	MS-A	R8	15	0.13		0.22	298	13	36	36	2	42	42	0	43	42	-2
DTC441B	MS-B	MR3	11	0.35		0.18	294	13	6	6	5	15	17	10	26	29	10
DTC480A	MS-B	MR8	14	0.29		0.22	298	13	27	22	-23	50	46	-10	66	61	-7
DTC481B	MS-B	R8	15	0.13		0.22	298	13	34	35	3	42	43	3	42	44	3
DTC440A	MS-C	MR3	11	0.36		0.18	296	13	6	7	10	18	19	6	32	34	4
DTC478A	MS-C	MR8	14	0.30		0.22	297	13	30	27	-11	52	50	-4	66	67	0

Table B-1 (continued)

Run	Run Type or VOC [a]	Rct'y Type [a]	Char Set [b]	NOx (ppm)	Pr.Eq. (ppm) [c]	k1 (min^{-1}) [d]	T (K) [e]	Ref [f]	Δ (O3-NO) Results (pphm) 2 Hour Expt	2 Hour Calc	2 Hour Δ%	4 Hour Expt	4 Hour Calc	4 Hour Δ%	6 Hour Expt	6 Hour Calc	6 Hour Δ%
DTC479B	MS-C	R8	15	0.14		0.22	297	13	36	38	4	45	46	3	46	47	2
DTC439B	MS-D	MR3	11	0.35		0.18	297	13	7	6	-9	21	19	-10	36	33	-8
DTC476A	MS-D	MR8	14	0.31		0.22	298	13	30	23	-30	53	46	-14	68	62	-10
DTC477B	MS-D	R8	15	0.13		0.22	297	13	36	38	4	43	44	3	43	44	3
DTC753A	D95	MR3	18	0.41		0.16	299	25	4	4	6	13	12	-12	26	22	-17
DTC757A	D95	MR3	18	0.38		0.16	299	25	6	6	-12	20	16	-30	37	29	-29
DTC754B	D95	MR8	18	0.30		0.16	299	25	17	17	2	40	40	1	51	52	2
DTC772B	D95	MR8	18	0.30		0.16	299	25	15	17	14	40	43	8	51	57	11
DTC756B	D95	R8	0	0.13		0.16	299	25	28	30	9	35	39	10	36	41	12
DTC778A	D95	R8	18	0.09		0.16	300	25	25	27	8	29	31	4	29	30	3
DTC719A	ISOPARM	MRX	18	0.40		0.16	294	25	8	7	-15	24	18	-31	42	32	-29
DTC724B	ISOPARM	MR3	18	0.33		0.16	294	25	4	4	1	12	10	-18	24	19	-27
DTC720B	ISOPARM	MR8	18	0.32		0.16	296	25	20	13	-56	43	33	-31	55	46	-20
DTC771A	ISOPARM	MR8	18	0.29		0.16	299	25	18	15	-19	44	40	-10	57	53	-6
DTC723A	ISOPARM	R8	18	0.11		0.16	295	25	29	28	-1	34	34	2	34	35	4
DTC775B	ISOPARM	R8	0	0.09		0.16	299	25	27	27	0	31	30	-2	30	30	0
DTC760B	OC10ACET	MR3	18	0.39		0.16	298	25	10	6	-75	23	14	-58	37	25	-46
DTC773A	OC10ACET	MR3	0	0.38		0.16	300	25	5	5	-17	16	12	-30	31	23	-35
DTC769A	OC10ACET	MR8	18	0.27		0.16	299	25	14	21	34	40	44	9	53	56	7
DTC776A	OC10ACET	MR8	18	0.30		0.16	300	25	21	19	-8	44	41	-9	57	53	-8
DTC770B	OC10ACET	R8	18	0.08		0.16	299	25	20	26	23	23	29	21	23	29	21
DTC771A	OC10ACET	R8	18	0.29		0.16	299	25	18	15	-19	44	40	-10	57	53	-6
VOC Mixture - NOx Runs (Including Base Case Reactivity Experiments)																	
EC166	MIX-A		1	0.11	0.25	0.35	301	1	26	18	-45	44	33	-36	53	44	-21
EC172	MIX-A		1	0.10	0.08	0.37	301	1	14	11	-24	23	20	-19	33	27	-23
EC144	MIX-E		1	0.51	0.88	0.31	301	1	130	94	-38	136	125	-9	116	113	-2
EC145	MIX-E		1	1.00	0.77	0.31	301	1	65	61	-7	107	103	-4	151	137	-11
EC149	MIX-E		1	1.00	0.89	0.31	301	1	77	65	-19	94	90	-4	107	103	-4
EC150	MIX-E		1	1.02	0.90	0.32	301	1	78	72	-8	116	108	-8	157	136	-16
EC151	MIX-E		1	2.06	1.47	0.31	301	1	91	94	3	128	136	6	152	161	5
EC152	MIX-E		1	0.51	0.96	0.32	301	1	93	86	-7	117	111	-5	108	109	1
EC153	MIX-E		1	0.99	1.70	0.33	302	1	153	140	-9	174	172	-1	157	160	1
EC160	MIX-E		1	1.01	0.73	0.34	301	1	75	57	-31	117	95	-23	163	125	-30
EC161	MIX-E		1	0.54	0.83	0.34	301	1	96	75	-29	123	104	-18	-		
XTC111	MIX-AE		1	0.22	1.14	0.25	303	1	7	5	-30	26	16	-65	65	39	-65
EC163	MIX-AO		1	0.51	0.47	0.34	300	1	40	33	-19	61	50	-21	80	63	-26
EC217	MIX-EO		1	0.48	0.19	0.43	301	1	12	20	41	19	32	39	26	40	36
EC257	MIX-EO		1	0.52	0.25	0.29	303	1	33	33	-1	46	47	2	52	53	3
EC272	MIX-RO		1	0.48	0.35	0.34	302	1	43	47	9	65	74	13	81	92	13
EC335	MIX-RO		1	0.50	0.42	0.38	302	1	54	63	15	77	96	20	73	93	22
EC336	MIX-RO		1	0.49	0.34	0.38	302	1	67	87	23	70	94	26	63	88	28
EC337	MIX-RO		1	0.51	0.30	0.38	302	1	34	35	2	66	72	8	62	77	19
EC338	MIX-RO		1	0.50	0.42	0.37	302	1	61	64	4	86	107	20	78	105	25
EC339	MIX-RO		1	0.50	0.21	0.37	302	1	19	16	-20	41	37	-13	60	54	-10
DTC073B	MIX-AR		1	0.49	0.44	0.39	302	1	5	6	20	12	13	6	23	22	-7
DTC076A	MIX-AR		1	0.48	0.31	0.39	302	1	6	9	38	18	22	20	33	35	7
EC328	MIX-AR		1	0.50	0.33	0.42	303	1	46	50	8	74	89	18	89	112	20
EC331	MIX-AR		1	0.52	0.65	0.41	302	1	91	110	17	81	103	21	73	94	22
ETC218	MIX-ER		2	0.47	0.61	0.35	299	1	79	75	-4	114	108	-6	106	101	-5
EC329	MIX-ER		1	0.50	0.22	0.41	302	1	42	46	10	69	80	14	76	95	20
EC330	MIX-ER		1	0.32	0.22	0.42	302	1	45	51	12	53	69	22	49	65	25
EC334	MIX-ER		1	0.50	0.32	0.39	302	1	63	70	10	75	96	22	69	91	24
ITC437	SURG-4		2	0.08	0.35	0.46	305	1	37	41	10	42	45	6	46	47	3
ITC438	SURG-4		2	0.08	0.37	0.46	302	1	30	40	25	33	43	23	36	45	22
ITC440	SURG-4		2	0.08	0.17	0.45	302	1	20	29	31	31	41	24	37	46	19
ITC442	SURG-4		2	0.14	0.34	0.45	303	1	37	49	25	55	62	11	60	66	9
ITC444	SURG-4		2	0.14	0.16	0.44	303	1	15	24	36	29	42	33	41	56	27
ITC446	SURG-4		2	0.07	0.39	0.44	302	1	29	36	20	29	37	20	30	36	17
ITC450	SURG-4		2	0.08	0.35	0.43	302	1	33	39	17	38	42	9	40	44	9
ITC452	SURG-4		2	0.08	0.33	0.43	302	1	31	39	21	38	43	12	40	45	11
ITC456	SURG-4		2	0.08	0.41	0.42	301	1	31	41	25	37	44	17	39	46	15
ITC459	SURG-4		2	0.08	0.35	0.42	301	1	31	38	19	37	40	7	39	42	8

Table B-1 (continued)

Run	Run Type or VOC [a]	Rct'y Type [a]	Char Set [b]	NOx (ppm)	Pr.Eq. (ppm) [c]	k1 (min^{-1}) [d]	T (K) [e]	Ref [f]	Δ (O3-NO) Results (pphm) 2 Hour Expt	2 Hour Calc	2 Hour Δ%	4 Hour Expt	4 Hour Calc	4 Hour Δ%	6 Hour Expt	6 Hour Calc	6 Hour Δ%
ITC461	SURG-4		2	0.09	0.35	0.41	302	1	30	39	23	37	42	12	39	44	12
ITC465	SURG-4		2	0.09	0.33	0.41	301	1	32	40	21	39	44	13	40	46	13
ITC467	SURG-4		2	0.09	0.33	0.40	302	1	29	41	30	36	46	20	38	47	21
ITC471	SURG-4		2	0.09	0.33	0.40	302	1	29	39	27	36	43	18	37	46	20
ITC483	SURG-4		2	0.08	0.34	0.39	302	1	30	38	22	35	41	15	39	43	8
ITC488	SURG-4		2	0.08	0.39	0.38	303	1	28	39	27	34	42	18	35	44	19
ITC489	SURG-4		2	0.09	0.35	0.38	302	1	28	38	27	34	41	17	36	43	16
ITC497	SURG-4		2	0.09	0.34	0.38	301	1	27	38	29	34	41	17	36	43	16
ITC501	SURG-4		2	0.09	0.34	0.38	302	1	30	39	23	37	42	13	39	44	12
ITC503	SURG-4		2	0.09	0.34	0.37	302	1	27	40	32	33	44	24	35	46	23
ITC571	SURG-4		4	0.11	0.33	0.36	298	1	28	38	28	39	46	16	-	48	
ITC572	SURG-4		4	0.12	0.34	0.36	299	1	34	39	14	40	48	16	45	50	9
ITC574	SURG-4		4	0.09	0.33	0.36	301	1	33	38	14	39	44	12	41	46	11
ITC578	SURG-4		4	0.09	0.32	0.36	299	1	30	36	17	38	40	5	42	42	0
ITC580	SURG-4		4	0.09	0.33	0.36	299	1	31	37	18	42	42	1	44	43	0
ITC581	SURG-4		4	0.09	0.48	0.35	300	1	37	41	10	41	41	1	43	42	-2
ITC584	SURG-4		4	0.09	0.36	0.35	300	1	34	38	11	43	42	-2	45	44	-4
ITC586	SURG-4		4	0.08	0.34	0.35	301	1	34	36	6	40	39	-3	43	41	-6
ITC590	SURG-4		4	0.09	0.33	0.35	302	1	31	37	17	40	42	4	44	44	-1
ITC598	SURG-4		4	0.10	0.37	0.35	300	1	34	39	14	42	43	4	44	45	1
ITC603	SURG-4		4	0.09	0.34	0.35	300	1	31	38	18	39	41	6	41	42	4
ITC607	SURG-4		4	0.10	0.37	0.35	302	1	34	40	15	43	44	3	45	46	1
ITC609	SURG-4		4	0.09	0.37	0.35	301	1	32	39	18	41	42	4	44	44	1
ITC613	SURG-4		4	0.08	0.37	0.35	301	1	31	37	17	38	40	5	40	42	3
EC676	SURG-4		1	0.09	0.40	0.37	301	1	20	38	47	19	39	50	16	41	61
ITC573	SURG-4R		4	0.11	0.18	0.36	300	1	24	26	7	-	40		43	47	8
EC231	SURG-7		1	0.68	0.97	0.29	302	1	78	105	26	104	131	21	96	119	19
EC232	SURG-7		1	0.48	0.47	0.29	302	1	37	33	-11	60	66	9	75	90	17
EC233	SURG-7		1	0.09	0.48	0.29	302	1	36	42	14	41	50	17	41	50	18
EC237	SURG-7		1	0.46	0.84	0.29	302	1	74	93	21	101	112	10	94	103	9
EC238	SURG-7		1	0.91	0.82	0.29	303	1	61	82	26	97	135	28	128	158	19
EC241	SURG-7		1	0.47	0.40	0.28	302	1	34	43	21	56	73	23	76	95	20
EC242	SURG-7		1	0.46	1.47	0.29	302	1	102	107	4	83	86	3	77	76	-1
EC243	SURG-7		1	0.47		0.29	302	1	107	111	4	-			-		
EC245	SURG-7		1	0.94	1.47	0.29	302	1	136	164	17	151	151	0	133	131	-2
EC246	SURG-7		1	0.48	0.44	0.29	302	1	35	37	5	55	62	11	73	84	13
EC247	SURG-7		1	0.48	0.72	0.29	302	1	77	94	18	100	106	5	-		
ITC626	SURG-8S		5	0.29	0.51	0.35	296	1	26	29	10	53	68	23	73	87	16
ITC630	SURG-8S		5	0.31	0.25	0.35	298	1	13	11	-17	22	23	4	31	35	11
ITC631	SURG-8S		5	0.32	0.14	0.35	300	1	8	5	-58	12	10	-19	17	15	-14
ITC633	SURG-8S		5	0.61	0.51	0.35	299	1	17	14	-20	31	34	9	42	53	20
ITC635	SURG-8S		5	1.19	0.52	0.35	300	1	13	8	-69	23	20	-19	31	32	3
ITC637	SURG-8S		5	0.30	0.51	0.35	299	1	28	28	1	54	68	20	71	88	19
ITC865	SURG-8S		9	0.31	0.63	0.35	296	1	30	33	10	62	79	21	80	95	16
ITC867	SURG-8S		9	0.28	0.52	0.35	297	1	29	47	39	52	80	35	68	93	27
ITC868	SURG-8S		9	0.37	0.39	0.35	296	1	28	13	-118	47	28	-65	61	44	-39
ITC871	SURG-8S		9	0.37	0.29	0.35	296	1	16	10	-67	29	21	-40	40	31	-31
ITC872	SURG-8S		9	0.36	0.25	0.35	297	1	16	16	-3	26	26	-1	34	33	-1
ITC873	SURG-8S		9	0.37	0.19	0.35	296	1	12	5	-119	20	11	-75	27	17	-63
ITC874	SURG-8S		9	0.36	0.22	0.35	296	1	11	6	-97	21	12	-74	28	18	-52
ITC877	SURG-8S		9	0.38	0.26	0.35	296	1	16	17	3	27	28	5	34	36	6
ITC880	SURG-8S		9	0.66	0.31	0.35	295	1	10	6	-71	20	13	-46	28	21	-31
ITC881	SURG-8S		9	0.67	0.25	0.35	296	1	10	10	5	18	18	1	25	24	-5
ITC885	SURG-8S		9	0.64	0.19	0.35	295	1	6	4	-59	11	7	-46	16	11	-38
ITC888	SURG-8S		9	0.32	0.40	0.35	296	1	19	11	-78	40	24	-64	57	38	-50
ITC891	SURG-8S		9	0.32	0.57	0.35	296	1	31	27	-17	64	66	3	81	89	9
DTC312B	SURG-X		11	0.31	0.68	0.21	299	24	21	18	-16	49	44	-12	77	72	-7
DTC345A	SURG-X		11	0.34	0.49	0.20	300	10	14	14	4	38	38	-2	65	64	-1
DTC363B	SURG-X		11	0.32	0.49	0.20	298	10	14	14	0	37	36	-1	62	62	1
DTC568B	SURG-X		15	0.46	0.51	0.20	298	16	8	13	41	25	34	27	44	54	19
DTC569B	SURG-X		15	0.36	0.49	0.20	298	16	9	14	40	-	40		58	66	12
DTC572B	SURG-X		15	0.38	0.44	0.20	298	16	7	10	30	25	28	12	46	47	3
DTC573B	SURG-X		15	0.13	0.38	0.20	297	16	32	33	4	40	40	1	41	42	1

Table B-1 (continued)

Run	Run Type or VOC [a]	Rct'y Type [a]	Char Set [b]	NOx (ppm)	Pr.Eq. (ppm) [c]	k1 (min^{-1}) [d]	T (K) [e]	Ref [f]	Δ (O3-NO) Results (pphm) 2 Hour Expt	2 Hour Calc	2 Hour Δ%	4 Hour Expt	4 Hour Calc	4 Hour Δ%	6 Hour Expt	6 Hour Calc	6 Hour Δ%
DTC576B	SURG-X		15	0.41	0.49	0.20	299	16	8	12	28	28	32	13	50	56	9
DTC577B	SURG-X		15	0.33	0.37	0.20	298	16	22	23	8	40	40	1	51	51	0
DTC581B	SURG-X		15	0.40	0.50	0.20	298	16	7	13	45	25	35	28	43	57	24
DTC583B	SURG-X		15	0.35	0.51	0.19	298	16	-	13		26	33	23	46	58	21
DTC586B	SURG-X		15	0.32	0.43	0.19	297	16	22	30	25	41	47	12	52	59	12
DTC589B	SURG-X		15	0.42	0.53	0.19	298	16	6	12	45	21	30	32	37	53	31
DTC591B	SURG-X		15	0.35	0.42	0.19	296	16	20	27	24	40	45	12	50	57	12
DTC593B	SURG-X		15	0.45	0.52	0.19	297	16	6	11	45	22	32	31	40	53	24
DTC594B	SURG-X		15	0.32	0.42	0.19	298	16	-	29		42	46	9	54	58	8
DTC596B	SURG-X		15	0.29	0.52	0.19	297	16	9	15	36	29	38	24	55	65	16
DTC598A	SURG-X		14	0.03	0.15	0.19	298	16	11	12	15	12	14	16	13	15	18
DTC598B	SURG-X		15	0.14	0.15	0.19	298	16	8	10	23	15	18	14	21	23	11
DTC615B	SURG-X		17	0.72	0.41	0.19	298	23	23	13	-74	36	26	-36	43	36	-21
DTC719B	SURG-X		18	0.41	0.53	0.16	294	0	11	10	-10	32	27	-20	51	41	-24
ETC090	SURG-3M		2	0.55	0.37	0.36	301	1	9	13	31	27	37	26	46	60	22
ETC091	SURG-3M		2	0.51	0.33	0.36	301	1	9	12	27	27	34	22	43	55	21
ETC093	SURG-3M		2	0.51	0.34	0.36	301	1	11	13	16	30	36	18	47	58	18
ETC095	SURG-3M		2	0.51	0.35	0.36	301	1	9	13	28	28	36	23	46	59	21
ETC098	SURG-3M		2	0.51	0.33	0.36	301	1	10	12	17	29	34	15	44	54	18
ETC100	SURG-3M		2	0.51	0.34	0.36	300	1	9	12	24	27	34	21	45	55	18
ETC102	SURG-3M		2	0.51	0.34	0.36	300	1	12	12	0	29	34	14	48	55	12
ETC104	SURG-3M		2	0.50	0.34	0.36	300	1	10	12	19	27	33	21	44	54	19
ETC107	SURG-3M		2	0.50	0.36	0.36	300	1	12	13	5	31	37	17	47	59	20
ETC109	SURG-3M		2	0.52	0.34	0.36	300	1	8	11	32	24	33	28	41	53	24
ETC113	SURG-3M		2	0.51	0.35	0.36	300	1	9	12	28	26	34	24	42	55	24
ETC114	SURG-3M		2	0.49	0.34	0.36	300	1	8	12	32	26	34	24	41	54	25
ETC115	SURG-3M		2	0.53	0.33	0.36	300	1	8	11	31	24	32	25	40	51	21
ETC116	SURG-3M		2	0.51	0.37	0.36	301	1	12	15	24	34	42	20	56	69	18
ETC117	SURG-3M		2	0.52	0.33	0.36	301	1	9	12	25	27	34	20	43	55	21
ETC119	SURG-3M		2	0.52	0.35	0.35	302	1	11	13	19	31	37	15	50	60	16
ETC122	SURG-3M		2	0.53	0.31	0.35	304	1	9	11	18	28	33	13	48	53	10
ETC124	SURG-3M		2	0.50	0.31	0.35	303	1	8	11	24	27	33	17	45	53	15
ETC126	SURG-3M		2	0.52	0.31	0.35	302	1	8	11	25	27	32	18	43	52	18
ETC128	SURG-3M		2	0.53	0.31	0.35	301	1	8	10	20	24	30	19	40	49	17
ETC129	SURG-3M		2	0.53	0.31	0.35	301	1	7	10	27	24	30	19	41	49	16
ETC130	SURG-3M		2	0.52	0.30	0.35	302	1	8	10	21	26	31	17	43	50	14
ETC132	SURG-3M		2	0.54	0.31	0.35	302	1	8	10	26	24	30	18	43	48	11
ETC134	SURG-3M		2	0.53	0.31	0.35	303	1	8	11	29	25	32	20	43	51	15
ETC137	SURG-3M		2	0.52	0.29	0.35	300	1	8	9	10	23	27	13	39	44	12
ETC139	SURG-3M		2	0.53	0.31	0.35	301	1	9	10	11	25	30	15	42	48	13
ETC143	SURG-3M		2		0.29	0.35	301	1	11	11	0	30	32	7	48	51	5
ETC145	SURG-3M		2	0.51	0.28	0.35	301	1	8	10	20	23	28	19	39	45	14
ETC147	SURG-3M		2	0.50	0.28	0.35	301	1	8	10	15	23	28	16	38	44	13
ETC149	SURG-3M		2	0.51	0.28	0.35	302	1	8	10	22	24	28	14	41	45	10
ETC156	SURG-3M		2	0.51	0.40	0.35	300	1	16	16	-1	43	44	3	69	72	4
ETC158	SURG-3M		2	0.50	0.40	0.35	300	1	14	15	11	37	43	14	60	70	13
ETC160	SURG-3M		2	0.50	0.44	0.35	300	1	16	18	12	42	49	14	68	82	17
ETC161	SURG-3M		2	0.52	0.43	0.35	301	1	16	18	12	43	48	11	70	79	12
ETC162	SURG-3M		2	0.50	0.43	0.35	301	1	15	18	17	43	48	11	70	80	13
ETC165	SURG-3M		2	0.50	0.43	0.35	303	1	16	18	10	45	50	9	79	84	6
ETC168	SURG-3M		2	0.52	0.39	0.35	301	1	16	15	-7	44	42	-5	73	68	-8
ETC170	SURG-3M		2	0.51	0.40	0.35	301	1	16	16	3	43	44	3	72	72	0
ETC172	SURG-3M		2	0.50	0.41	0.35	300	1	14	16	10	40	44	9	68	73	7
ETC174	SURG-3M		2	0.50	0.44	0.35	299	1	13	16	19	40	46	15	67	79	15
ETC186	SURG-3M		2	0.40	0.08	0.35	299	1	13	3	-353	39	6	-561	67	9	-680
ETC188	SURG-3M		2		0.18	0.35	300	1	16	5	-200	44	18	-148	78	31	-153
ETC197	SURG-3M		2		0.17	0.35	300	1	28	5	-489	54	16	-236	84	28	-203
ETC208	SURG-3M		2	0.49	0.40	0.35	299	1	14	16	10	45	44	-2	-	71	
ETC210	SURG-3M		2	0.50	0.41	0.35	299	1	13	15	12	40	43	7	66	71	6
ETC215	SURG-3M		2	0.48	0.39	0.35	300	1	13	16	17	39	43	10	64	70	8
ETC223	SURG-3M		2	0.50	0.40	0.35	300	1	17	16	-6	44	44	0	71	71	1
ETC225	SURG-3M		2	0.50	0.40	0.35	299	1	11	15	23	34	41	19	55	67	19
ETC227	SURG-3M		2	0.50	0.43	0.35	300	1	12	17	26	37	46	19	62	77	20

Table B-1 (continued)

Run	Run Type or VOC [a]	Rct'y Type [a]	Char Set [b]	NOx (ppm)	Pr.Eq. (ppm) [c]	k1 (min^{-1}) [d]	T (K) [e]	Ref [f]	Δ (O3-NO) Results (pphm) 2 Hour Expt	2 Hour Calc	2 Hour Δ%	4 Hour Expt	4 Hour Calc	4 Hour Δ%	6 Hour Expt	6 Hour Calc	6 Hour Δ%
ETC229	SURG-3M		2	0.51	0.43	0.35	300	1	12	16	24	38	45	17	63	75	17
ETC231	SURG-3M		2	0.50	0.42	0.35	299	1	13	15	13	39	43	10	63	71	11
ETC234	SURG-3M		2	0.50	0.39	0.35	302	1	14	15	10	41	42	4	70	70	1
ETC236	SURG-3M		2	0.50	0.38	0.35	301	1	14	15	2	41	41	1	69	68	-3
ETC238	SURG-3M		2	0.47	0.37	0.35	301	1	13	15	8	39	41	4	67	67	0
ETC240	SURG-3M		2	0.48	0.37	0.35	300	1	12	14	15	36	39	9	62	64	3
ETC242	SURG-3M		2	0.48	0.38	0.35	301	1	15	15	1	41	42	1	72	69	-4
ETC244	SURG-3M		2	0.47	0.37	0.35	302	1	13	15	14	40	42	5	69	69	0
ETC246	SURG-3M		2	0.49	0.38	0.35	302	1	14	16	10	41	44	6	72	73	1
ETC248	SURG-3M		2	0.49	0.42	0.35	301	1	16	17	4	46	47	1	83	79	-4
ETC250	SURG-3M		2	0.50	0.44	0.35	299	1	14	15	8	42	44	4	73	74	1
ETC252	SURG-3M		2	0.50	0.41	0.35	300	1	13	16	16	39	45	14	67	75	11
ETC254	SURG-3M		2	0.42	0.37	0.35	299	1	12	14	17	34	40	14	59	67	13
ETC256	SURG-3M		2	0.49	0.41	0.35	302	1	17	16	-9	44	44	-1	77	75	-2
ETC258	SURG-3M		2	0.48	0.41	0.35	301	1	16	15	-4	44	44	0	76	75	0
ETC260	SURG-3M		2	0.49	0.41	0.35	300	1	15	15	1	41	42	3	70	72	3
ETC262	SURG-3M		2	0.47	0.40	0.35	302	1	17	17	1	44	46	5	75	78	4
ETC264	SURG-3M		2	0.49	0.41	0.35	301	1	17	15	-15	45	43	-4	75	74	-2
ETC266	SURG-3M		2	0.48	0.40	0.35	300	1	17	15	-17	44	42	-4	74	71	-4
ETC268	SURG-3M		2	0.48	0.39	0.35	302	1	19	16	-15	49	45	-9	83	76	-9
ETC270	SURG-3M		2	0.49	0.39	0.35	301	1	16	15	-7	44	42	-3	74	70	-6
ETC272	SURG-3M		2	0.48	0.40	0.35	301	1	16	15	-3	45	43	-4	76	72	-6
ETC274	SURG-3M		2	0.52	0.39	0.35	302	1	16	16	-1	49	45	-8	83	74	-13
ETC276	SURG-3M		2	0.49	0.38	0.35	302	1	16	16	-1	46	44	-4	80	72	-10
ETC278	SURG-3M		2	0.51	0.38	0.35	302	1	15	15	0	45	43	-5	80	70	-14
ETC280	SURG-3M		2	0.50	0.38	0.35	303	1	16	16	2	47	45	-4	84	75	-13
ETC282	SURG-3M		2	0.50	0.37	0.35	302	1	16	16	1	46	44	-5	81	72	-14
ETC284	SURG-3M		2	0.49	0.38	0.35	302	1	16	17	4	46	46	-2	83	75	-10
ETC286	SURG-3M		2	0.48	0.39	0.35	303	1	15	18	14	46	48	3	84	80	-5
ETC288	SURG-3M		2	0.49	0.37	0.35	303	1	16	17	4	48	45	-6	88	76	-16
ETC290	SURG-3M		2	0.49	0.39	0.35	304	1	17	18	4	51	48	-6	90	80	-13
ETC292	SURG-3M		2	0.49	0.38	0.35	301	1	16	16	1	46	44	-4	79	73	-8
ETC294	SURG-3M		2	0.48	0.38	0.35	301	1	15	17	10	45	45	-1	79	74	-8
ETC296	SURG-3M		2	0.47	0.37	0.35	301	1	16	16	2	47	44	-7	83	73	-13
ETC298	SURG-3M		2	0.49	0.40	0.35	302	1	18	19	7	51	51	-1	89	83	-6
ETC300	SURG-3M		2	0.48	0.40	0.35	300	1	16	18	8	47	48	2	80	79	-1
ETC302	SURG-3M		2	0.46	0.38	0.35	300	1	10	13	22	33	38	13	57	63	10
ETC304	SURG-3M		2	0.49	0.37	0.35	300	1	11	14	23	35	40	12	60	64	7
ETC306	SURG-3M		2	0.54	0.37	0.35	301	1	11	11	1	36	33	-9	61	55	-13
ETC308	SURG-3M		2	0.53	0.37	0.35	301	1	12	12	0	38	35	-7	65	58	-10
ETC310	SURG-3M		2	0.53	0.37	0.35	299	1	11	12	7	34	35	1	58	56	-3
ETC312	SURG-3M		2	0.52	0.38	0.35	297	1	10	10	9	32	33	3	55	55	0
ETC314	SURG-3M		2	0.53	0.37	0.35	298	1	11	11	-2	35	33	-5	59	54	-8
ETC316	SURG-3M		2	0.50	0.36	0.35	298	1	12	12	0	36	35	-4	60	56	-7
ETC323	SURG-3M		2	0.54	0.43	0.35	304	1	24	22	-6	59	55	-8	101	89	-14
ETC324	SURG-3M		2	0.62	0.42	0.35	302	1	15	16	5	43	45	4	68	70	2
ETC325	SURG-3M		2	0.53	0.42	0.35	302	1	18	19	2	49	49	0	81	80	-2
ETC326	SURG-3M		2	0.53	0.42	0.35	302	1	21	19	-12	52	50	-5	85	80	-6
ETC327	SURG-3M		2	0.49	0.44	0.35	302	1	19	21	8	51	54	5	88	91	3
ETC328	SURG-3M		2	0.52	0.42	0.35	303	1	18	19	8	49	50	2	80	81	1
ETC329	SURG-3M		2	0.52	0.41	0.35	303	1	19	19	3	51	50	-2	84	81	-5
ETC330	SURG-3M		2	0.50	0.41	0.35	303	1	20	20	-1	53	51	-4	88	83	-6
ETC331	SURG-3M		2	0.51	0.40	0.35	303	1	18	18	-1	49	47	-4	82	77	-7
ETC334	SURG-3M		2	0.52	0.41	0.35	303	1	19	19	-1	50	49	-1	84	81	-4
ETC336	SURG-3M		2	0.53	0.43	0.35	303	1	20	21	3	52	53	2	87	87	0
ETC339	SURG-3M		2	0.52	0.45	0.35	303	1	22	21	-3	55	54	-3	93	90	-3
ETC345	SURG-3M		2	0.52	0.44	0.35	303	1	21	21	-1	56	54	-3	91	89	-2
ETC347	SURG-3M		2	0.52	0.43	0.35	303	1	20	21	2	53	53	0	87	87	1
ETC349	SURG-3M		2	0.51	0.42	0.35	304	1	22	20	-7	56	52	-9	92	86	-7
ETC351	SURG-3M		2	0.57	0.42	0.35	303	1	18	18	0	49	48	-2	78	77	-2
ETC353	SURG-3M		2	0.51	0.42	0.35	303	1	18	19	2	49	49	0	84	81	-3
ETC356	SURG-3M		2	0.51	0.39	0.35	302	1	17	15	-15	47	41	-16	77	67	-16
ETC376	SURG-3M		3	0.50	0.41	0.35	302	1	17	19	11	46	48	4	78	79	1

Table B-1 (continued)

Run	Run Type or VOC [a]	Rct'y Type [a]	Char Set [b]	NOx (ppm)	Pr.Eq. (ppm) [c]	k1 (min^{-1}) [d]	T (K) [e]	Ref [f]	Δ (O3-NO) Results (pphm) 2 Hour Expt	2 Hour Calc	2 Hour Δ%	4 Hour Expt	4 Hour Calc	4 Hour Δ%	6 Hour Expt	6 Hour Calc	6 Hour Δ%
ETC408	SURG-3M		3	0.53	0.41	0.35	300	1	17	16	-8	43	43	2	67	68	2
ETC411	SURG-3M		3	0.52	0.43	0.35	300	1	16	18	11	43	47	8	69	76	10
ETC413	SURG-3M		3	0.54	0.42	0.35	299	1	16	15	-7	42	42	1	66	68	3
ETC415	SURG-3M		3	0.53	0.42	0.35	298	1	12	16	23	37	44	16	60	69	14
ETC419	SURG-3M		3	0.54	0.45	0.35	299	1	15	18	18	42	49	14	66	78	16
DTC233B	SURG-3M		10	0.30	0.49	0.23	296	3	13	17	27	34	43	22	58	72	20
DTC235A	SURG-3M		10	0.31	0.46	0.23	297	3	13	16	20	34	40	14	59	68	14
DTC237B	SURG-3M		10	0.30	0.47	0.23	298	3	12	17	32	33	43	23	58	71	18
DTC239A	SURG-3M		10	0.33	0.49	0.23	297	3	13	17	21	34	40	13	59	65	10
DTC240B	SURG-3M		10	0.31	0.49	0.23	296	3	12	16	29	33	42	22	56	71	21
DTC241A	SURG-3M		10	0.33	0.48	0.23	295	3	14	15	8	33	38	13	54	65	17
DTC242B	SURG-3M		10	0.32	0.48	0.23	296	3	13	16	20	34	41	17	57	70	18
DTC243B	SURG-3M		10	0.31	0.47	0.23	296	3	12	14	17	31	37	16	52	64	19
DTC244A	SURG-3M		10	0.33	0.47	0.23	295	3	11	16	29	30	38	21	49	65	25
DTC264A	SURG-3M		10	0.31	0.47	0.22	298	3	11	16	31	32	40	21	53	69	23
DTC271A	SURG-3M		10	0.30	0.47	0.22	298	4	12	14	14	34	38	12	55	66	18
DTC273B	SURG-3M		10	0.31	0.48	0.22	298	4	14	14	5	37	37	2	63	66	4
DTC275B	SURG-3M		10	0.31	0.46	0.22	298	4	12	14	12	34	37	8	60	64	6
DTC277A	SURG-3M		10	0.33	0.51	0.22	298	4	13	22	42	35	51	31	61	80	24
DTC279A	SURG-3M		10	0.32	0.49	0.22	298	4	9	17	49	31	44	29	56	73	23
DTC282B	SURG-3M		10	0.34	0.48	0.22	299	4	15	16	5	39	40	2	68	68	1
DTC283A	SURG-3M		10	0.31	0.50	0.22	297	4	12	17	33	33	43	24	58	72	21
DTC289A	SURG-3M		10	0.35	0.50	0.22	297	4	12	16	28	33	40	19	55	68	20
DTC291A	SURG-3M		10	0.33	0.51	0.22	297	4	12	16	28	33	41	20	57	71	20
DTC302A	SURG-3M		11	0.35	0.47	0.21	297	24	8	14	42	27	35	25	46	60	23
DTC302B	SURG-3M		11	0.35	0.47	0.21	297	24	7	14	47	26	36	26	48	61	22
DTC303A	SURG-3M		11	0.33	0.51	0.21	298	24	11	16	35	33	41	19	59	70	17
DTC305B	SURG-3M		11	0.33	0.49	0.21	299	24	12	16	27	37	40	8	66	69	3
DTC315A	SURG-3M		11	0.33	0.47	0.21	298	5	15	15	-5	38	37	-2	62	63	2
DTC324B	SURG-3M		11	0.31	0.49	0.21	298	5	16	19	18	41	47	13	68	75	9
DTC327B	SURG-3M		11	0.33	0.51	0.21	297	9	12	16	24	34	40	14	60	69	13
DTC328A	SURG-3M		11	0.32	0.51	0.21	297	9	11	16	27	33	40	17	56	68	17
DTC336B	SURG-3M		11	0.32	0.50	0.21	296	9	13	15	16	33	38	12	57	65	13
DTC352B	SURG-3M		11	0.34	0.50	0.20	298	10	14	15	9	38	39	2	65	66	2
DTC358B	SURG-3M		11	0.33	0.50	0.20	298	10	15	16	4	39	40	3	64	67	3
DTC375B	SURG-3M		11	0.35	0.46	0.20	300	16	14	13	-7	34	34	0	57	58	2
DTC377A	SURG-3M		11	0.36	0.47	0.20	297	16	12	13	9	32	34	7	52	57	9
DTC380A	SURG-3M		11	0.37	0.47	0.20	298	16	11	10	-15	31	27	-14	52	46	-14
DTC385B	SURG-3M		11	0.39	0.44	0.19	298	11	11	11	-2	31	29	-6	50	47	-7
DTC389A	SURG-3M		11	0.37	0.45	0.19	299	11	13	11	-10	34	31	-12	56	51	-11
DTC395B	SURG-3M		11	0.41	0.45	0.19	299	10	14	11	-29	37	30	-24	61	48	-27
DTC398A	SURG-3M		11	0.43	0.47	0.19	297	10	13	11	-20	35	29	-19	57	47	-21
DTC401B	SURG-3M		11	0.36	0.44	0.19	298	10	11	12	2	32	31	-4	54	51	-6
DTC402A	SURG-3M		11	0.37	0.49	0.19	299	10	13	14	5	37	37	0	61	62	1
DTC426A	SURG-3M		11	0.36	0.53	0.18	297	12	10	14	24	33	36	9	56	62	10
DTC433B	SURG-3M		11	0.47	0.48	0.18	297	12	14	9	-60	39	24	-62	66	40	-67
DTC438B	SURG-3M		11	0.36	0.49	0.18	296	13	10	11	7	30	29	-5	50	46	-8
DTC439A	SURG-3M		11	0.35	0.48	0.18	297	13	11	11	7	31	31	0	51	51	-1
DTC440B	SURG-3M		11	0.35	0.48	0.18	296	13	10	12	13	30	30	2	50	49	-2
DTC441A	SURG-3M		11	0.35	0.48	0.18	294	13	9	10	13	25	27	6	40	44	8
DTC442B	SURG-3M		11	0.35	0.50	0.17	294	13	7	10	32	22	28	21	40	47	15
DTC447B	SURG-3M		11	0.39	0.51	0.17	297	14	11	11	1	32	29	-12	48	47	-1
DTC449A	SURG-3M		12	0.35	0.48	0.17	297	14	17	17	2	41	38	-7	64	61	-4
DTC449B	SURG-3M		11	0.35	0.48	0.17	297	14	13	10	-24	35	29	-19	55	47	-17
DTC450B	SURG-3M		11	0.37	0.52	0.17	297	14	12	11	-7	35	30	-16	57	49	-15
DTC467B	SURG-3M		13	0.36	0.48	0.16	294	14	9	12	20	26	27	2	39	43	9
DTC489B	SURG-3M		15	0.38		0.22	298	15	15	16	5	42	40	-3	74	70	-5
DTC491A	SURG-3M		14	0.38	0.52	0.22	298	15	17	17	-1	46	43	-7	81	74	-9
DTC495B	SURG-3M		15	0.38	0.51	0.22	299	15	15	17	11	42	43	1	75	74	-1
DTC498A	SURG-3M		14	0.38	0.31	0.22	299	15	8	8	0	26	23	-12	42	37	-12
DTC505A	SURG-3M		14	0.39	0.48	0.22	298	15	13	16	19	40	39	0	70	67	-5
DTC508A	SURG-3M		14	0.37	0.48	0.22	299	10	13	16	17	40	40	1	71	69	-3
DTC510A	SURG-3M		14	0.39	0.50	0.22	299	10	17	16	-5	46	40	-14	79	68	-16

Table B-1 (continued)

Run	Run Type or VOC [a]	Rct'y Type [a]	Char Set [b]	NOx (ppm)	Pr.Eq. (ppm) [c]	k1 (min^{-1}) [d]	T (K) [e]	Ref [f]	Δ (O3-NO) Results (pphm) 2 Hour Expt	2 Hour Calc	2 Hour Δ%	4 Hour Expt	4 Hour Calc	4 Hour Δ%	6 Hour Expt	6 Hour Calc	6 Hour Δ%
DTC512A	SURG-3M		14	0.38	0.47	0.21	299	10	14	14	6	40	36	-9	70	62	-14
DTC514A	SURG-3M		14	0.39	0.48	0.21	299	10	13	15	10	39	37	-7	71	61	-15
DTC517B	SURG-3M		15	0.37	0.49	0.21	299	10	12	14	15	37	37	1	68	65	-4
DTC522B	SURG-3M		15	0.37	0.48	0.21	299	10	12	14	10	36	36	-2	65	61	-5
DTC528A	SURG-3M		14	0.38	0.49	0.21	299	10	14	14	1	40	36	-10	71	62	-14
DTC529B	SURG-3M		15	0.36	0.45	0.21	299	10	12	12	-1	34	31	-11	63	54	-17
DTC532A	SURG-3M		14	0.36	0.49	0.21	299	10	11	14	24	34	37	7	64	65	2
DTC533B	SURG-3M		15	0.36	0.48	0.21	299	10	11	14	20	36	37	5	64	64	0
DTC537B	SURG-3M		15	0.35	0.46	0.21	299	10	10	13	20	33	34	2	61	59	-4
DTC541B	SURG-3M		15	0.38	0.49	0.21	299	10	11	13	17	35	34	-1	62	59	-6
DTC549A	SURG-3M		14	0.37	0.45	0.20	300	10	14	13	-8	39	33	-18	70	57	-23
DTC551B	SURG-3M		15	0.38	0.44	0.20	300	10	12	11	-4	35	29	-20	63	48	-31
DTC554A	SURG-3M		14	0.38	0.47	0.20	299	10	13	14	5	37	35	-4	66	60	-9
DTC558B	SURG-3M		15	0.34	0.49	0.20	300	10	11	13	18	33	35	8	61	63	3
DTC565B	SURG-3M		15	0.40	0.47	0.20	299	16	9	12	21	26	31	17	44	53	18
DTC570A	SURG-3M		14	0.37	0.51	0.20	298	16	11	14	18	34	36	4	59	61	2
DTC570B	SURG-3M		15	0.37	0.51	0.20	298	16	10	13	22	32	35	7	56	59	5
DTC590A	SURG-3M		14	0.42	0.56	0.19	297	16	10	15	32	31	38	18	52	63	18
DTC590B	SURG-3M		15	0.42	0.56	0.19	297	16	8	14	42	27	36	26	46	60	23
DTC600A	SURG-3M		14	0.37	0.49	0.19	298	23	10	13	23	31	33	7	54	55	2
DTC600B	SURG-3M		15	0.37	0.49	0.19	298	23	9	12	28	28	32	12	50	53	6
DTC601B	SURG-3M		15	0.38	0.49	0.19	298	23	-	12		30	31	4	52	52	1
DTC602B	SURG-3M		15	0.39	0.51	0.19	298	23	10	11	16	30	31	4	54	54	0
DTC603A	SURG-3M		16	0.38	0.49	0.19	298	23	14	16	17	36	39	7	62	64	3
DTC603B	SURG-3M		15	0.37	0.50	0.19	298	23	8	12	30	27	31	13	50	54	8
DTC618B	SURG-3M		17	0.42	0.50	0.18	297	23	8	9	1	27	25	-6	48	44	-9
DTC688A	SURG-3M		18	0.42	0.52	0.17	294	20	13	10	-29	37	29	-29	60	47	-28
DTC692A	SURG-3M		18	0.44	0.53	0.16	298	0	13	11	-21	38	28	-34	64	46	-38
DTC694B	SURG-3M		18	0.41	0.54	0.16	298	0	11	11	6	32	29	-10	55	47	-17
DTC701A	SURG-3M		18	0.40	0.49	0.16	296	0	11	9	-18	33	25	-32	56	40	-38
DTC703A	SURG-3M		18	0.43	0.52	0.16	296	0	10	10	-3	33	27	-24	57	44	-31
DTC724A	SURG-3M		18	0.34	0.46	0.16	294	0	7	10	29	27	28	7	47	47	1
DTC734A	SURG-3M		18	0.39	0.50	0.16	295	21	10	10	-1	32	28	-12	54	46	-16
DTC741B	SURG-3M		18	0.38	0.48	0.16	295	21	9	9	-3	29	25	-16	47	40	-17
DTC750A	SURG-3M		18	0.36	0.51	0.16	300	0	13	10	-21	34	29	-17	55	48	-13
DTC753B	SURG-3M		18	0.41	0.47	0.16	299	0	8	9	8	29	26	-12	48	42	-14
DTC757B	SURG-3M		18	0.38	0.47	0.16	299	0	10	9	-5	31	26	-17	51	43	-19
DTC759B	SURG-3M		18	0.37	0.47	0.16	299	0	9	10	6	29	26	-11	49	43	-13
DTC760A	SURG-3M		18	0.39	0.49	0.16	298	0	15	9	-61	33	23	-44	54	39	-38
DTC766B	SURG-3M		18	0.37	0.52	0.16	300	0	8	11	24	29	31	5	53	51	-3
DTC773B	SURG-3M		18	0.38	0.50	0.16	300	0	10	11	4	31	29	-5	51	48	-5
DTC783A	SURG-3M		18	0.40	0.55	0.16	300	0	13	12	-10	35	32	-10	55	54	-2
XTC104	SURG-3M		1	0.51	0.33	0.25	301	1	11	12	8	37	36	-1	58	55	-4
CTC100A	SURG-3M		4	0.45	0.35	0.19	295	2	5	6	26	16	22	27	-	37	
CTC100B	SURG-3M		4	0.45	0.36	0.19	295	2	5	7	28	18	24	24	-	40	
CTC101A	SURG-3M		4	0.36	0.44	0.19	295	2	8	12	33	26	35	26	43	58	25
CTC101B	SURG-3M		4	0.35	0.44	0.19	295	2	8	12	29	28	35	21	45	59	23
CTC103A	SURG-3M		5	0.30	0.46	0.19	295	2	10	16	34	30	41	27	-	66	
CTC103B	SURG-3M		5	0.30	0.46	0.19	295	2	11	16	34	31	44	29	-	69	
CTC104B	SURG-3M		5	0.29	0.45	0.19	295	2	11	15	28	31	42	26	52	68	24
CTC105A	SURG-3M		5	0.30	0.45	0.19	296	2	11	16	32	32	41	24	53	66	20
CTC107B	SURG-3M		5	0.30	0.44	0.19	295	2	10	15	29	32	40	20	-	65	
CTC108A	SURG-3M		5	0.31	0.44	0.19	295	2	10	13	29	30	38	21	-	63	
CTC109B	SURG-3M		5	0.31	0.43	0.19	295	2	11	13	16	33	38	14	-	64	
CTC110A	SURG-3M		5	0.30	0.46	0.19	296	2	11	15	26	34	43	20	-	69	
CTC112B	SURG-3M		5	0.29	0.43	0.19	296	2	11	14	22	31	39	20	-	64	
CTC113A	SURG-3M		5	0.30	0.20	0.19	297	2	13	6	-118	34	21	-61	-	33	
CTC113B	SURG-3M		5	0.30	0.21	0.19	297	2	12	6	-93	34	23	-47	-	35	
CTC119A	SURG-3M		5	0.31	0.43	0.19	294	2	12	12	6	30	34	12	-	57	
CTC121B	SURG-3M		5	0.31	0.42	0.19	292	2	9	12	25	27	34	20	-		
CTC142A	SURG-3M		6	0.37	0.34	0.18	295	2	6	6	9	18	21	16	-	35	
CTC172A	SURG-3M		7	0.32	0.44	0.17	294	10	7	9	22	26	28	8	-	49	
CTC172B	SURG-3M		7	0.32	0.44	0.17	294	10	8	9	11	27	28	3	-	50	

Table B-1 (continued)

Run	Run Type or VOC [a]	Rct'y Type [a]	Char Set [b]	NOx (ppm)	Pr.Eq. (ppm) [c]	k1 (min^{-1}) [d]	T (K) [e]	Ref [f]	Δ (O3-NO) Results (pphm) 2 Hour Expt	2 Hour Calc	2 Hour Δ%	4 Hour Expt	4 Hour Calc	4 Hour Δ%	6 Hour Expt	6 Hour Calc	6 Hour Δ%
CTC181B	SURG-3M		7	0.23	0.43	0.16	298	10	13	11	-19	39	33	-17	63	54	-16
CTC183B	SURG-3M		7	0.23	0.43	0.16	298	10	12	11	-8	37	34	-9	61	55	-11
CTC184A	SURG-3M		7	0.23	0.43	0.16	298	17	11	10	-8	35	32	-11	60	53	-13
CTC185B	SURG-3M		7	0.28	0.43	0.16	301	17	12	11	-7	36	34	-5	60	56	-7
CTC192B	SURG-3M		7	0.22	0.41	0.16	298	17	9	9	-2	32	28	-14	57	49	-17
CTC196B	SURG-3M		8	0.22	0.42	0.15	297	10	10	11	6	34	34	-1	-	54	
CTC197A	SURG-3M		8	0.25		0.15	297	18	10	10	7	33	31	-5	57	53	-9
CTC201B	SURG-3M		8	0.24	0.54	0.15	298	18	9	8	-16	29	27	-8	51	49	-3
CTC209A	SURG-3M		8	0.25	0.45	0.15	298	18	10	10	9	32	32	0	55	53	-4
CTC211A	SURG-3M		8	0.23	0.46	0.15	298	18	8	11	27	30	34	10	54	54	-1
CTC216A	SURG-3M		8	0.24	0.44	0.14	298	19	10	10	1	33	31	-6	57	52	-10
CTC221B	SURG-3M		8	0.24	0.42	0.14	299	19	9	9	1	32	30	-6	55	51	-9
CTC231B	SURG-3M		9	0.27	0.51	0.14	303	5	8	14	47	27	39	32	-	58	
CTC246B	SURG-3M		9	0.25	0.48	0.13	295	6	6	10	36	30	31	4	53	50	-6
CTC250A	SURG-3M		9	0.24	0.45	0.13	296	6	7	10	30	27	29	8	50	48	-3
CTC255B	SURG-3M		9	0.22	0.44	0.13	296	20	7	10	33	26	30	14	48	48	1
CTC257B	SURG-3M		10	0.24	0.46	0.13	297	20	7	8	18	26	28	7	47	47	0
DTC725B	SURG-4M		18		0.51	0.16	295	21	10	10	4	30	27	-14	48	41	-16
DTC730B	SURG-4M		18	0.31	0.52	0.16	296	21	9	11	25	26	29	11	44	48	8
DTC733B	SURG-4M		18	0.30	0.53	0.16	296	21	9	12	29	27	30	10	47	50	7
DTC749B	SURG-4M		18	0.38	0.54	0.16	298	21	12	11	-1	34	30	-13	54	48	-12
CTC266B	SURG-4M		10	0.24	0.46	0.12	299	6	10	7	-49	33	23	-44	53	40	-32
ETC217	SURG-3		2	0.26	0.39	0.35	299	1	18	23	20	55	59	7	84	87	3
ETC219	SURG-3		2	0.25	0.38	0.35	300	1	20	22	10	58	58	0	85	85	0
ETC387	SURG-3		3	0.15	0.28	0.35	301	1	21	22	2	52	51	-1	62	65	5
ETC388	SURG-3		3	0.15	0.34	0.35	301	1	25	27	7	58	59	2	65	67	4
ETC390	SURG-3		3	0.14	0.34	0.35	300	1	23	26	15	56	57	3	64	65	2
ETC392	SURG-3		3	0.15	0.32	0.35	300	1	24	23	-4	58	55	-5	68	69	2
ETC395	SURG-3		3	0.14	0.34	0.35	299	1	24	26	9	57	57	-1	66	64	-2
ETC399	SURG-3		3	0.15	0.35	0.35	300	1	23	28	18	54	60	9	60	68	12
ETC401	SURG-3		3	0.15	0.35	0.35	300	1	20	27	27	53	59	10	60	66	9
ETC403	SURG-3		3	0.15	0.31	0.35	299	1	19	22	15	50	53	6	62	65	5
ETC405	SURG-3		3	0.13	0.33	0.35	299	1	21	26	17	53	55	5	61	63	2
ETC407	SURG-3		3	0.16	0.34	0.35	300	1	23	27	18	56	61	8	67	71	5
DTC318A	SURG-3		11	0.34	0.49	0.21	297	5	12	14	13	32	36	10	55	62	11
DTC360A	SURG-3		11	0.25	0.52	0.20	297	10	12	18	35	32	45	29	57	67	15
DTC360B	SURG-3		11	0.24	0.52	0.20	297	10	11	18	39	31	45	30	57	67	15
DTC362A	SURG-3		11	0.30	0.50	0.20	298	10	12	15	18	34	39	13	60	66	9
DTC364A	SURG-3		11	0.32	0.48	0.20	298	10	14	14	-5	37	36	-5	63	62	-2
DTC365B	SURG-3		11	0.32	0.49	0.20	298	10	13	15	12	35	38	6	61	65	5
DTC366A	SURG-3		11	0.33	0.50	0.20	298	10	13	15	15	35	39	10	60	67	10
DTC368A	SURG-3		11	0.35	0.49	0.20	299	10	13	14	6	35	35	0	61	60	-1
DTC369B	SURG-3		11	0.35	0.49	0.20	298	10	12	14	10	34	35	3	59	60	2
DTC415A	SURG-3		11	0.20	0.48	0.19	297	10	15	16	4	42	40	-5	61	58	-5
DTC421B	SURG-3		11	0.39	0.52	0.19	297	12	13	12	-11	37	32	-17	64	53	-21
DTC011A	SURG-8M		1	0.52	0.39	0.39	301	1	38	35	-7	60	56	-8	-	71	
DTC011B	SURG-8M		1	0.52	0.38	0.39	301	1	39	36	-9	61	55	-11	78	69	-13
DTC012A	SURG-8M		1	0.52	0.41	0.39	301	1	42	37	-14	63	57	-11	81	73	-11
DTC012B	SURG-8M		1	0.51	0.41	0.39	301	1	42	38	-12	64	58	-10	-	74	
DTC013A	SURG-8M		1	0.45	0.40	0.39	300	1	40	38	-5	61	58	-4	79	75	-4
DTC013B	SURG-8M		1	0.45	0.40	0.39	300	1	41	37	-9	62	57	-8	-	74	
DTC014B	SURG-8M		1	0.48	0.39	0.39	301	1	41	37	-12	62	57	-10	80	72	-11
DTC015A	SURG-8M		1	0.50	0.41	0.39	301	1	43	37	-16	66	58	-13	-	76	
DTC016B	SURG-8M		1	0.48	0.38	0.39	300	1	40	35	-14	62	55	-13	78	69	-13
DTC017B	SURG-8M		1	0.48	0.38	0.39	300	1	40	36	-11	61	55	-11	78	71	-10
DTC018B	SURG-8M		1	0.48	0.41	0.39	301	1	44	38	-14	66	59	-10	84	77	-9
DTC019A	SURG-8M		1	0.46	0.40	0.39	300	1	39	38	-3	60	59	-3	77	77	-1
DTC020A	SURG-8M		1	0.50	0.38	0.39	300	1	32	26	-24	53	48	-11	68	63	-8
DTC021A	SURG-8M		1	0.49	0.42	0.39	300	1	41	40	-2	61	60	-1	77	78	1
DTC022A	SURG-8M		1	0.50	0.40	0.39	300	1	40	37	-7	61	58	-6	77	74	-4
DTC023B	SURG-8M		1	0.47	0.40	0.39	301	1	40	39	-2	61	60	-2	80	78	-2
DTC024A	SURG-8M		1	0.50	0.41	0.39	301	1	41	38	-6	63	59	-6	82	77	-6
DTC025B	SURG-8M		1	0.47	0.42	0.39	302	1	40	41	1	64	64	0	85	85	0

Table B-1 (continued)

Run	Run Type or VOC [a]	Rct'y Type [a]	Char Set [b]	NOx (ppm)	Pr.Eq. (ppm) [c]	k1 (min^{-1}) [d]	T (K) [e]	Ref [f]	Δ (O3-NO) Results (pphm) 2 Hour Expt	2 Hour Calc	2 Hour Δ%	4 Hour Expt	4 Hour Calc	4 Hour Δ%	6 Hour Expt	6 Hour Calc	6 Hour Δ%
DTC028B	SURG-8M		1	0.49	0.41	0.39	301	1	39	40	3	61	62	1	80	80	1
DTC064A	SURG-8M		1	0.49	0.40	0.39	302	1	38	38	0	60	59	-1	77	78	1
DTC065B	SURG-8M		1	0.48	0.40	0.39	301	1	37	38	4	58	60	3	75	79	5
DTC068A	SURG-8M		1	0.48	0.38	0.39	301	1	34	36	4	56	56	1	72	74	2
DTC069B	SURG-8M		1	0.48	0.36	0.39	302	1	37	35	-6	58	55	-5	75	73	-3
DTC070B	SURG-8M		1	0.49	0.40	0.39	301	1	37	38	2	58	60	3	74	79	6
DTC249B	SURG-8M		10	0.26	0.36	0.23	297	3	24	28	16	36	44	16	47	57	18
DTC250A	SURG-8M		10	0.27	0.34	0.23	297	3	23	25	8	36	41	12	45	54	16
DTC251A	SURG-8M		10	0.26	0.34	0.23	297	3	24	26	9	37	41	10	46	53	13
DTC251B	SURG-8M		10	0.26	0.35	0.23	297	3	24	26	9	37	41	11	46	54	14
DTC252B	SURG-8M		10	0.26	0.37	0.23	297	3	25	29	13	38	45	16	48	58	19
DTC255A	SURG-8M		10	0.27	0.34	0.23	297	3	22	25	14	33	40	16	42	52	20
DTC256B	SURG-8M		10	0.27	0.36	0.23	297	3	24	27	12	35	42	17	46	56	17
DTC272B	SURG-8M		10	0.14	0.33	0.22	298	4	26	30	14	37	42	11	11	46	75
DTC274A	SURG-8M		10	0.16	0.35	0.22	298	4	30	31	5	43	45	5	47	50	6
DTC276A	SURG-8M		10	0.17	0.36	0.22	298	4	33	33	0	47	47	-1	51	52	2
DTC278B	SURG-8M		10	0.16	0.39	0.22	298	4	32	36	11	46	47	3	51	49	-2
DTC280B	SURG-8M		10	0.17	0.37	0.22	298	4	32	34	8	45	48	5	50	51	2
DTC281A	SURG-8M		10	0.16	0.37	0.22	298	4	30	34	11	44	46	6	48	50	5
DTC284B	SURG-8M		10	0.15	0.37	0.22	298	4	31	34	9	44	45	2	49	48	-3
DTC290B	SURG-8M		10	0.17	0.37	0.22	298	4	31	33	8	44	46	5	49	51	5
DTC292B	SURG-8M		10	0.16	0.56	0.22	297	4	23	27	13	38	44	14	46	51	11
DTC311A	SURG-8M		11	0.29	0.37	0.21	298	24	26	26	2	42	42	1	52	55	5
DTC317B	SURG-8M		11	0.18	0.37	0.21	297	5	30	33	8	43	46	7	48	52	8
DTC319A	SURG-8M		11	0.18	0.34	0.21	297	5	27	29	8	40	42	6	-	50	
DTC320B	SURG-8M		11	0.30	0.38	0.21	297	24	25	27	5	41	43	3	52	56	6
DTC332B	SURG-8M		11	0.57	0.38	0.21	297	9	15	16	10	29	31	8	37	40	8
DTC335A	SURG-8M		11	0.43	0.40	0.21	297	9	21	22	8	37	40	6	46	50	8
DTC338B	SURG-8M		11	0.29	0.39	0.21	297	10	24	28	14	40	44	10	50	57	11
DTC359A	SURG-8M		11	0.28	0.39	0.20	298	10	26	29	8	43	45	6	54	58	8
DTC370A	SURG-8M		11	0.28	0.36	0.20	298	10	24	24	2	40	40	1	50	52	3
DTC378A	SURG-8M		11	0.26	0.55	0.20	298	16	44	42	-6	63	63	0	71	74	4
DTC381B	SURG-8M		11	0.27	0.34	0.20	298	16	26	24	-7	41	38	-7	51	49	-5
DTC390B	SURG-8M		11	0.28	0.36	0.19	297	11	25	24	-6	41	39	-5	52	51	-2
DTC396A	SURG-8M		11	0.29	0.35	0.19	299	10	28	22	-26	44	37	-18	56	49	-15
DTC399B	SURG-8M		11	0.27	0.37	0.19	298	10	27	25	-7	42	39	-7	53	51	-5
DTC403B	SURG-8M		11	0.30	0.39	0.19	299	10	27	28	2	44	45	2	55	58	5
DTC408A	SURG-8M		11	0.28	0.36	0.19	298	10	30	24	-23	46	39	-18	57	51	-13
DTC410A	SURG-8M		11	0.28	0.37	0.19	298	10	29	26	-12	45	41	-10	56	53	-5
DTC414B	SURG-8M		11	0.27	0.39	0.19	298	10	28	27	-4	45	42	-6	56	53	-5
DTC419A	SURG-8M		11	0.29	0.45	0.19	297	12	31	32	2	47	49	5	58	63	8
DTC423A	SURG-8M		11	0.29	0.50	0.19	297	12	27	36	25	44	55	19	56	67	17
DTC427B	SURG-8M		11	0.26	0.47	0.18	298	12	28	36	21	47	54	13	59	64	8
DTC430B	SURG-8M		11	0.25	0.40	0.18	297	12	29	28	-4	46	43	-7	58	54	-7
DTC455A	SURG-8M		12	0.25	0.40	0.17	297	14	27	28	3	43	42	-1	52	53	2
DTC455B	SURG-8M		11	0.25	0.41	0.17	297	14	25	25	-1	42	40	-4	52	51	-2
DTC456B	SURG-8M		11	0.28	0.40	0.17	297	14	26	25	-3	41	41	-2	50	51	3
DTC459B	SURG-8M		11	0.29	0.41	0.16	298	14	24	24	1	41	40	-1	51	50	-1
DTC474A	SURG-8M		14	0.31	0.39	0.23	298	13	33	30	-11	51	46	-11	66	60	-10
DTC474B	SURG-8M		15	0.30	0.40	0.23	298	13	32	30	-8	51	46	-10	65	60	-9
DTC476B	SURG-8M		15	0.31	0.41	0.22	298	13	33	31	-8	52	48	-9	66	62	-7
DTC478B	SURG-8M		15	0.31	0.44	0.22	297	13	34	34	0	53	52	-2	67	66	-2
DTC480B	SURG-8M		15	0.30	0.41	0.22	298	13	33	31	-6	51	48	-7	66	63	-6
DTC486B	SURG-8M		15	0.30	0.41	0.22	298	13	33	31	-6	51	48	-8	66	62	-6
DTC488A	SURG-8M		14	0.30	0.38	0.22	298	13	32	23	-43	51	40	-26	66	53	-23
DTC488B	SURG-8M		15	0.30	0.38	0.22	298	13	32	22	-43	50	40	-25	64	53	-22
DTC492B	SURG-8M		15	0.30	0.38	0.22	298	15	29	28	-3	46	44	-4	59	58	-3
DTC493A	SURG-8M		14	0.30	0.38	0.22	297	15	29	28	-4	47	44	-5	61	58	-5
DTC500B	SURG-8M		15	0.30	0.42	0.22	298	15	32	32	0	50	49	-2	64	63	-1
DTC502B	SURG-8M		15	0.30	0.39	0.22	299	15	32	29	-11	50	46	-9	64	59	-7
DTC509B	SURG-8M		15	0.30	0.38	0.22	299	10	32	27	-18	50	44	-15	64	57	-13
DTC511B	SURG-8M		15	0.31	0.39	0.21	299	10	32	28	-16	51	45	-14	65	58	-12
DTC515B	SURG-8M		15	0.31	0.37	0.21	299	10	31	25	-24	49	41	-20	63	53	-18

Table B-1 (continued)

Run	Run Type or VOC [a]	Rct'y Type [a]	Char Set [b]	NOx (ppm)	Pr.Eq. (ppm) [c]	k1 (min^{-1}) [d]	T (K) [e]	Ref [f]	Δ (O3-NO) Results (pphm) 2 Hour Expt	2 Hour Calc	2 Hour Δ%	4 Hour Expt	4 Hour Calc	4 Hour Δ%	6 Hour Expt	6 Hour Calc	6 Hour Δ%
DTC516A	SURG-8M		14	0.32	0.40	0.21	299	10	31	28	-9	49	45	-10	64	59	-9
DTC521A	SURG-8M		14	0.30	0.39	0.21	299	10	32	28	-14	50	45	-12	64	58	-10
DTC530A	SURG-8M		14	0.31	0.37	0.21	299	10	29	26	-15	47	41	-13	60	54	-11
DTC534A	SURG-8M		14	0.29	0.38	0.21	299	10	29	27	-7	48	44	-9	62	57	-8
DTC538A	SURG-8M		14	0.29	0.37	0.21	299	10	28	27	-3	46	43	-6	59	56	-5
DTC547A	SURG-8M		14	0.31	0.36	0.20	300	10	31	25	-21	49	41	-18	63	54	-16
DTC552A	SURG-8M		14	0.31	0.37	0.20	300	10	32	26	-26	52	43	-21	67	56	-20
DTC556B	SURG-8M		15	0.28	0.42	0.20	300	10	26	33	20	44	50	11	58	63	9
DTC610B	SURG-8M		17	0.31	0.43	0.19	297	23	26	30	13	43	46	7	54	58	7
DTC616A	SURG-8M		16	0.81	0.37	0.19	297	23	9	11	18	19	22	14	26	30	13
DTC616B	SURG-8M		17	0.80	0.38	0.19	297	23	8	10	16	16	19	15	23	27	16
DTC689B	SURG-8M		18	0.33	0.44	0.16	294	20	27	25	-10	46	41	-12	58	50	-15
DTC693B	SURG-8M		18	0.31	0.45	0.16	298	0	29	29	0	48	46	-3	60	58	-3
DTC695A	SURG-8M		18	0.32	0.50	0.16	299	0	29	31	9	49	50	3	63	63	1
DTC697B	SURG-8M		18	0.32	0.42	0.16	296	20	30	24	-22	49	41	-17	60	52	-17
DTC702B	SURG-8M		18	0.32	0.44	0.16	297	0	26	25	-3	45	42	-6	57	53	-6
DTC705B	SURG-8M		18	0.29	0.45	0.16	296	0	25	27	9	42	44	4	56	55	-2
DTC720A	SURG-8M		18	0.33	0.40	0.16	296	0	28	21	-34	46	39	-18	58	50	-17
DTC726A	SURG-8M		18	0.29	0.42	0.16	294	21	24	24	1	43	42	-1	55	53	-3
DTC729A	SURG-8M		18	0.24	0.40	0.16	294	21	18	25	30	36	41	13	47	52	10
DTC737B	SURG-8M		18	0.32	0.43	0.16	294	21	24	22	-7	41	40	-5	51	49	-5
DTC738A	SURG-8M		18	0.31	0.42	0.16	293	21	25	23	-11	43	41	-4	54	52	-4
DTC746A	SURG-8M		18	0.30	0.44	0.16	298	21	25	28	11	42	45	6	54	57	6
DTC747B	SURG-8M		18	0.29	0.43	0.16	299	21	24	27	12	42	44	6	52	55	6
DTC754A	SURG-8M		18	0.31	0.43	0.16	299	0	26	27	5	44	44	1	56	56	0
DTC755B	SURG-8M		18	0.29	0.43	0.16	299	0	26	27	4	44	43	-1	55	54	-1
DTC762B	SURG-8M		18	0.30	0.42	0.16	299	0	25	25	-3	44	42	-4	54	53	-1
DTC769B	SURG-8M		18	0.28	0.43	0.16	299	0	19	28	32	39	45	13	50	57	11
DTC771B	SURG-8M		18	0.29	0.44	0.16	299	0	24	29	19	42	46	8	53	58	9
DTC772A	SURG-8M		18	0.30	0.44	0.16	299	0	26	27	4	45	44	-1	56	56	-1
DTC776B	SURG-8M		18	0.30	0.40	0.16	300	0	24	24	-3	43	42	-3	54	54	0
DTC780A	SURG-8M		18	0.30	0.42	0.16	300	0	25	24	-5	44	42	-5	56	53	-5
DTC786B	SURG-8M		18	0.30	0.47	0.16	300	0	23	30	24	39	47	16	47	58	19
CTC123B	SURG-8M		5	0.40	0.53	0.18	293	2	35	34	0	52	58	10	64	74	13
CTC124A	SURG-8M		5	0.39	0.51	0.18	293	2	33	33	0	49	54	9	-	69	
CTC126B	SURG-8M		5	0.38	0.51	0.18	294	2	32	33	2	50	54	9	-		
CTC127A	SURG-8M		5	0.39	0.51	0.18	293	2	33	31	-6	50	53	6	-	67	
CTC128B	SURG-8M		5	0.40	0.55	0.18	294	2	35	36	2	53	58	9	-	75	
CTC130A	SURG-8M		5	0.39	0.53	0.18	293	2	32	33	2	50	55	8	63	70	10
CTC131B	SURG-8M		5	0.40	0.54	0.18	293	2	33	34	3	51	56	9	64	72	11
CTC138A	SURG-8M		6	0.40	0.55	0.18	293	2	34	35	3	51	56	9	64	71	11
CTC140B	SURG-8M		6	0.37	0.55	0.18	294	2	30	37	18	49	59	18	-	74	
CTC149A	SURG-8M		6	0.42	0.47	0.18	299	4	25	23	-8	42	42	-1	-	51	
CTC149B	SURG-8M		6	0.42	0.46	0.18	299	4	25	22	-13	42	41	-2	-	52	
CTC150A	SURG-8M		6	0.43	0.54	0.18	299	4	36	33	-9	59	57	-3	75	73	-4
CTC151B	SURG-8M		6	0.51	0.54	0.18	303	4	37	33	-11	57	55	-4	71	68	-4
CTC152A	SURG-8M		6	0.38	0.45	0.18	301	4	27	25	-7	43	42	-3	52	51	-2
CTC154B	SURG-8M		6	0.42	0.54	0.18	301	4	41	35	-15	62	60	-4	78	77	-1
CTC156A	SURG-8M		6	0.41	0.52	0.18	303	4	36	34	-6	58	58	0	-	74	
CTC158B	SURG-8M		6	0.36	0.52	0.18	304	4	35	39	11	60	64	7	-	79	
CTC165A	SURG-8M		7	0.57	0.57	0.18	305	5	31	36	14	51	61	16	-	80	
CTC165B	SURG-8M		7	0.57	0.58	0.18	305	5	32	36	9	51	60	15	-	80	
CTC167B	SURG-8M		7	0.41	0.57	0.18	300	5	36	39	8	58	63	9	-	80	
CTC168A	SURG-8M		7	0.41	0.58	0.18	300	5	37	40	9	59	64	9	-	80	
CTC171A	SURG-8M		7	0.39	0.56	0.17	300	5	38	36	-5	61	60	-2	-	73	
CTC171B	SURG-8M		7	0.39	0.55	0.17	300	5	37	35	-6	61	59	-3	-	74	
CTC180A	SURG-8M		7	0.39	0.57	0.16	298	10	35	35	1	57	57	0	72	71	-2
CTC182A	SURG-8M		7	0.39	0.57	0.16	298	10	36	34	-5	58	56	-3	74	70	-5
CTC186A	SURG-8M		7	0.38	0.53	0.16	298	17	32	30	-5	54	53	-3	70	67	-4
CTC193A	SURG-8M		7	0.37	0.55	0.16	298	17	35	32	-11	57	54	-7	72	67	-8
CTC198B	SURG-8M		8	0.39	0.58	0.15	298	18	34	33	-5	56	56	0	71	71	0
CTC204B	SURG-8M		8	0.44	0.60	0.15	298	18	32	31	-5	56	57	1	71	72	3
CTC208B	SURG-8M		8	0.43	0.61	0.15	298	18	32	34	4	56	59	6	70	74	6

Table B-1 (continued)

Run	Run Type or VOC [a]	Rct'y Type [a]	Char Set [b]	NOx (ppm)	Pr.Eq. (ppm) [c]	k1 (min^{-1}) [d]	T (K) [e]	Ref [f]	Δ (O3-NO) Results (pphm) 2 Hour Expt	2 Hour Calc	2 Hour Δ%	4 Hour Expt	4 Hour Calc	4 Hour Δ%	6 Hour Expt	6 Hour Calc	6 Hour Δ%
CTC212A	SURG-8M		8			0.15	298	18	29	29	0	52	53	2	66	67	1
CTC217B	SURG-8M		8	0.43	0.58	0.14	297	19	31	28	-13	55	53	-3	70	67	-3
CTC222A	SURG-8M		8	0.45	0.55	0.14	299	19	32	26	-24	56	50	-11	71	64	-12
CTC232A	SURG-8M		9	0.46	0.57	0.14	301	5	20	27	27	42	51	17	-	65	
CTC239A	SURG-8M		9	0.44	0.59	0.13	301	5	28	30	7	52	55	6	-	69	
CTC248A	SURG-8M		9	0.32	0.60	0.13	292	6	32	41	22	54	62	13	66	70	5
CTC251B	SURG-8M		9	0.34	0.63	0.13	294	6	32	36	13	52	58	9	66	68	4
CTC260A	SURG-8M		10	0.40	0.65	0.12	295	20	28	32	12	50	57	13	63	70	10
CTC262B	SURG-8M		10	0.38	0.60	0.12	294	20	29	29	0	50	53	4	64	64	0
DTC027A	SURG-8		1	0.15	0.40	0.39	302	1	52	49	-6	61	59	-4	63	61	-3
DTC027B	SURG-8		1	0.15	0.41	0.39	302	1	52	50	-4	61	59	-4	63	61	-3
DTC029B	SURG-8		1	0.17	0.43	0.39	301	1	54	53	-2	63	64	2	64	66	3
DTC030A	SURG-8		1	0.17	0.40	0.39	300	1	50	50	-1	59	62	4	60	64	6
DTC031B	SURG-8		1	0.17	0.43	0.39	301	1	52	53	1	61	63	4	62	66	5
DTC032A	SURG-8		1	0.17	0.42	0.39	300	1	51	52	3	60	63	5	61	65	7
DTC033B	SURG-8		1	0.17	0.41	0.39	300	1	51	51	0	60	62	2	62	64	4
DTC034A	SURG-8		1	0.16	0.41	0.39	301	1	50	50	0	60	62	4	60	64	7
DTC035B	SURG-8		1	0.17	0.40	0.39	301	1	51	49	-3	60	62	4	61	65	6
DTC036B	SURG-8		1	0.18	0.44	0.39	300	1	54	53	-2	-	65		63	67	6
DTC037A	SURG-8		1	0.17	0.42	0.39	301	1	51	52	1	61	64	5	61	66	7
DTC038B	SURG-8		1	0.17	0.39	0.39	301	1	51	49	-4	59	62	4	61	64	6
DTC039A	SURG-8		1	0.18	0.41	0.39	301	1	52	51	-3	61	64	6	61	67	9
DTC066A	SURG-8		1	0.17	0.37	0.39	302	1	49	47	-4	59	62	5	60	66	9
DTC067A	SURG-8		1	0.17	0.38	0.39	301	1	48	48	-1	59	62	5	60	65	8
DTC071A	SURG-8		1	0.18	0.39	0.39	302	1	49	49	0	60	64	7	61	68	11
DTC258A	SURG-8		10	0.14	0.36	0.23	297	3	28	33	15	35	43	17	36	44	19
DTC258B	SURG-8		10	0.13	0.36	0.23	297	3	29	33	14	36	42	16	-	44	
DTC259B	SURG-8		10	0.16	0.35	0.23	297	3	27	32	16	37	44	16	41	49	16
DTC260A	SURG-8		10	0.17	0.36	0.22	297	3	28	32	14	39	46	16	42	52	18
DTC261B	SURG-8		10	0.16	0.34	0.22	296	3	25	31	18	36	44	18	39	48	19
DTC266B	SURG-8		10	0.16	0.34	0.22	298	3	25	31	18	36	44	20	39	50	21
DTC267A	SURG-8		10	0.16	0.36	0.22	299	3	29	33	12	40	46	13	43	51	16
DTC268B	SURG-8		10	0.16	0.47	0.22	299	3	34	40	15	46	54	14	49	58	15
DTC269B	SURG-8		10	0.17	0.36	0.22	299	3	30	33	7	42	46	9	45	52	13
DTC293B	SURG-8		10	0.08	0.39	0.22	297	4	28	29	4	32	30	-5	32	30	-6
DTC298A	SURG-8		10	0.09	0.38	0.22	298	4	29	30	4	31	31	0	31	31	1
DTC308A	SURG-8		11	0.17	0.37	0.21	301	24	32	33	3	45	48	6	48	54	11
DTC309B	SURG-8		11	0.17	0.53	0.21	299	24	42	45	5	49	52	6	49	53	6
DTC321A	SURG-8		11	0.11	0.38	0.21	298	24	30	32	7	33	36	8	32	37	12
DTC325A	SURG-8		11	0.18	0.42	0.21	299	5	31	37	17	44	50	13	47	54	13
DTC329B	SURG-8		11	0.18	0.39	0.21	296	9	29	34	13	43	47	8	49	51	5
DTC330A	SURG-8		11	0.17	0.39	0.21	296	9	30	34	12	43	46	6	48	49	4
DTC386A	SURG-8		11	0.29	0.34	0.19	298	11	26	20	-31	41	34	-21	52	44	-18
DTC388B	SURG-8		11	0.11	0.37	0.19	298	11	29	30	2	34	34	-1	34	34	0
DTC391A	SURG-8		11	0.11	0.36	0.19	297	11	30	29	-2	35	34	-3	35	34	-3
DTC394B	SURG-8		11	0.11	0.36	0.19	296	10	29	30	2	34	35	2	34	36	5
DTC397B	SURG-8		11	0.13	0.36	0.19	298	10	32	31	-3	38	39	3	38	41	8
DTC400A	SURG-8		11	0.12	0.36	0.19	298	10	31	30	-4	36	37	1	36	38	5
DTC406B	SURG-8		11	0.13	0.39	0.19	299	10	32	33	3	37	38	3	37	38	4
DTC409B	SURG-8		11	0.11	0.36	0.19	298	10	31	30	-3	35	36	2	34	37	7
DTC411B	SURG-8		11	0.11	0.36	0.19	297	10	30	29	-3	35	35	1	34	35	4
DTC412A	SURG-8		11	0.11	0.36	0.19	297	10	30	31	4	35	36	5	35	37	6
DTC418B	SURG-8		11	0.10	0.38	0.19	298	10	30	30	-1	34	34	-2	34	34	0
DTC420A	SURG-8		11	0.10	0.47	0.19	297	12	32	31	-3	35	31	-12	34	31	-11
DTC424B	SURG-8		11	0.10	0.44	0.18	297	12	31	30	-5	35	30	-15	34	30	-14
DTC428A	SURG-8		11	0.12	0.42	0.18	298	12	32	32	1	36	37	3	35	37	6
DTC432A	SURG-8		11	0.09	0.42	0.18	297	12	33	28	-18	37	29	-28	36	28	-27
DTC451A	SURG-8		12	0.10	0.43	0.17	297	14	31	30	-4	36	33	-9	36	33	-8
DTC451B	SURG-8		11	0.10	0.44	0.17	297	14	32	29	-8	37	31	-17	36	31	-17
DTC453B	SURG-8		11	0.14	0.40	0.17	295	14	29	30	3	35	37	5	35	38	10
DTC454B	SURG-8		11	0.12	0.40	0.17	297	14	29	29	1	34	34	-1	33	34	1
DTC462A	SURG-8		12	0.13	0.40	0.16	299	14	30	31	4	36	37	3	35	38	7
DTC466B	SURG-8		13	0.13	0.38	0.16	297	14	30	29	-5	-	34		34	34	2

Table B-1 (continued)

Run	Run Type or VOC [a]	Rct'y Type [a]	Char Set [b]	NOx (ppm)	Pr.Eq. (ppm) [c]	k1 (min^{-1}) [d]	T (K) [e]	Ref [f]	Δ (O3-NO) Results (pphm) 2 Hour Expt	2 Hour Calc	2 Hour Δ%	4 Hour Expt	4 Hour Calc	4 Hour Δ%	6 Hour Expt	6 Hour Calc	6 Hour Δ%
DTC477A	SURG-8		14	0.13	0.46	0.22	297	13	38	38	-1	43	42	-2	43	42	-2
DTC479A	SURG-8		14	0.14	0.44	0.22	297	13	37	38	2	44	44	0	44	44	0
DTC481A	SURG-8		14	0.13	0.41	0.22	298	13	37	36	-2	42	41	-2	42	41	-2
DTC487A	SURG-8		14	0.13	0.40	0.22	298	13	37	35	-3	42	41	-4	43	41	-4
DTC496A	SURG-8		14	0.13	0.41	0.22	299	15	37	36	-3	43	41	-4	44	42	-5
DTC497B	SURG-8		15	0.13	0.41	0.22	299	15	37	36	-3	43	42	-3	44	43	-3
DTC501A	SURG-8		14	0.13	0.40	0.22	299	15	37	35	-6	43	41	-5	44	42	-5
DTC506B	SURG-8		15	0.12	0.39	0.22	298	15	35	34	-2	41	40	-2	41	40	-2
DTC513B	SURG-8		15	0.13	0.36	0.21	298	10	35	33	-8	42	40	-4	43	42	-2
DTC519A	SURG-8		14	0.13	0.34	0.21	298	10	35	32	-8	41	39	-6	42	40	-5
DTC520B	SURG-8		15	0.12	0.39	0.21	299	10	35	34	-4	41	40	-2	42	41	-2
DTC524A	SURG-8		14	0.13	0.39	0.21	299	10	36	34	-6	42	40	-5	43	41	-4
DTC525B	SURG-8		15	0.13	0.38	0.21	299	10	37	34	-8	44	42	-6	45	43	-4
DTC531B	SURG-8		15	0.12	0.37	0.21	299	10	35	33	-7	42	39	-7	43	40	-6
DTC539B	SURG-8		15	0.13	0.38	0.21	299	10	34	34	-2	41	41	-1	42	42	0
DTC540A	SURG-8		14	0.12	0.37	0.21	299	10	35	33	-6	40	40	-2	42	41	-1
DTC543A	SURG-8		14	0.30	0.40	0.21	299	10	31	29	-5	48	45	-7	62	58	-7
DTC544B	SURG-8		15	0.13	0.38	0.21	299	10	36	34	-7	43	41	-3	44	43	-2
DTC548B	SURG-8		15	0.13	0.37	0.20	299	10	35	32	-9	42	41	-3	43	43	0
DTC553B	SURG-8		15	0.13	0.37	0.20	300	10	36	33	-7	43	42	-3	44	44	-1
DTC557A	SURG-8		14	0.12	0.42	0.20	300	10	35	35	0	42	40	-5	43	41	-6
DTC559B	SURG-8		15	0.28		0.20	299	10	26	32	17	43	50	15	54	64	15
DTC560B	SURG-8		15	0.12	0.41	0.20	299	16	30	33	11	37	37	1	38	37	-2
DTC604A	SURG-8		16	0.14	0.38	0.19	298	23	35	33	-6	40	41	3	41	43	5
DTC608B	SURG-8		17	0.15	0.43	0.19	297	23	32	35	9	40	43	7	41	44	7
DTC609A	SURG-8		16	0.14	0.42	0.19	298	23	31	35	10	37	41	10	-	42	
DTC609B	SURG-8		17	0.13	0.42	0.19	298	23	31	34	9	37	41	8	-	41	
DTC698A	SURG-8		18	0.10	0.43	0.16	295	0	30	29	-3	33	32	-1	33	32	-4
DTC700B	SURG-8		18	0.10	0.44	0.16	296	0	30	30	-2	33	32	-2	33	32	-2
DTC707A	SURG-8		18	0.10	0.41	0.16	297	0	30	28	-7	35	32	-8	35	32	-8
DTC723B	SURG-8		18	0.11	0.42	0.16	295	0	30	29	-1	33	33	-1	33	33	-1
DTC732A	SURG-8		18	0.08	0.42	0.16	296	21	26	25	-3	29	26	-9	29	26	-10
DTC739B	SURG-8		18	0.10	0.40	0.16	295	21	26	28	7	28	31	8	28	30	9
DTC740A	SURG-8		18	0.10	0.40	0.16	295	21	26	28	7	29	31	6	28	31	8
DTC748A	SURG-8		18	0.09	0.43	0.16	297	21	25	27	7	27	28	6	26	28	7
DTC758A	SURG-8		18	0.09	0.44	0.16	299	0	27	28	2	29	30	3	28	30	4
DTC763A	SURG-8		18	0.09	0.42	0.16	299	0	25	27	9	27	29	10	26	30	11
DTC763A	SURG-8		18	0.09	0.42	0.16	299	0	25	27	9	27	29	10	26	30	11
DTC770A	SURG-8		18	0.08	0.42	0.16	299	0	22	26	17	24	28	16	23	28	18
DTC778B	SURG-8		18	0.09	0.43	0.16	300	0	27	28	3	-	30		29	31	6
DTC782B	SURG-8		18	0.09	0.46	0.16	300	0	26	27	7	27	29	9	26	29	12
DTC787A	SURG-8		18	0.10	0.44	0.16	299	0	25	29	14	27	32	16	-	32	
XTC109	SURG-8		1	0.24	0.38	0.25	302	1	41	38	-7	63	60	-6	-	72	
XTC116	SURG-8		1	0.22	0.42	0.25	301	1	45	42	-6	64	62	-3	69	71	2
CTC187B	SURG-8		7	0.15	0.58	0.16	298	17	39	38	-3	44	42	-5	44	42	-5
CTC194B	SURG-8		8	0.15	0.58	0.16	297	17	39	38	-3	44	42	-5	44	42	-5
CTC195A	SURG-8		8	0.14	0.52	0.15	297	10	39	36	-9	44	41	-7	44	41	-5
CTC199A	SURG-8		8	0.16	0.58	0.15	298	18	39	39	-1	44	44	-1	44	44	-1
CTC205A	SURG-8		8	0.17	0.59	0.15	298	18	41	40	-2	46	45	-2	46	45	-3
CTC210B	SURG-8		8	0.16	0.60	0.15	298	18	40	39	-2	44	43	-3	44	43	-2
CTC215B	SURG-8		8	0.18	0.56	0.15	297	18	41	39	-5	47	46	-2	47	47	0
CTC220A	SURG-8		8	0.16	0.55	0.14	298	19	40	38	-4	46	44	-3	46	45	-2
CTC223B	SURG-8		8	0.17	0.56	0.14	298	19	40	39	-2	46	45	-1	46	46	0
CTC233B	SURG-8		9	0.17	0.62	0.14	299	5	38	40	5	43	44	4	43	45	5
CTC235B	SURG-8		9	0.15	0.60	0.14	301	10	36	37	3	40	41	2	41	42	4
CTC238B	SURG-8		9	0.16	0.58	0.13	301	10	37	39	4	43	44	4	43	45	5
CTC240B	SURG-8		9	0.16	0.60	0.13	300	5	37	39	6	42	44	3	-	44	
CTC249B	SURG-8		9	0.16	0.63	0.13	295	6	37	38	3	42	42	1	42	42	-1
CTC253A	SURG-8		9	0.16	0.63	0.13	295	6	39	39	-1	45	44	-3	45	44	-2
CTC258A	SURG-8		10	0.17	0.59	0.13	296	20	39	38	-1	44	44	0	43	45	5
CTC259B	SURG-8		10	0.17	0.64	0.12	295	20	37	39	4	43	44	2	43	44	3
CTC263A	SURG-8		10	0.16	0.62	0.12	294	20	37	38	1	42	43	1	41	43	4
CTC267A	SURG-8		10	0.16	0.59	0.12	300	6	36	37	2	40	42	6	39	43	8

Table B-1 (continued)

Run	Run Type or VOC [a]	Rct'y Type [a]	Char Set [b]	NOx (ppm)	Pr.Eq. (ppm) [c]	k1 (min^{-1}) [d]	T (K) [e]	Ref [f]	Δ (O3-NO) Results (pphm) 2 Hour Expt	2 Hour Calc	2 Hour Δ%	4 Hour Expt	4 Hour Calc	4 Hour Δ%	6 Hour Expt	6 Hour Calc	6 Hour Δ%
OTC275B	SURG-8		11	0.63	0.44	0.00	319	8	84	75	-11	148	137	-8	-	158	
OTC276A	SURG-8		11	0.58	0.44	0.00	315	8	80	69	-15	135	120	-13	144	144	0
OTC277A	SURG-8		11	0.51	0.40	0.00	312	8	67	61	-10	121	109	-12	-	131	
OTC277B	SURG-8		11	0.52	0.39	0.00	312	8	63	60	-6	115	109	-6	133	132	-1

[a] See Table 45 for the definitions of the codes used to designate run type and incremental reactivity experiment category.

[b] Characterization set. Runs with the same chamber and characterization set number are assumed to have the same chamber effects and (for CTC runs) light spectrum.

[c] "Propene equivalent" for all VOCs injected in experiment. Sum of measured initial VOC concentration times OH rate constant, divided by the OH rate constant for propene.

[d] NO_2 photolysis rate assigned for this experiment.

[e] Average measured temperature for this experiment.

[f] References for reports describing chamber experiments. These reports are (or will be) available at http://cert.ucr.edu/~carter/bycarter.htm.

0 Unpublished results from this laboratory.

1 Carter et al. (1995d)
2 Carter et al. (1997a)
3 Carter et al. (1996c)
4 Carter et al. (1996a)
5 Carter et al. (2000c)
6 Carter et al. (1999b)
7 Carter et al. (1995c)
8 Carter et al. (1993b). See also Carter et al, (1995c).
9 Carter et al. (1996b)
10 Carter et al. (2000a)
11 Carter et al. (1997b)
12 Carter et al. (1997d)
13 Carter et al. (1997f)
14 Carter et al. (1997i)
15 Carter et al. (2000f)
16 Carter et al. (1999c)
17 Carter et al. (1997c)
18 Carter et al. (1997e)
19 Carter et al. (1997g)
20 Carter et al. (2000e)
21 Carter et al. (2000b)
22 Carter et al. (2000d)
23 Carter et al. (1999a)
24 Carter et al. (1996d)
25 Carter et al. (2000g)

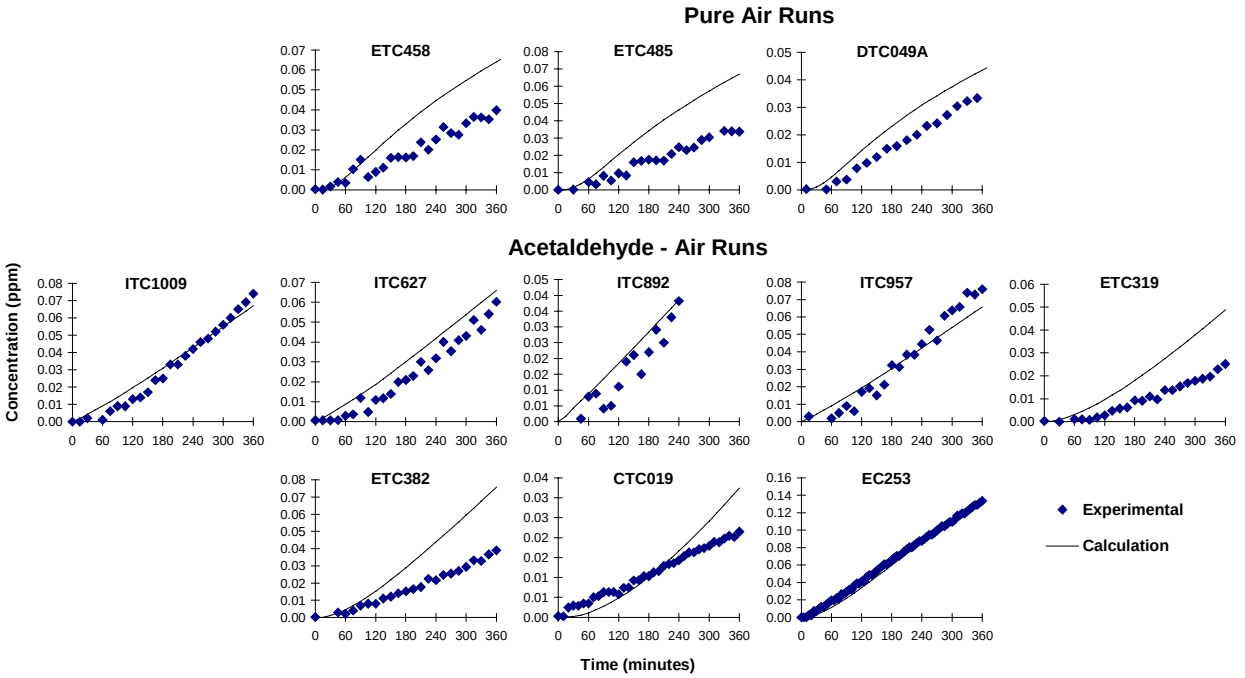

Figure B-1. Plots of experimental and calculated ozone data for the pure air and acetaldehyde - air runs.

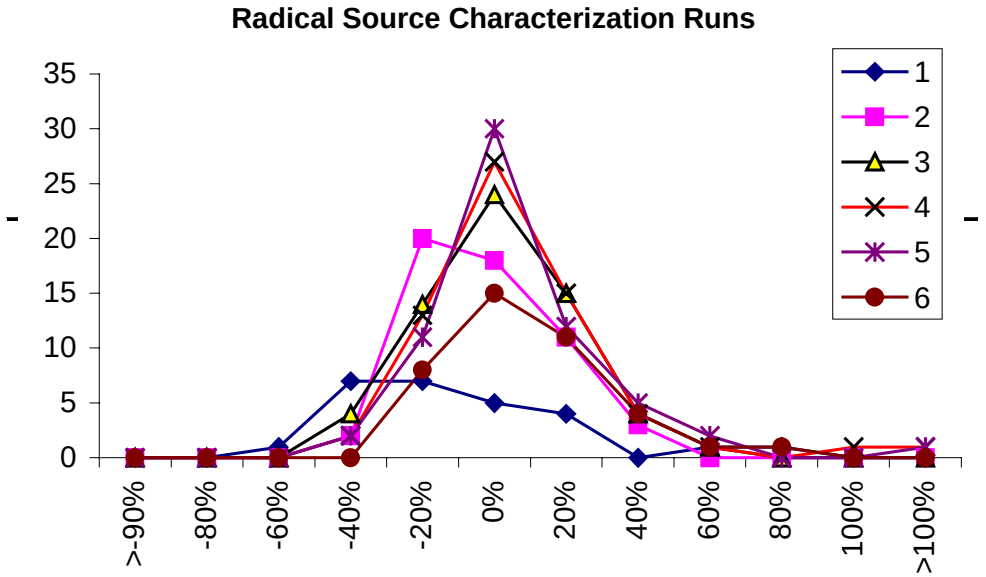

Figure B-2. Distribution plots of percentage errors of fits of calculated to experimental hourly $\Delta([O_3]-[NO])$ data for the radical source characterization (CO - NO_x and n-butane - NO_x) runs.

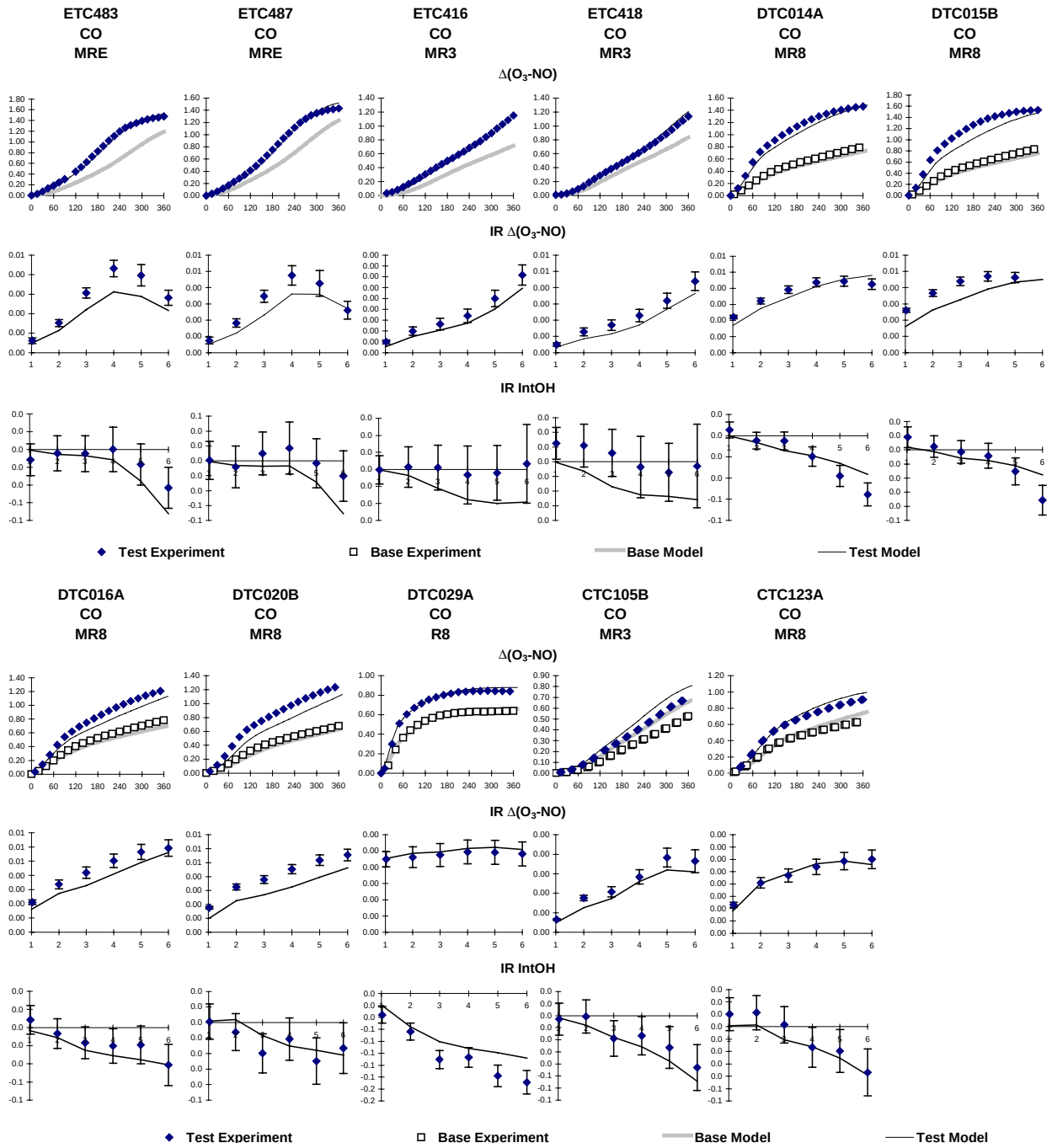

Figure B-3. Plots of experimental and calculated results of the incremental reactivity experiments with CO.

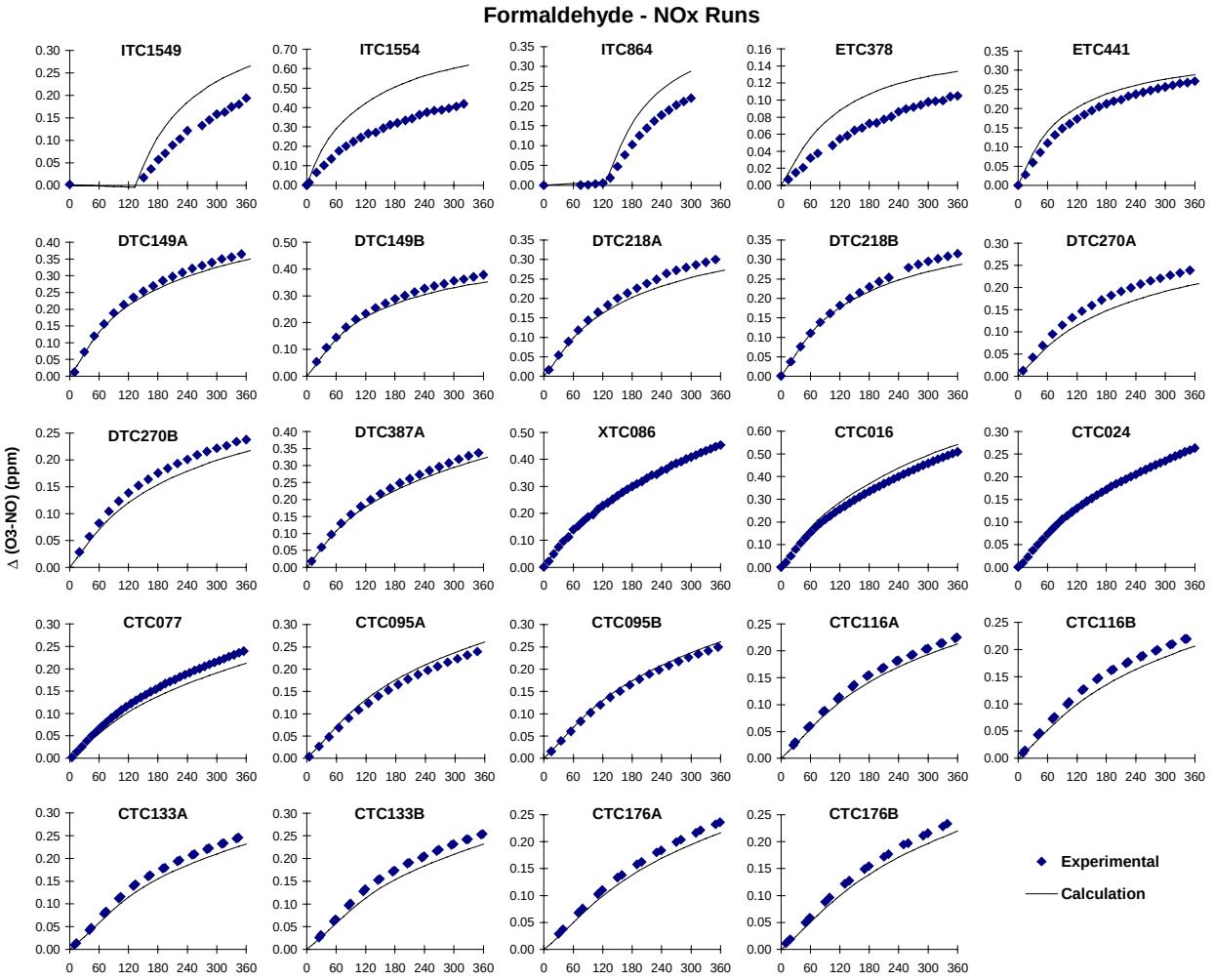

Figure B-4. Plots of experimental and calculated $\Delta([O_3]-[NO])$ data for the formaldehyde - NO_x experiments.

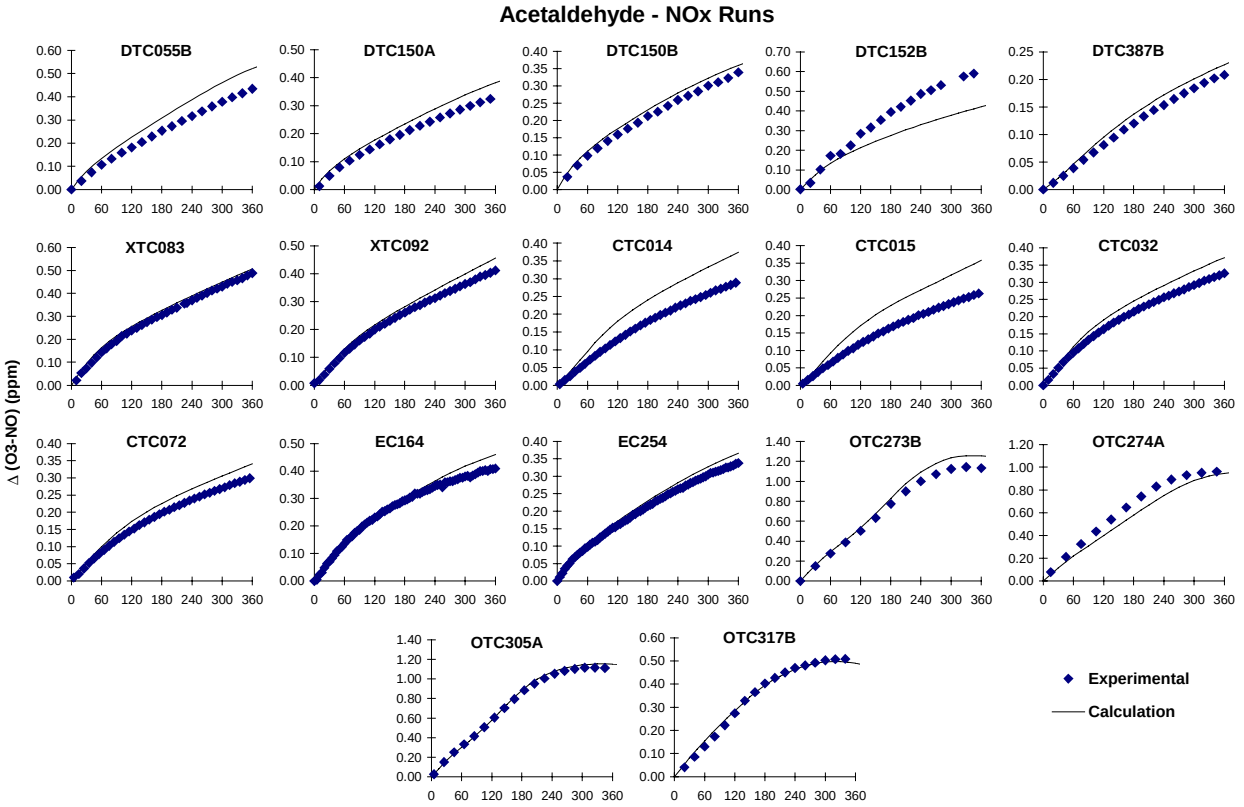

Figure B-5. Plots of experimental and calculated $\Delta([O_3]-[NO])$ data for the acetaldehyde - NO_x experiments.

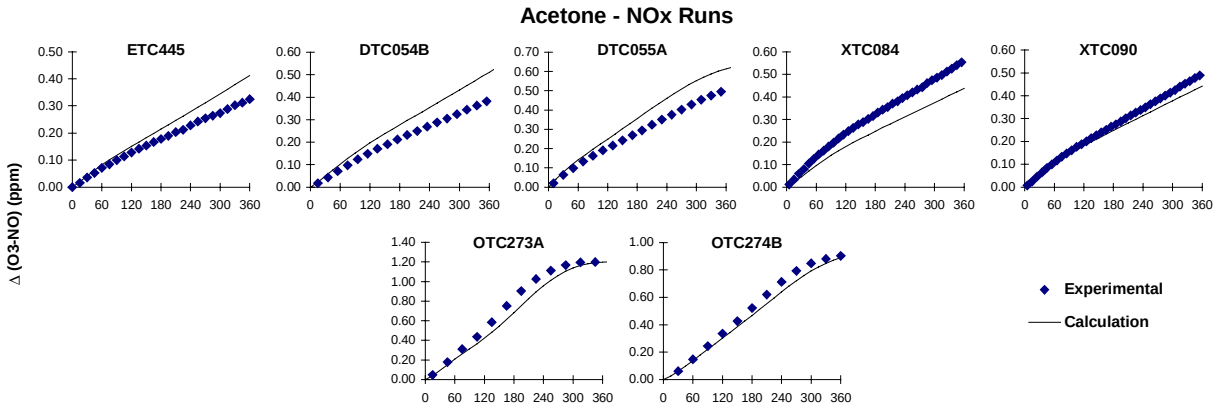

Figure B-6. Plots of experimental and calculated $\Delta([O_3]-[NO])$ data for the acetone - NO_x experiments.

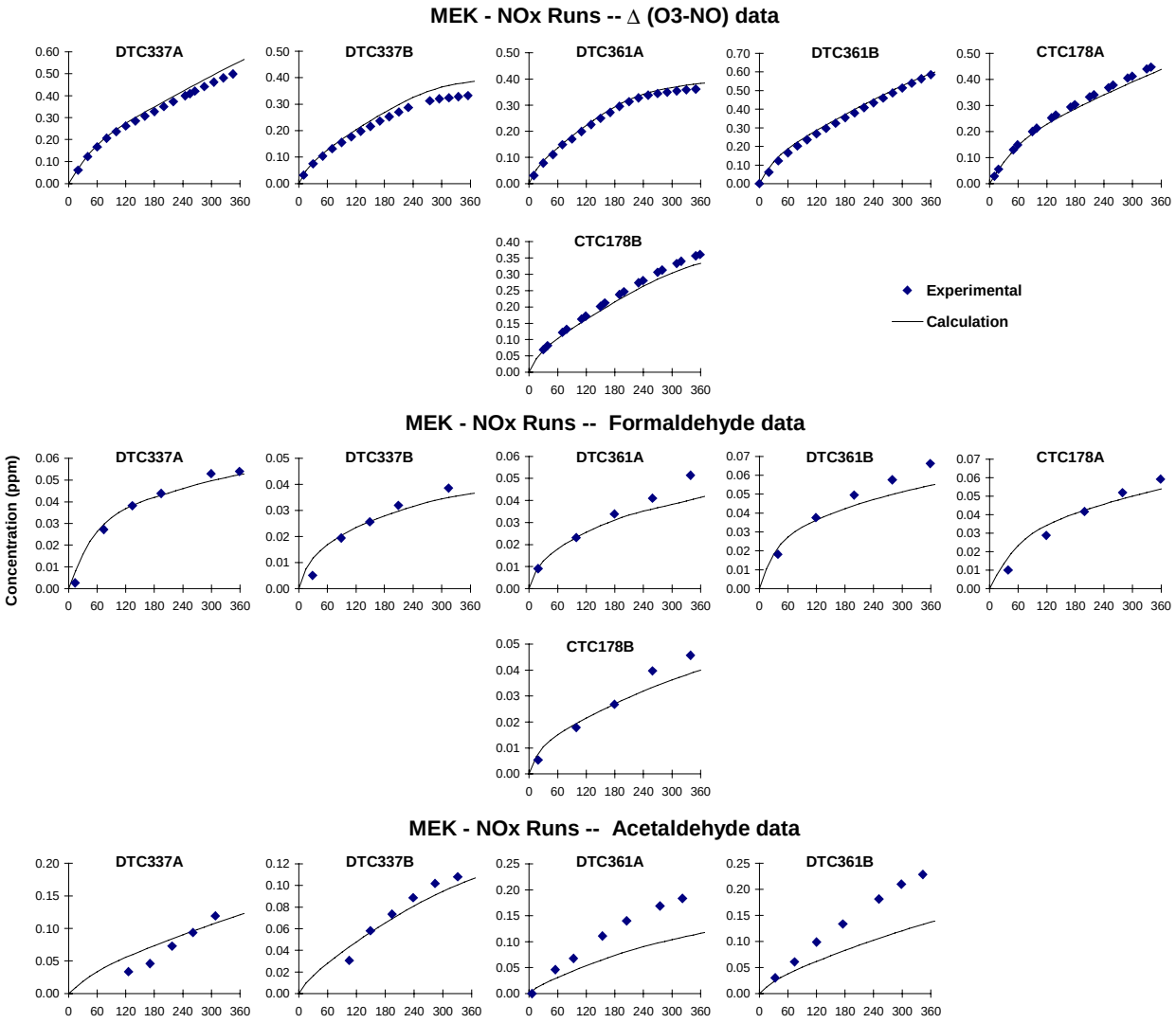

Figure B-7. Plots of experimental and calculated $\Delta([O_3]-[NO])$, formaldehyde, and acetaldehyde data for the methyl ethyl ketone (MEK) - NO_x experiments.

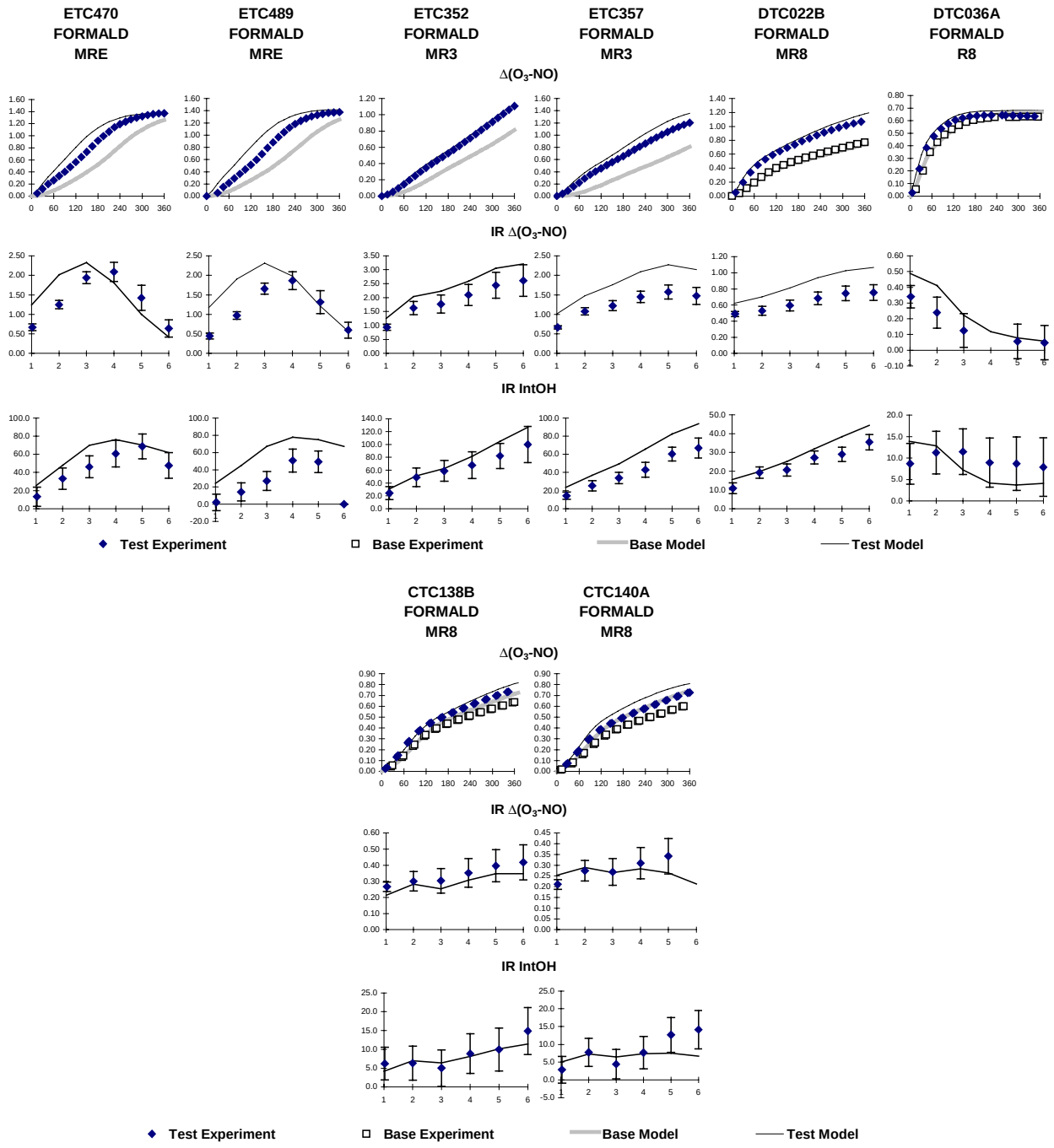

Figure B-8. Plots of experimental and calculated results of the incremental reactivity experiments with formaldehyde.

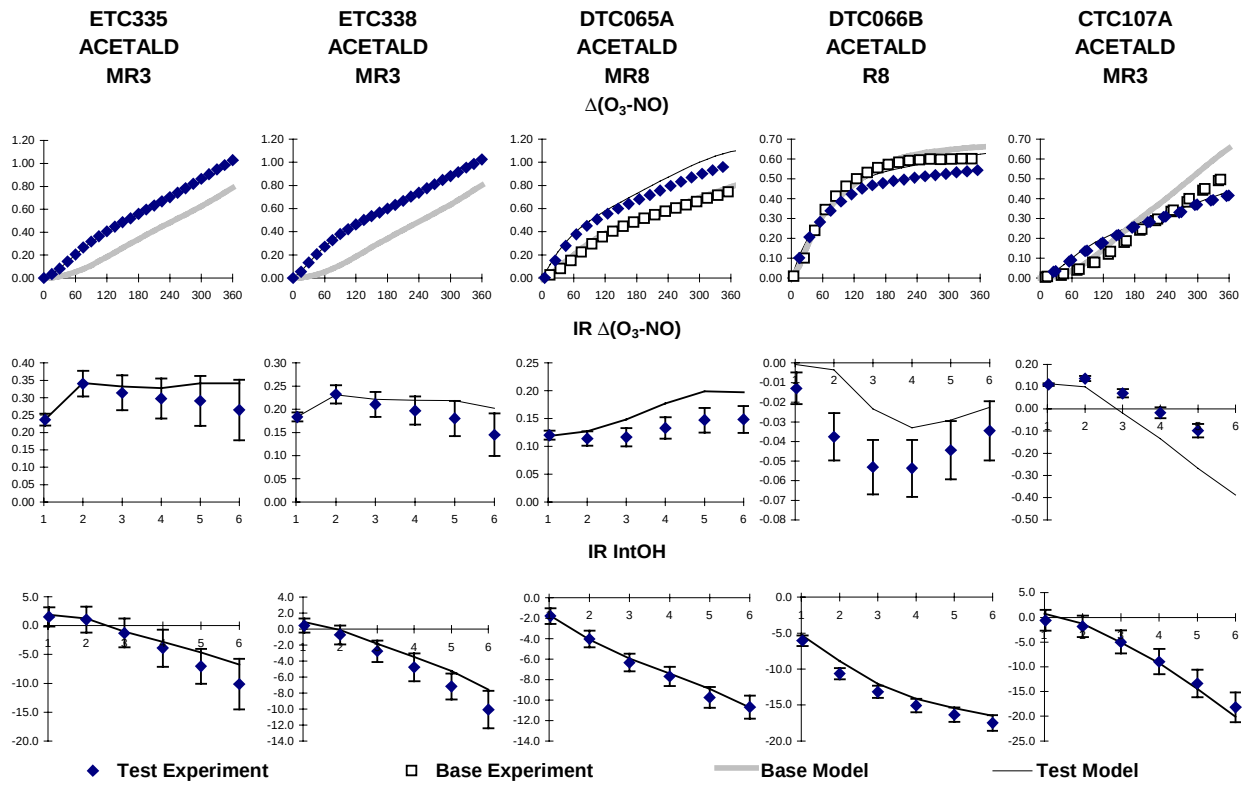

Figure B-9. Plots of experimental and calculated results of the incremental reactivity experiments with acetaldehyde.

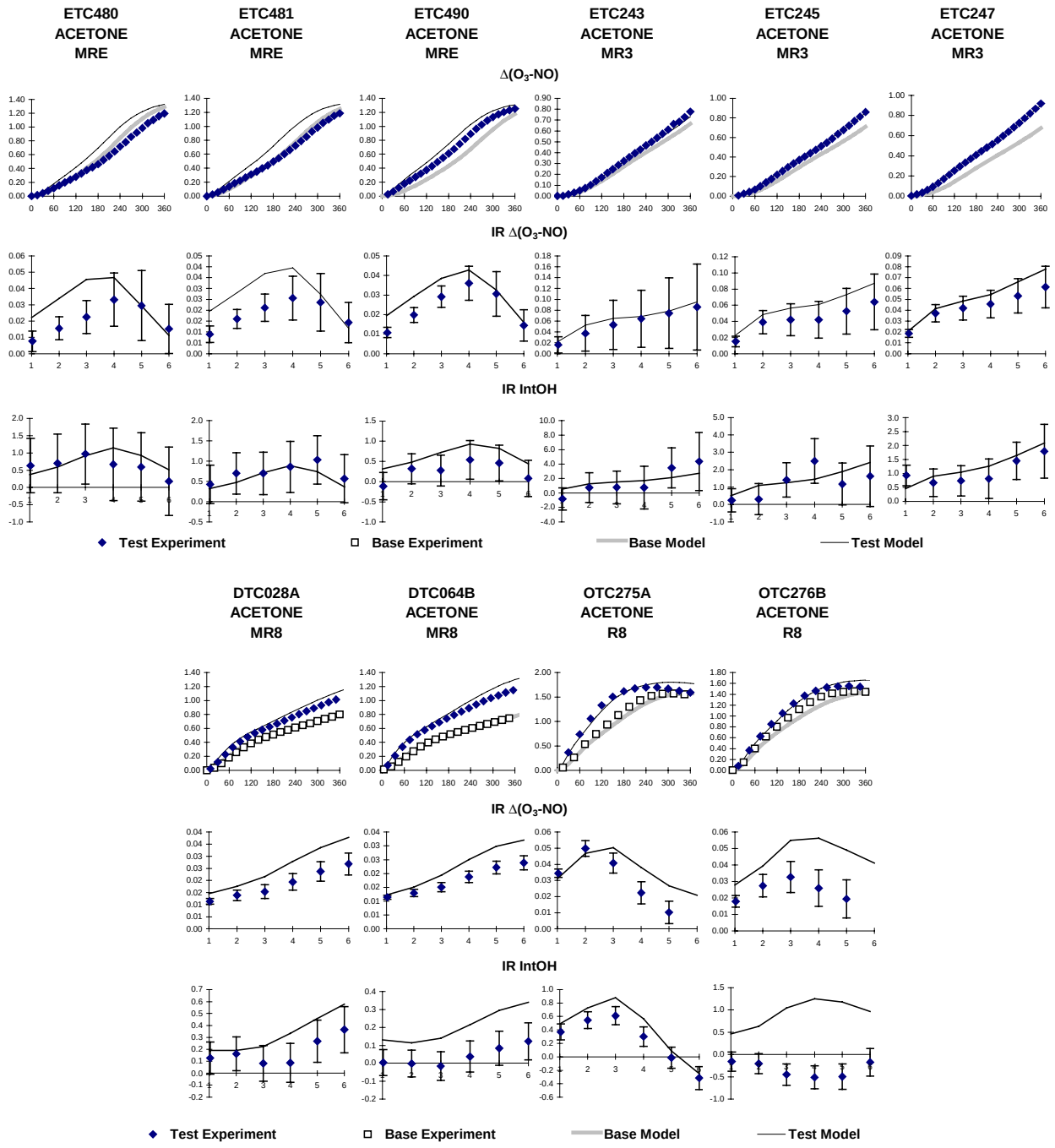

Figure B-10. Plots of experimental and calculated results of the incremental reactivity experiments with acetone.

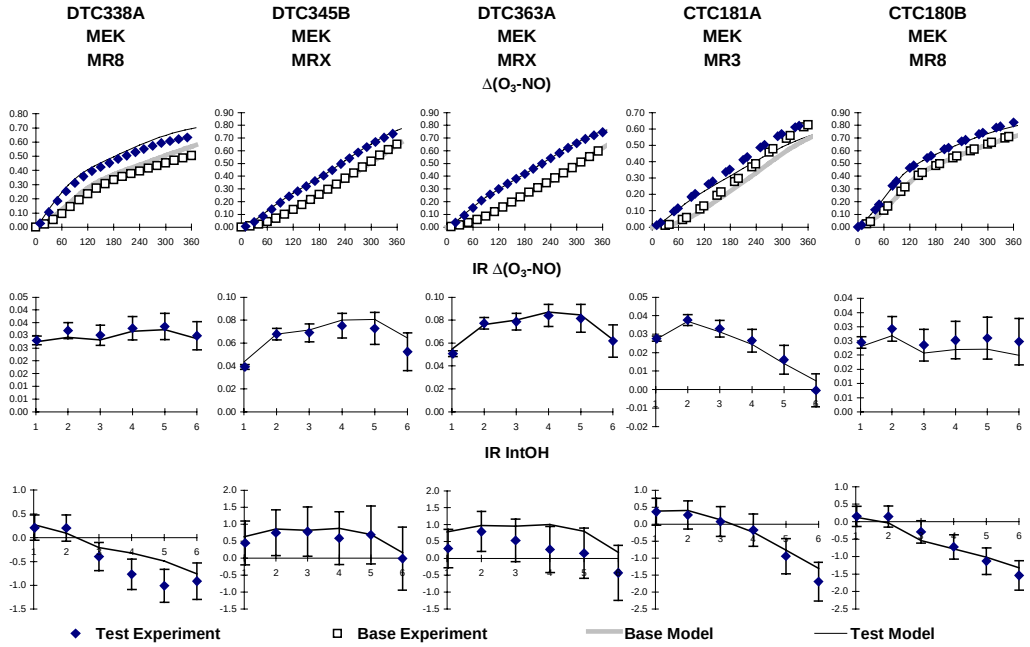

Figure B-11. Plots of experimental and calculated results of the incremental reactivity experiments with methyl ethyl ketone.

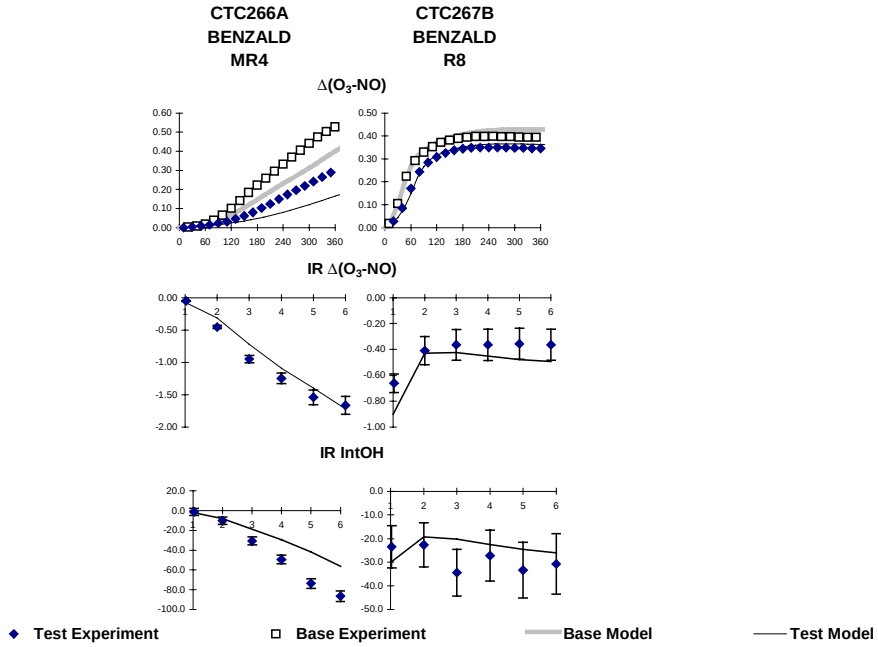

Figure B-12. Plots of experimental and calculated results of the incremental reactivity experiments with benzaldehyde.

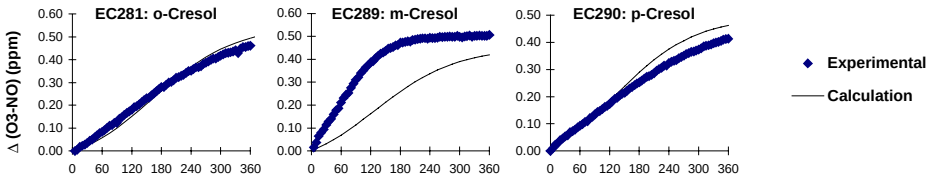

Figure B-13. Plots of experimental and calculated $\Delta([O_3]-[NO])$ data for the cresol - NO_x experiments.

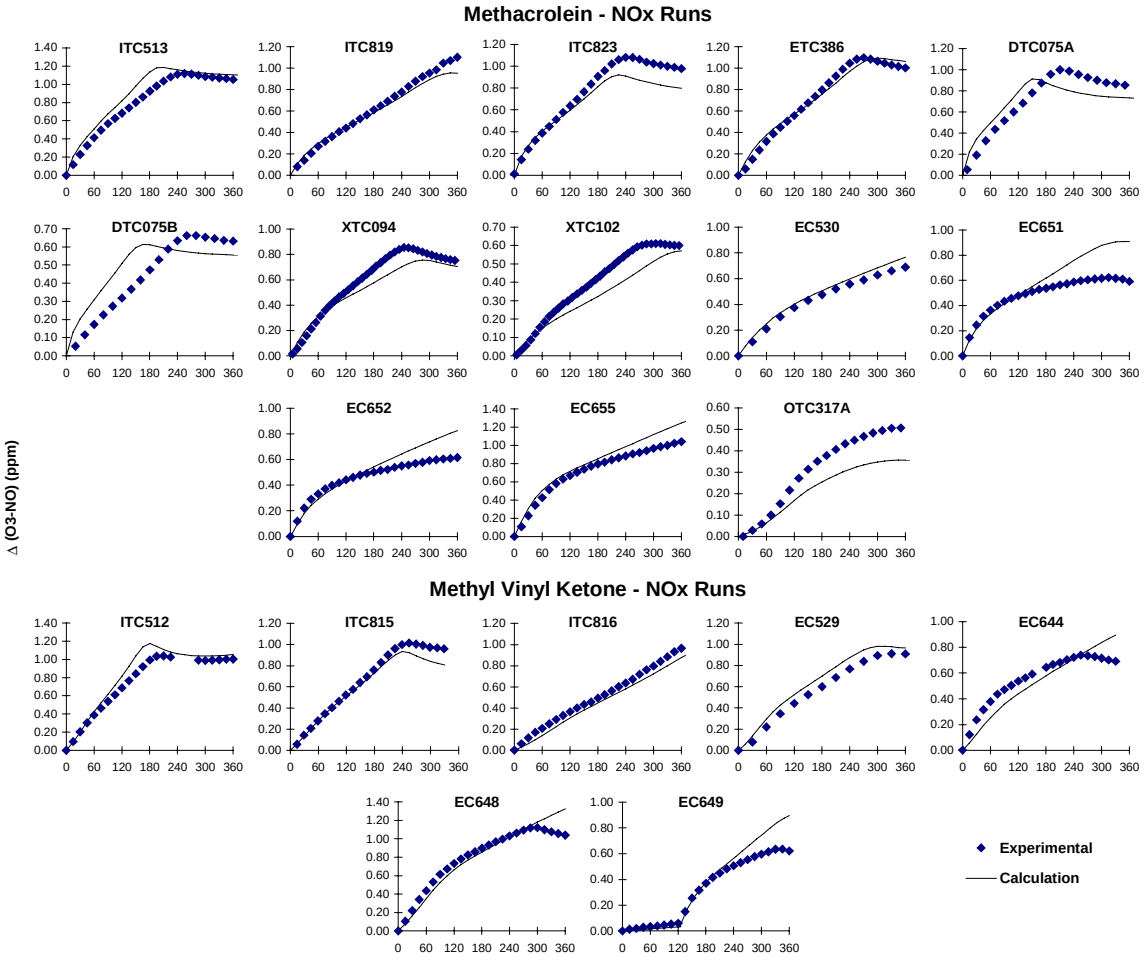

Figure B-14. Plots of experimental and calculated $\Delta([O_3]-[NO])$ data for the methacrolein - NO_x and the methyl vinyl ketone - NO_x experiments.

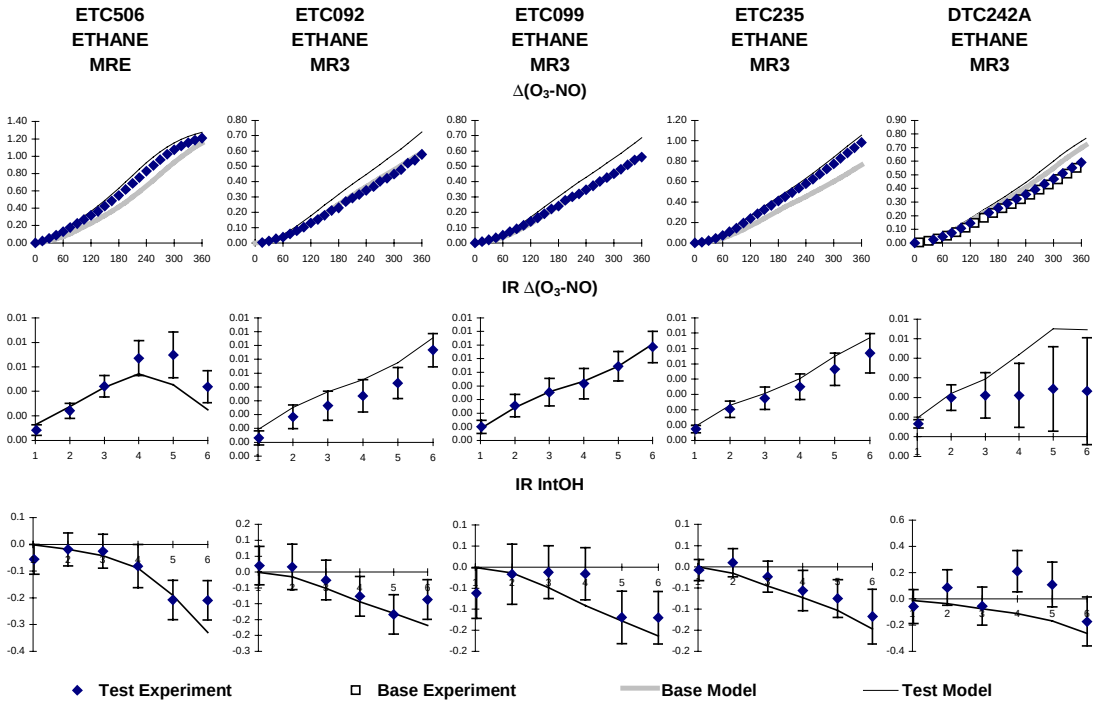

Figure B-15. Plots of experimental and calculated results of the incremental reactivity experiments with ethane

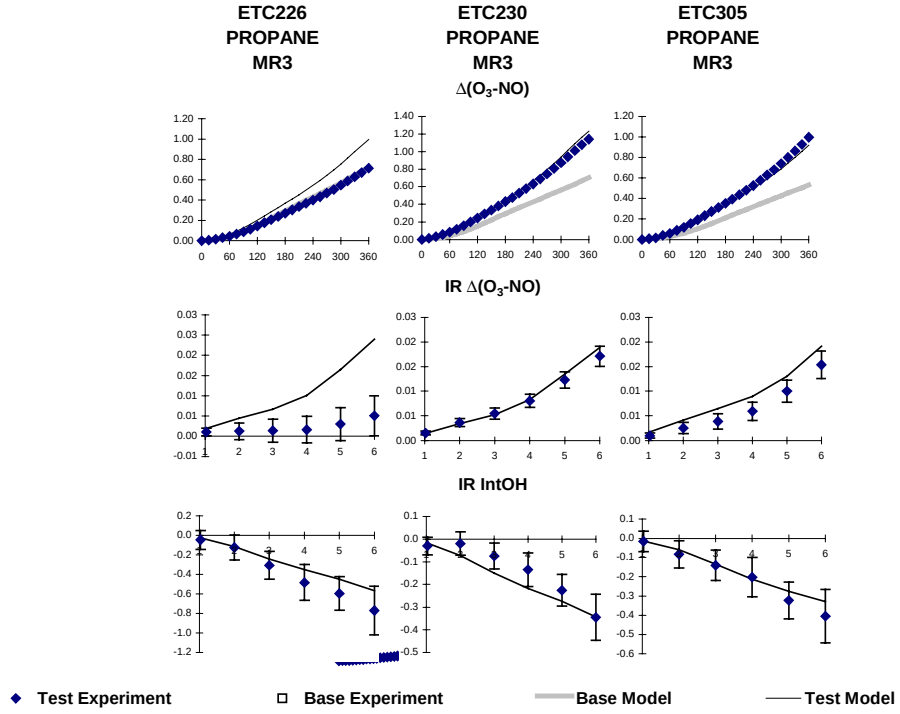

Figure B-16. Plots of experimental and calculated results of the incremental reactivity experiments with propane

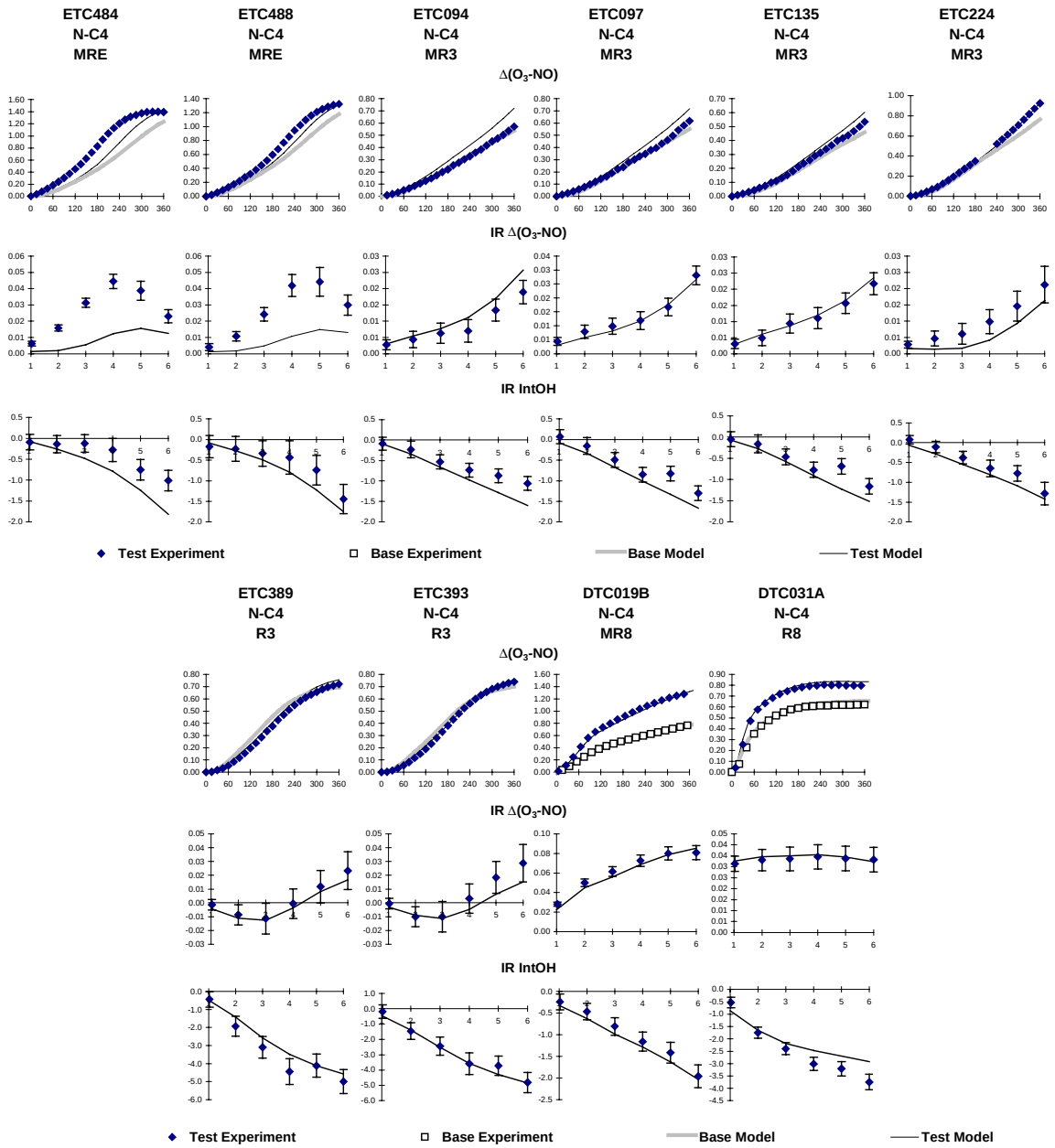

Figure B-17. Plots of experimental and calculated results of the incremental reactivity experiments with n-butane.

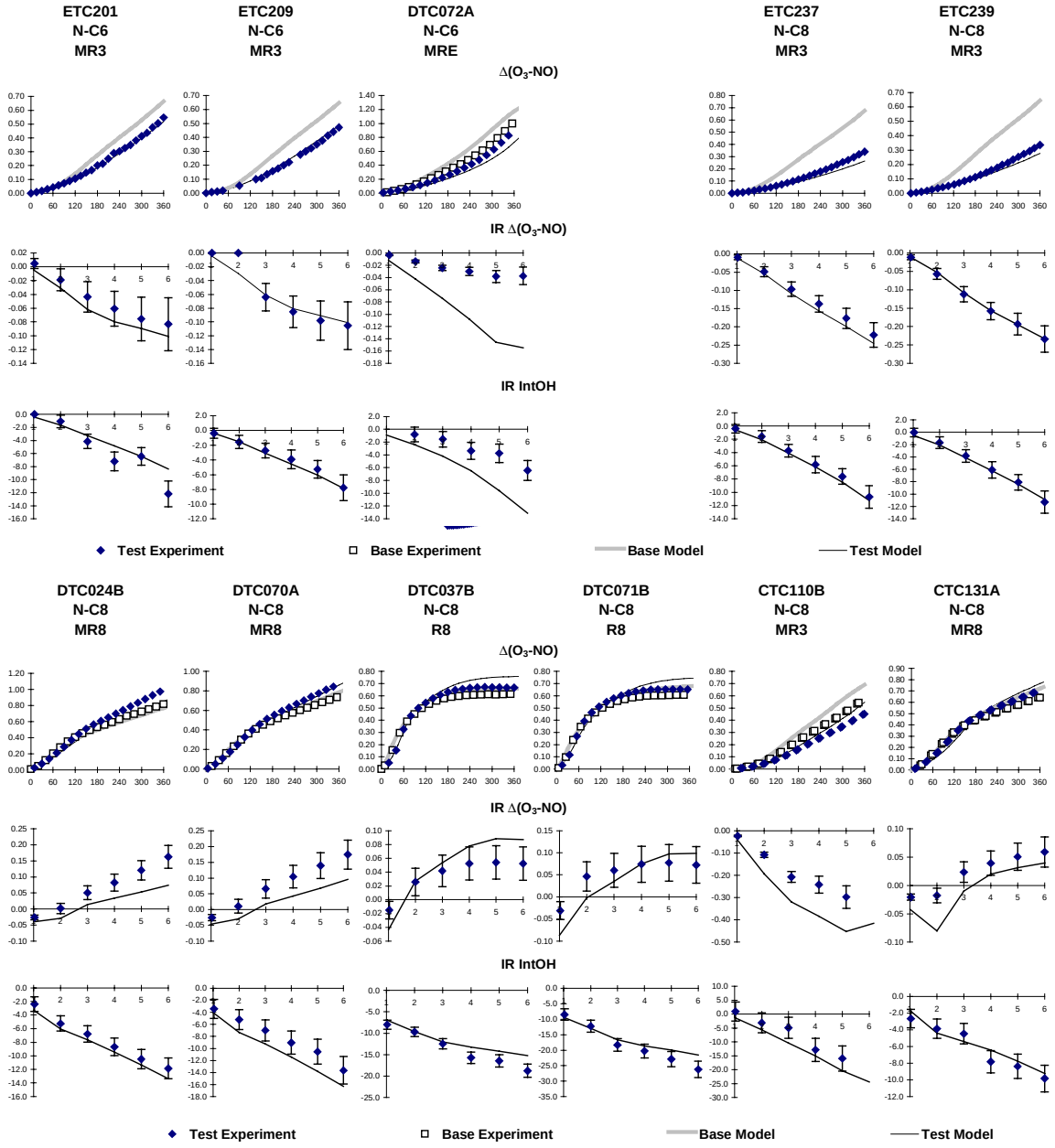

Figure B-18. Plots of experimental and calculated results of the incremental reactivity experiments with n-hexane and n-octane.

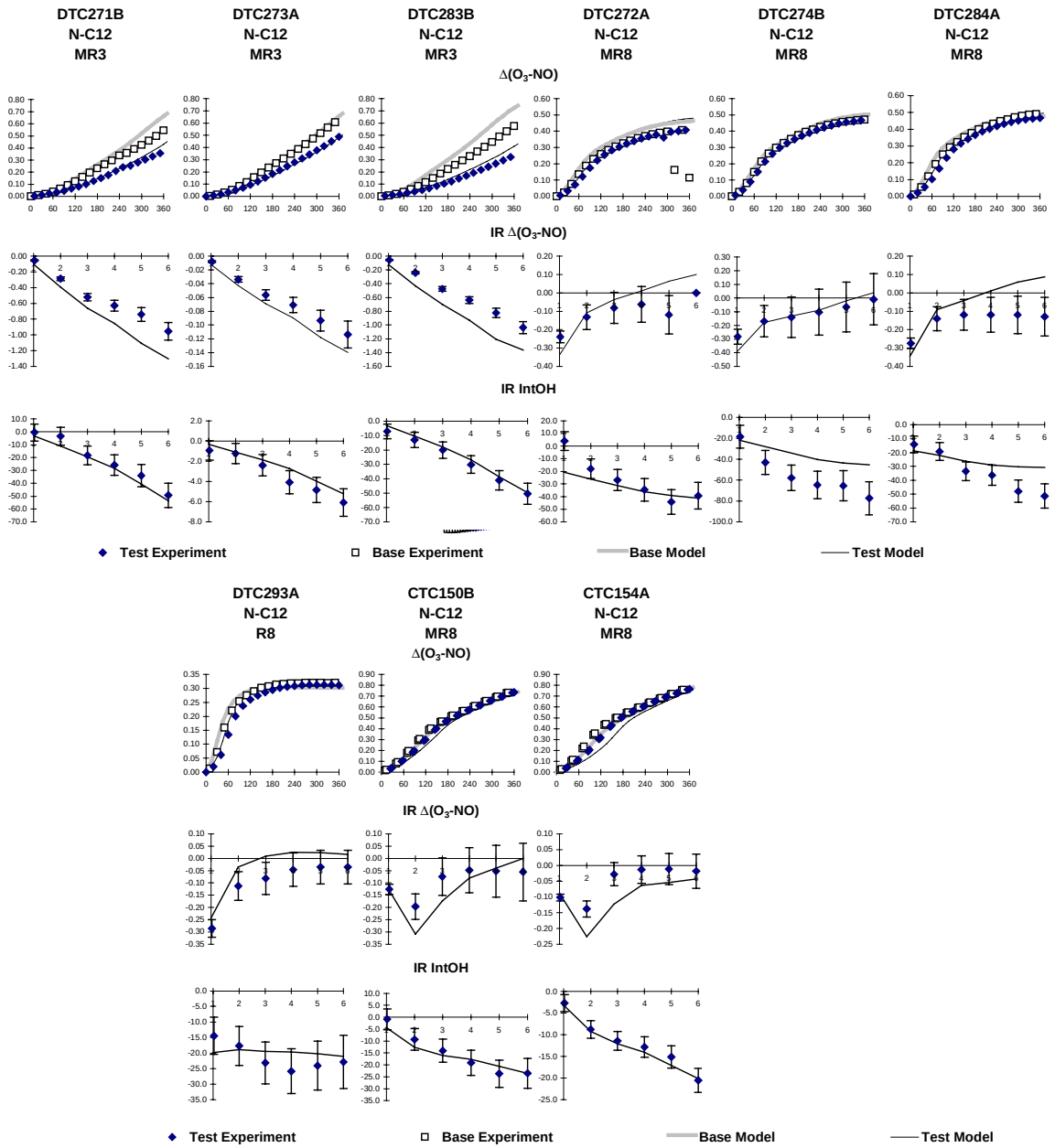

Figure B-19. Plots of experimental and calculated results of the incremental reactivity experiments with n-dodecane.

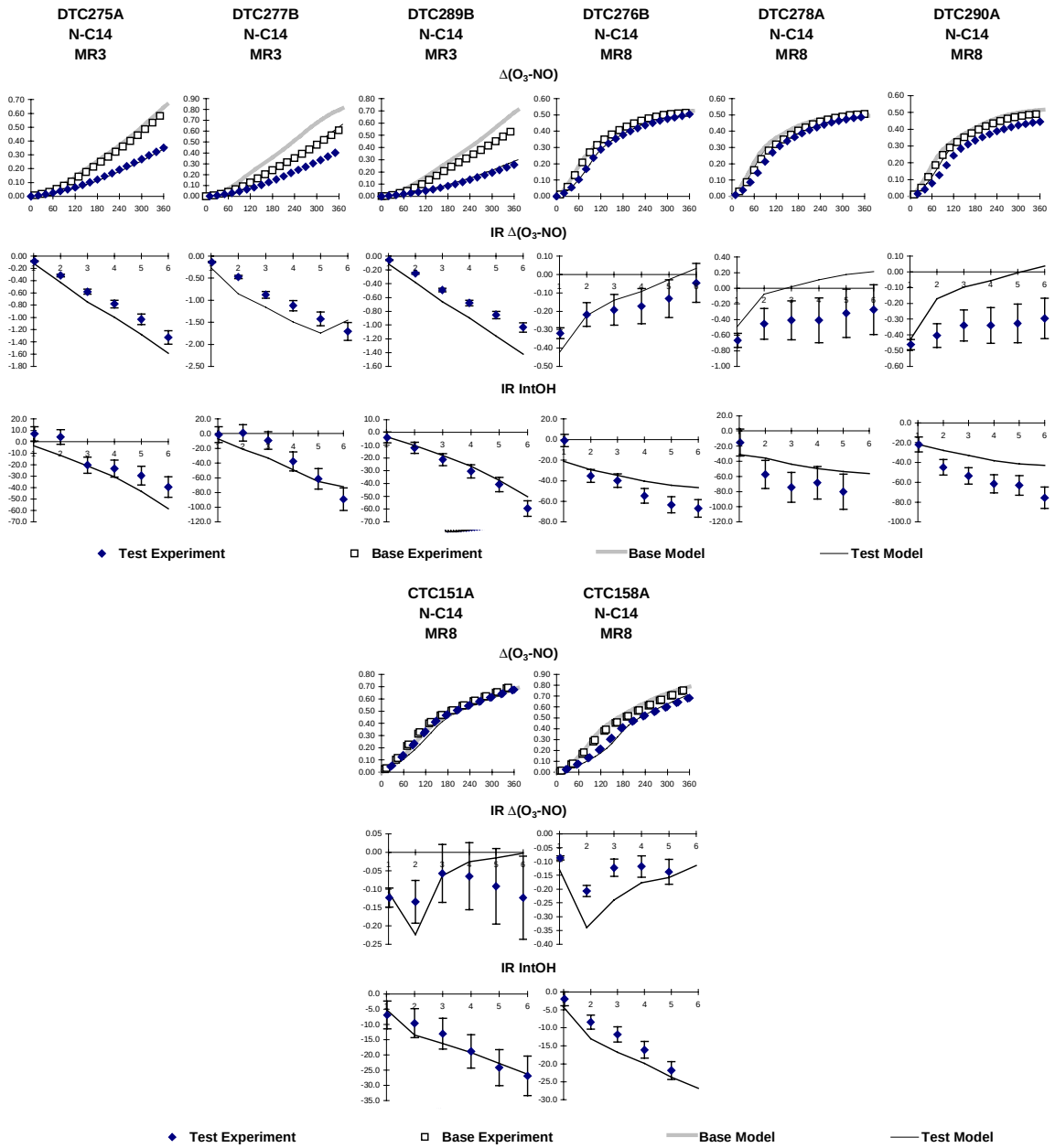

Figure B-20. Plots of experimental and calculated results of the incremental reactivity experiments with n-tetradecane.

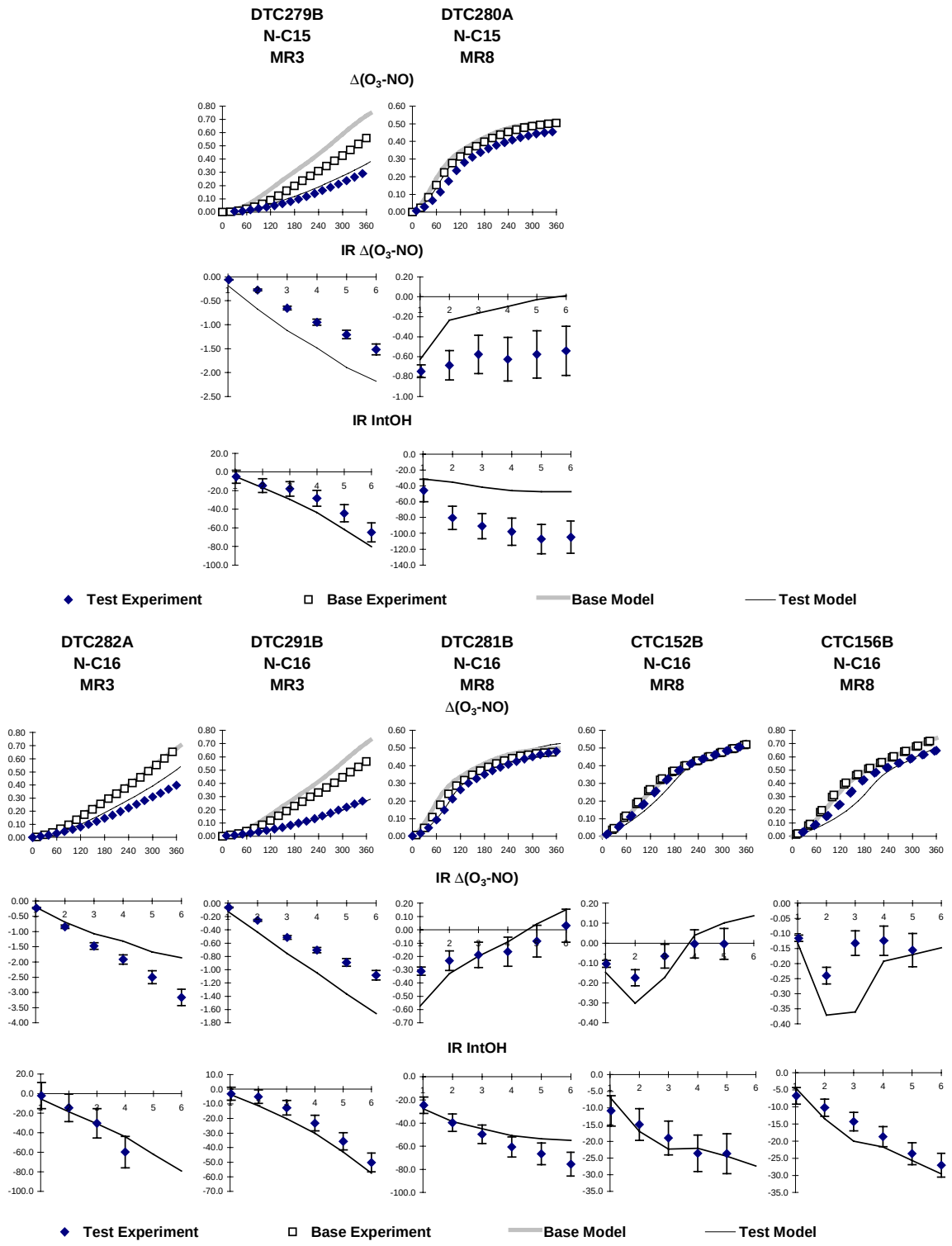

Figure B-21. Plots of experimental and calculated results of the incremental reactivity experiments with n-pentadecane and n-hexadecane.

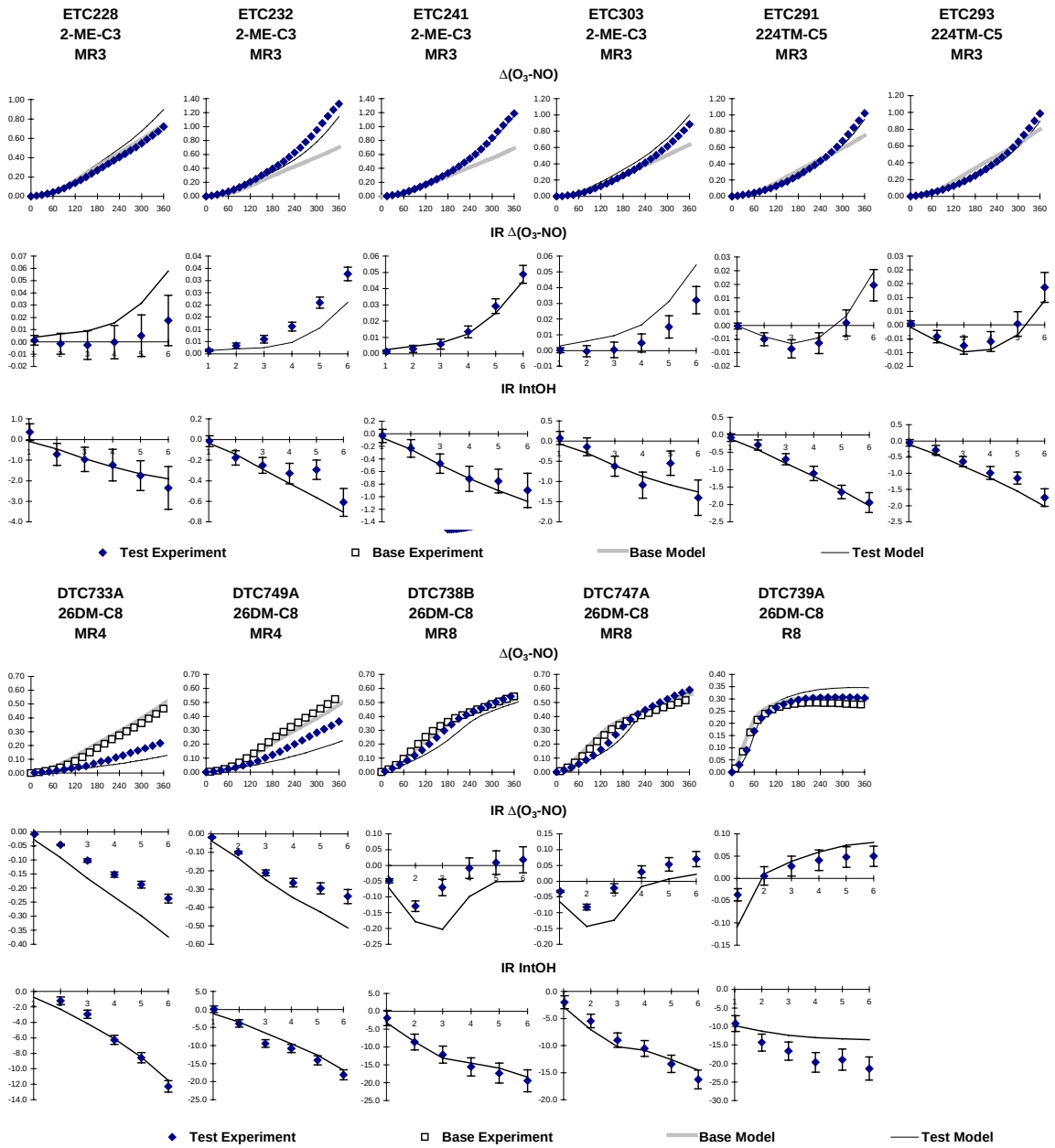

Figure B-22. Plots of experimental and calculated results of the incremental reactivity experiments with 2-methyl propene, 2,2,4-trimethyl butane and 2,5-dimethyl octane.

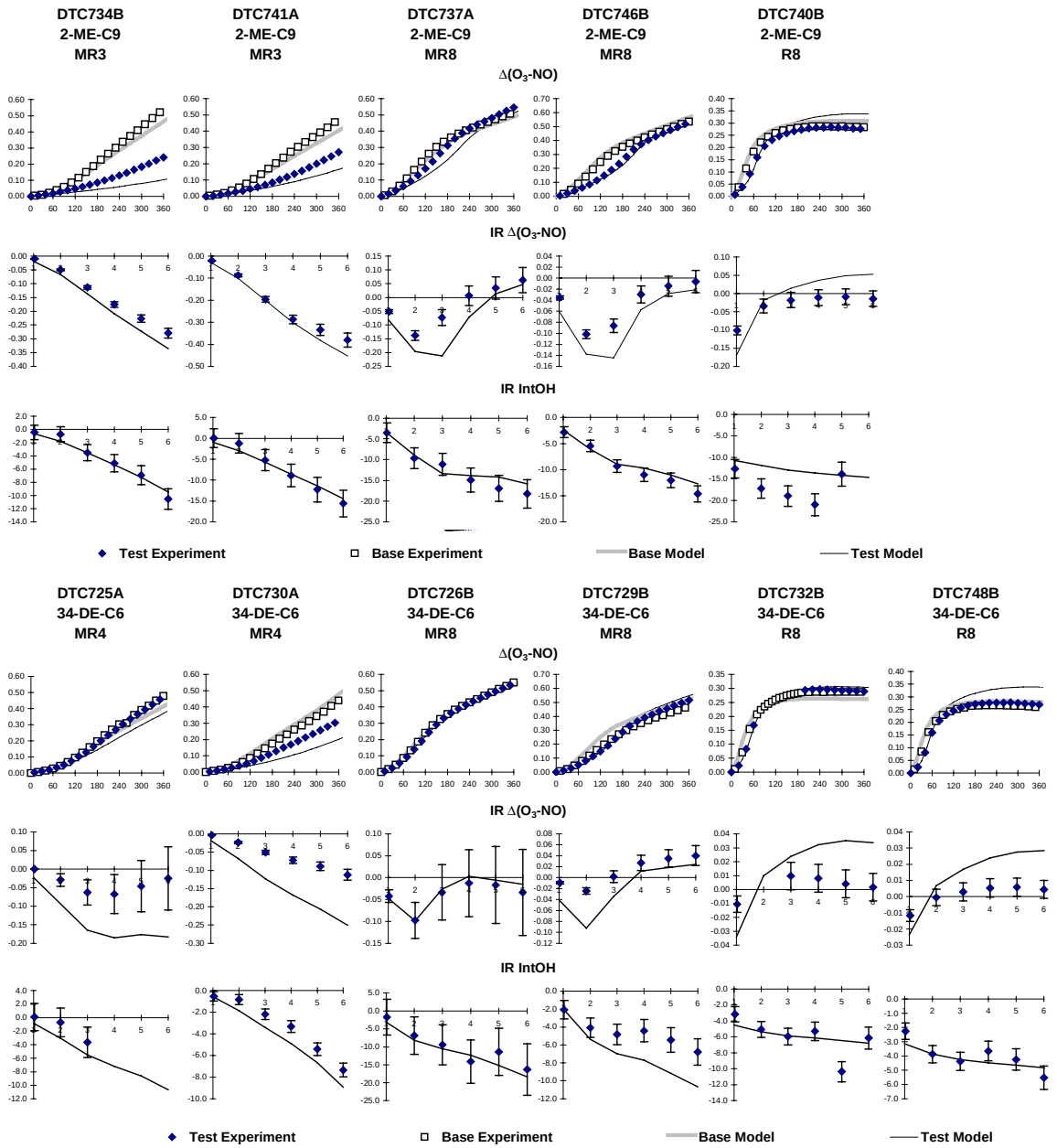

Figure B-23. Plots of experimental and calculated results of the incremental reactivity experiments with 2-methyl nonane and 3,4-diethyl hexane.

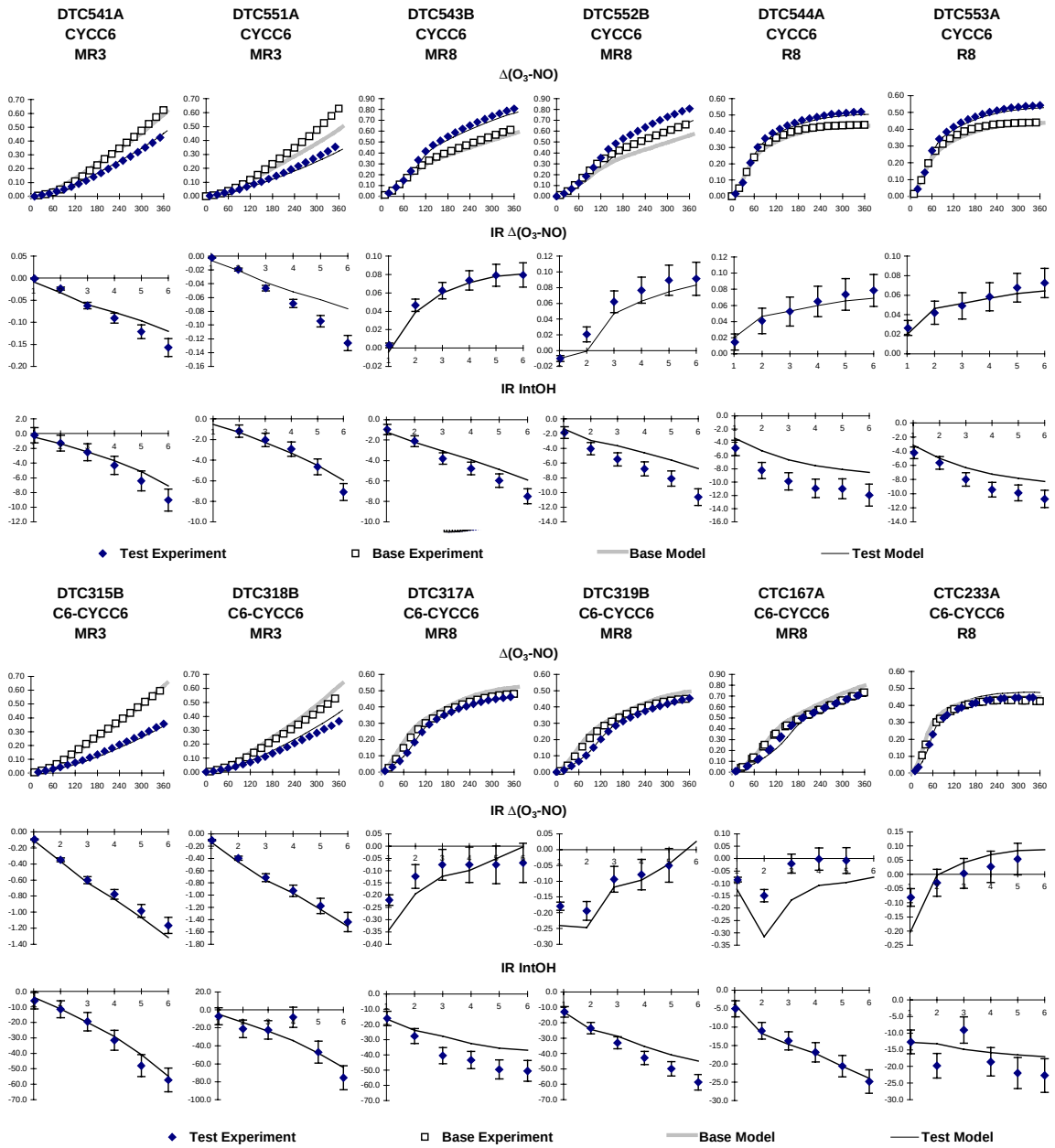

Figure B-24. Plots of experimental and calculated results of the incremental reactivity experiments with cyclohexane and n-hexyl cyclohexane.

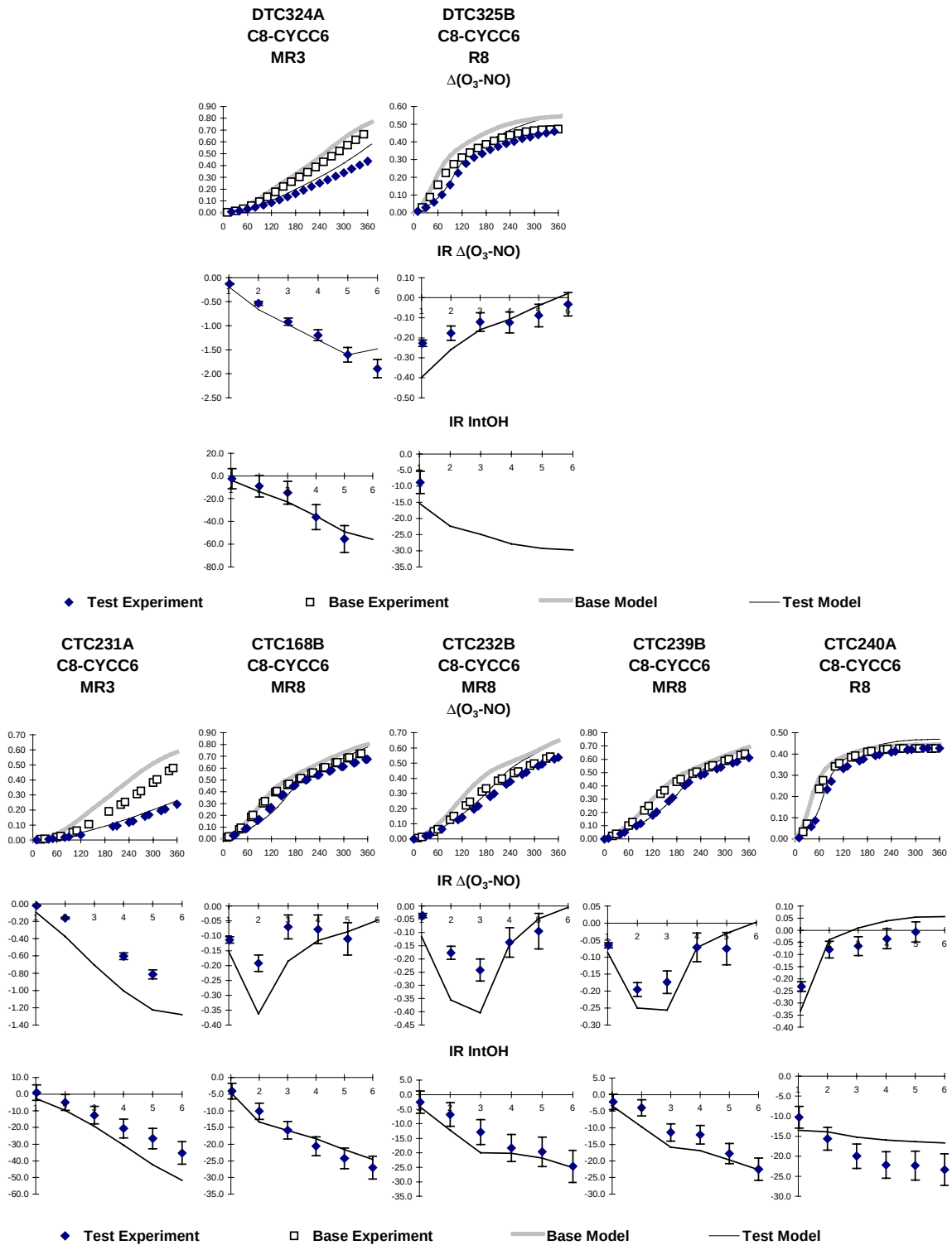

Figure B-25. Plots of experimental and calculated results of the incremental reactivity experiments with n-octyl cyclohexane.

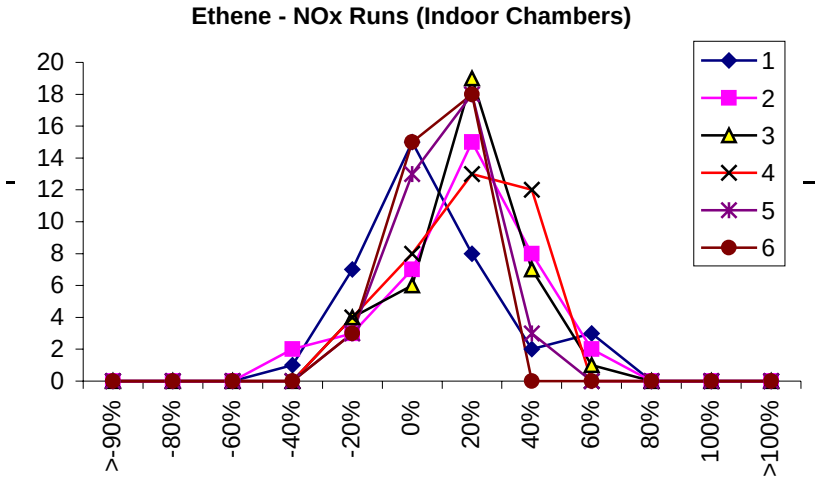

Figure B-26. Distribution plots of percentage errors of fits of calculated to experimental hourly $\Delta([O_3]-[NO])$ data for the ethene - NO_x runs carried out in indoor chambers.

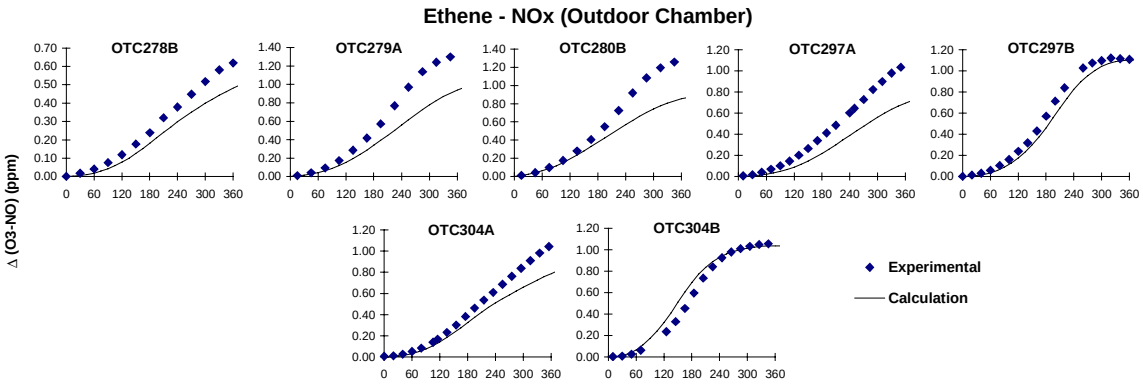

Figure B-27. Plots of experimental and calculated $\Delta([O_3]-[NO])$ data for the ethene - NO_x runs carried out in the SAPRC outdoor chamber (OTC).

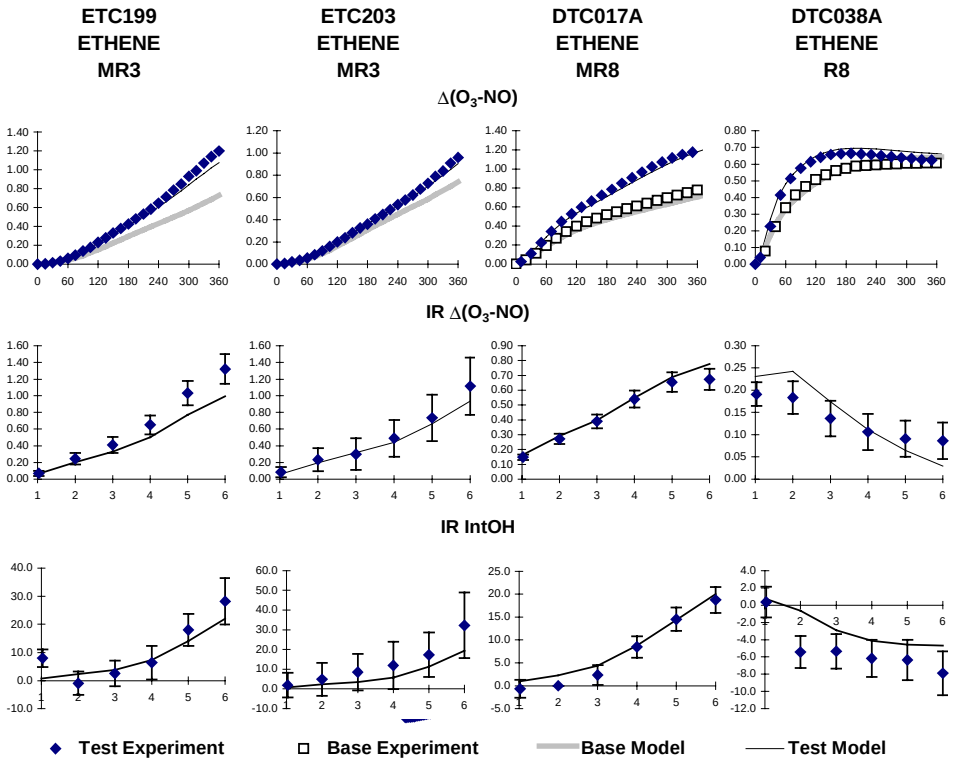

Figure B-28. Plots of experimental and calculated results of the incremental reactivity experiments with ethene.

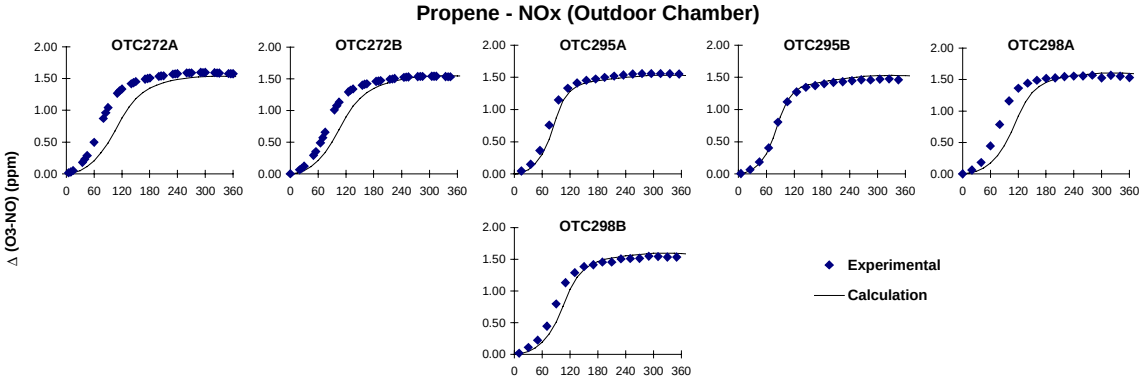

Figure B-29. Plots of experimental and calculated $\Delta([O_3]-[NO])$ data for the propene - NO_x runs using the SAPRC outdoor chamber.

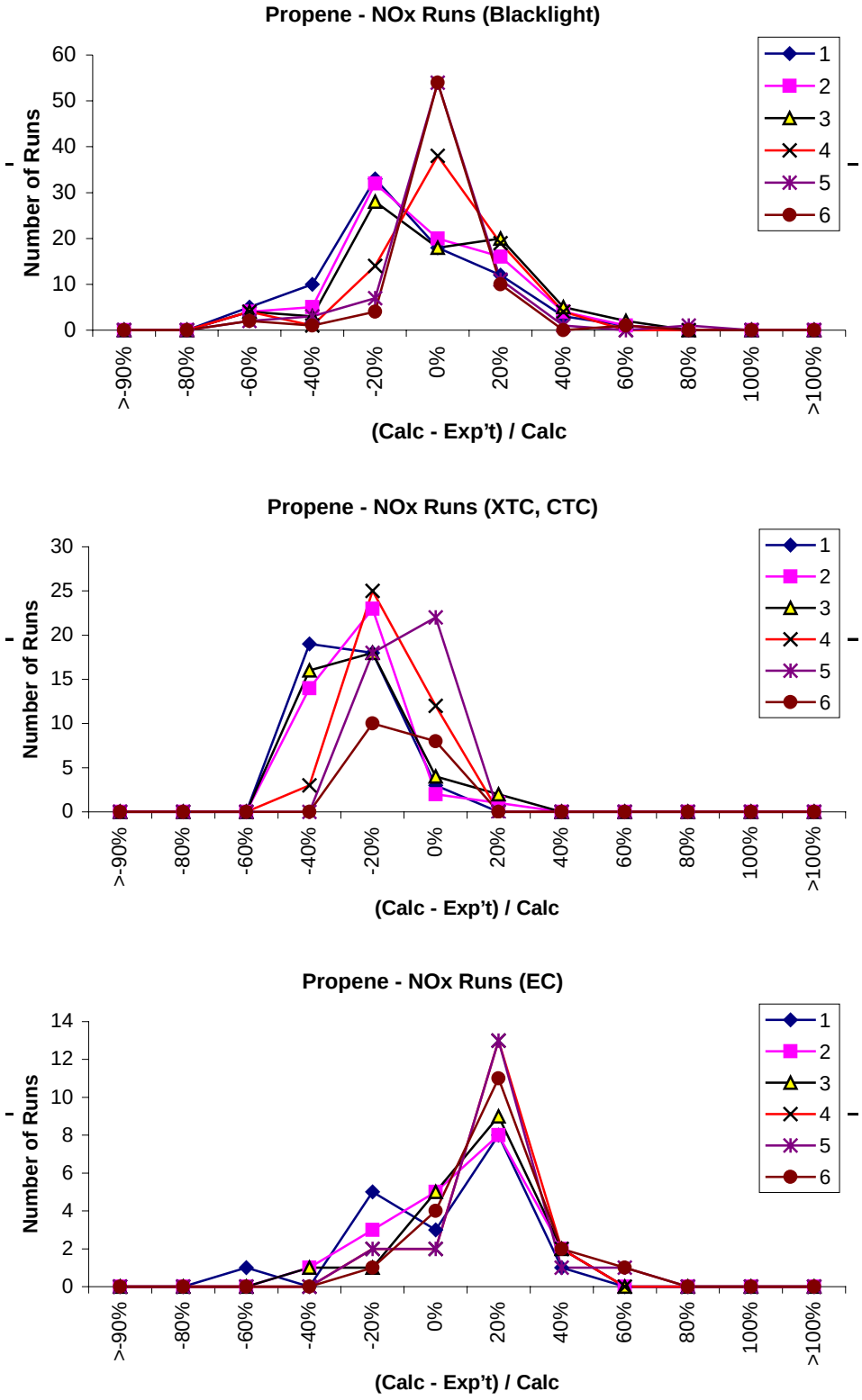

Figure B-30. Distribution plots of percentage errors of fits of calculated to experimental hourly $\Delta([O_3]-[NO])$ data for the propene - NO_x runs carried out using various chambers.

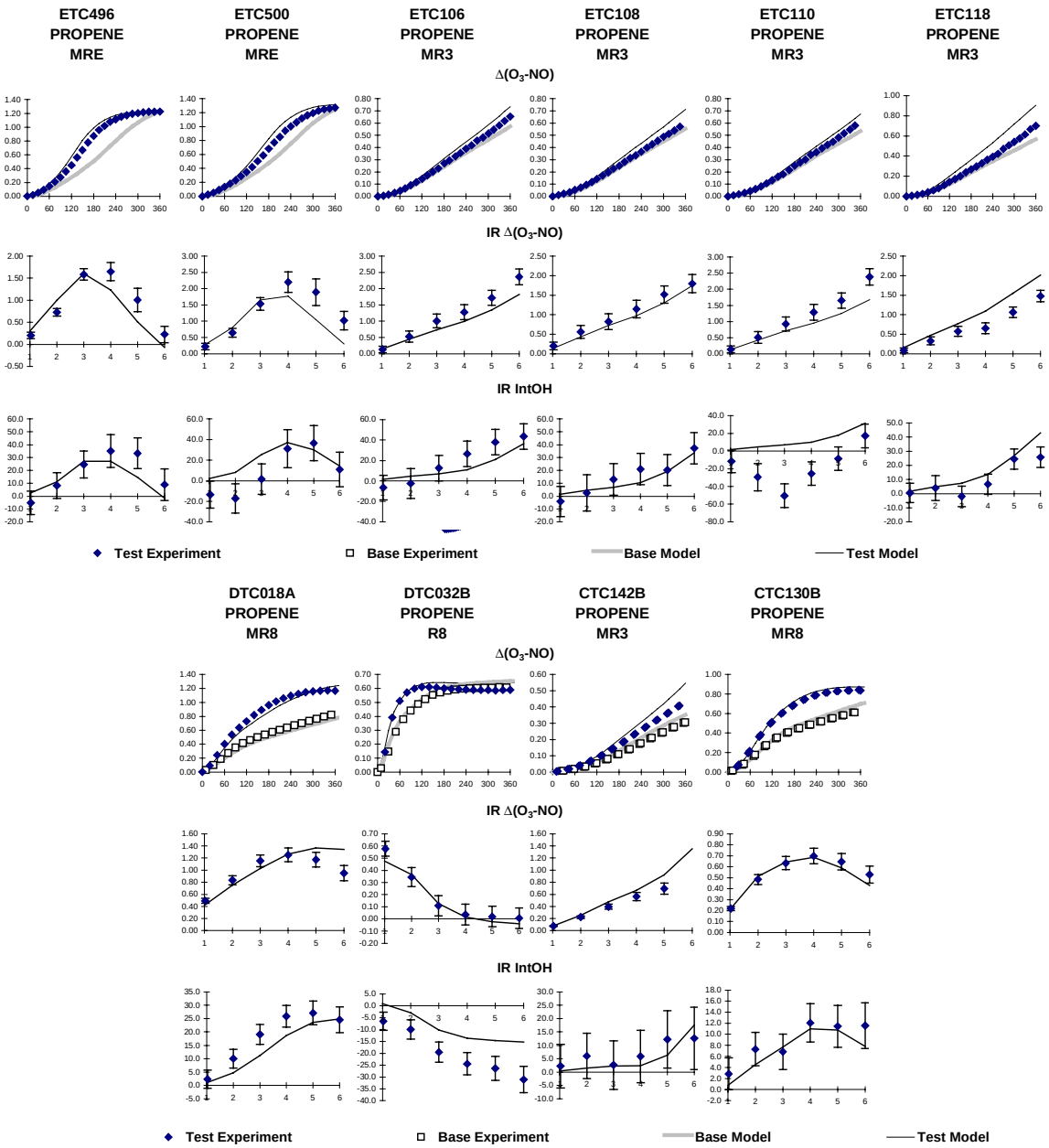

Figure B-31. Plots of experimental and calculated results of the incremental reactivity experiments with propene.

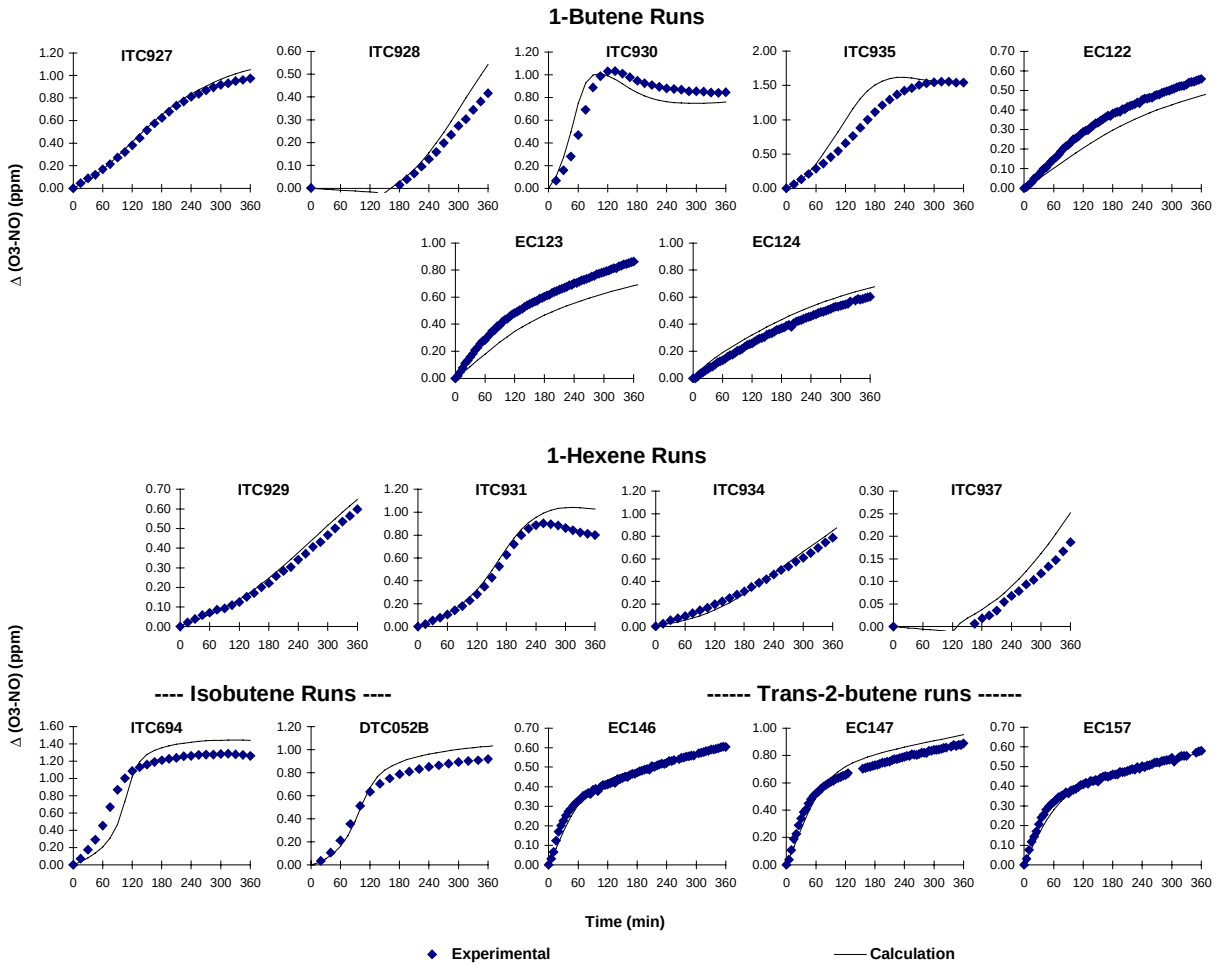

Figure B-32. Plots of experimental and calculated $\Delta([O_3]-[NO])$ data for the 1-butene, 1-hexene, isobutene, and trans-2-butene - NO_x experiments.

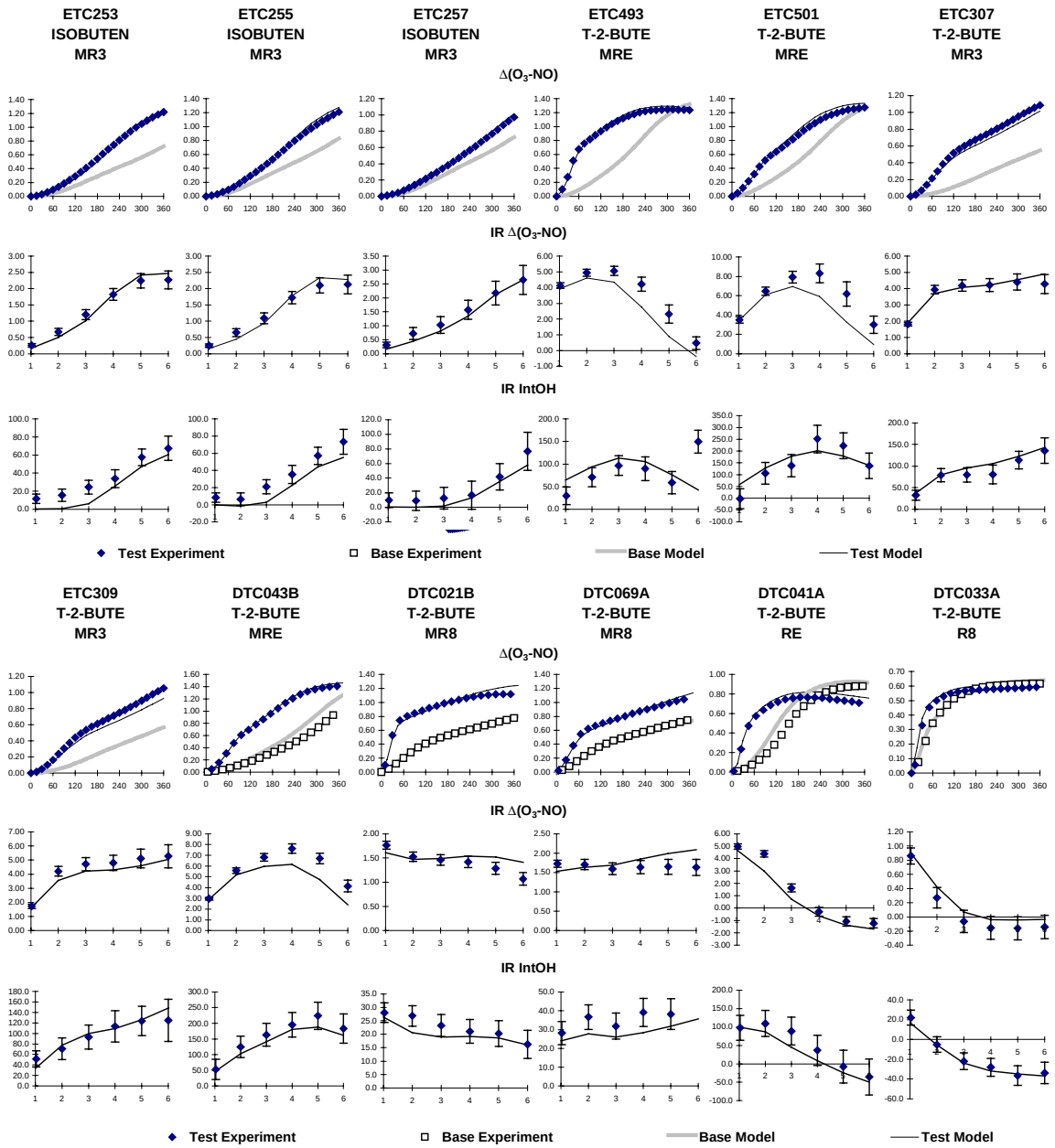

Figure B-33. Plots of experimental and calculated results of the incremental reactivity experiments with isobutene and trans-2-butene.

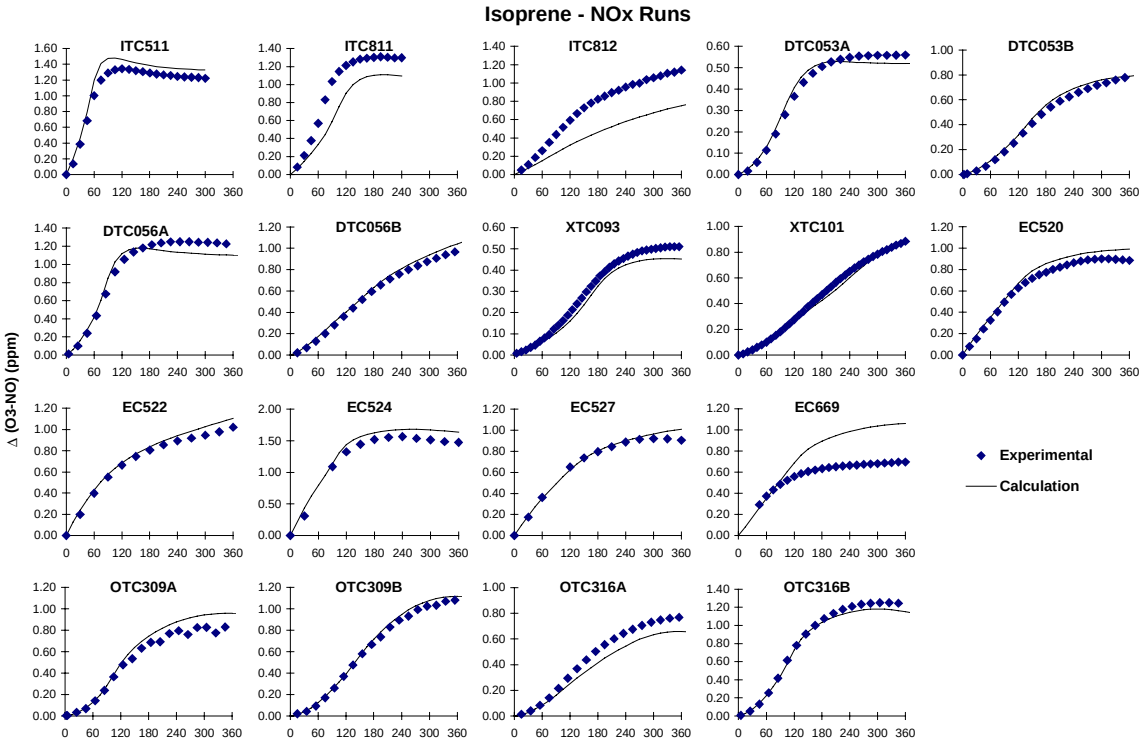

Figure B-34. Plots of experimental and calculated $\Delta([O_3]-[NO])$ data for the isoprene - NO_x experiments.

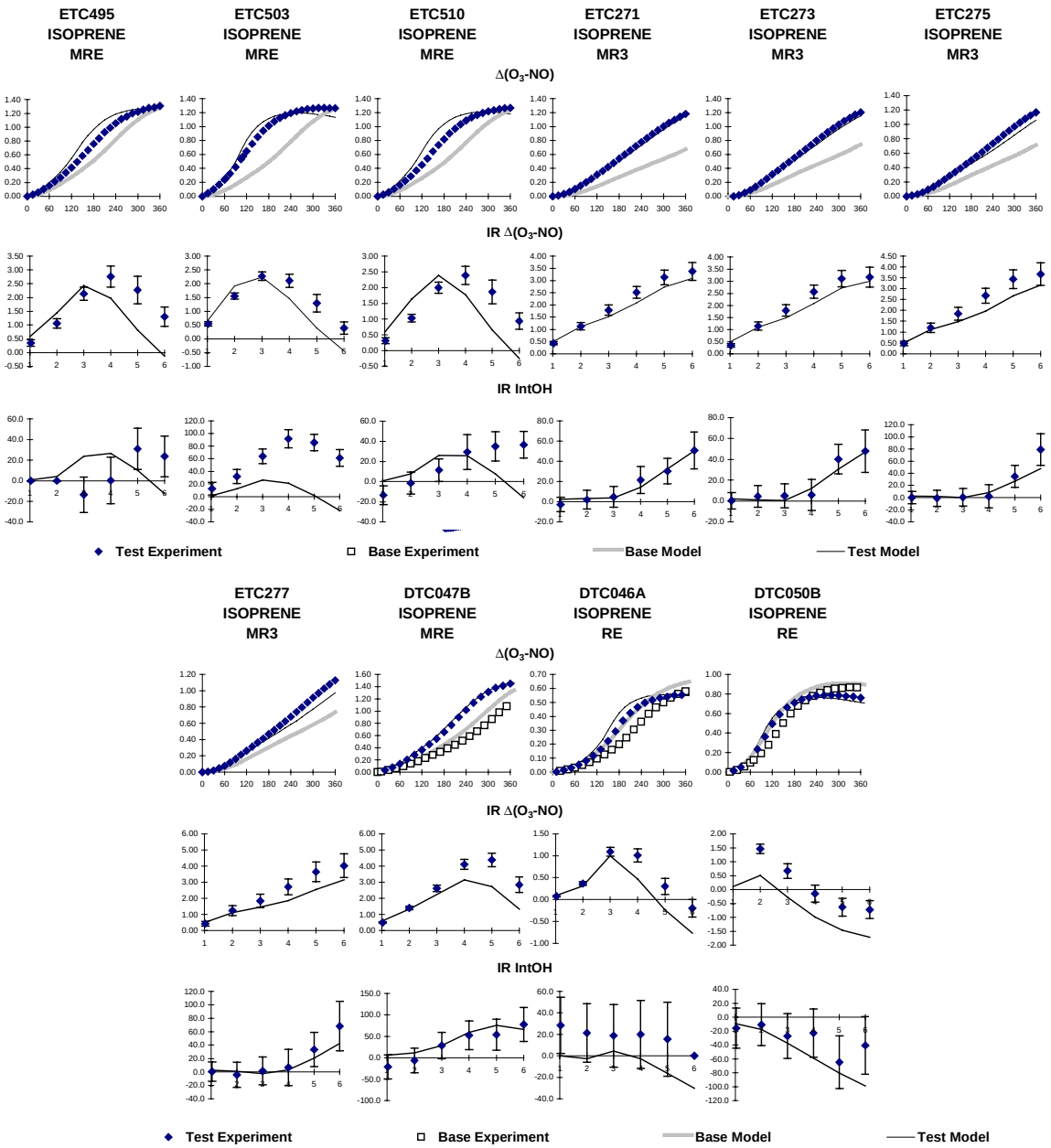

Figure B-35. Plots of experimental and calculated results of the incremental reactivity experiments with isoprene.

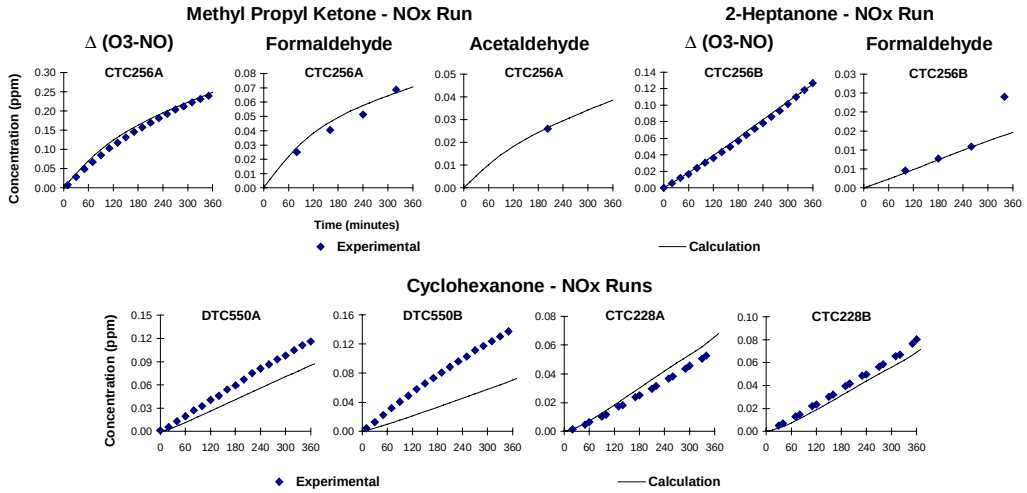

Figure B-36. Plots of experimental and calculated $\Delta([O_3]-[NO])$ data for the methyl propyl ketone - NO_x, 2 -heptanone - NO_x and cyclohexanone - NO_x experiments.

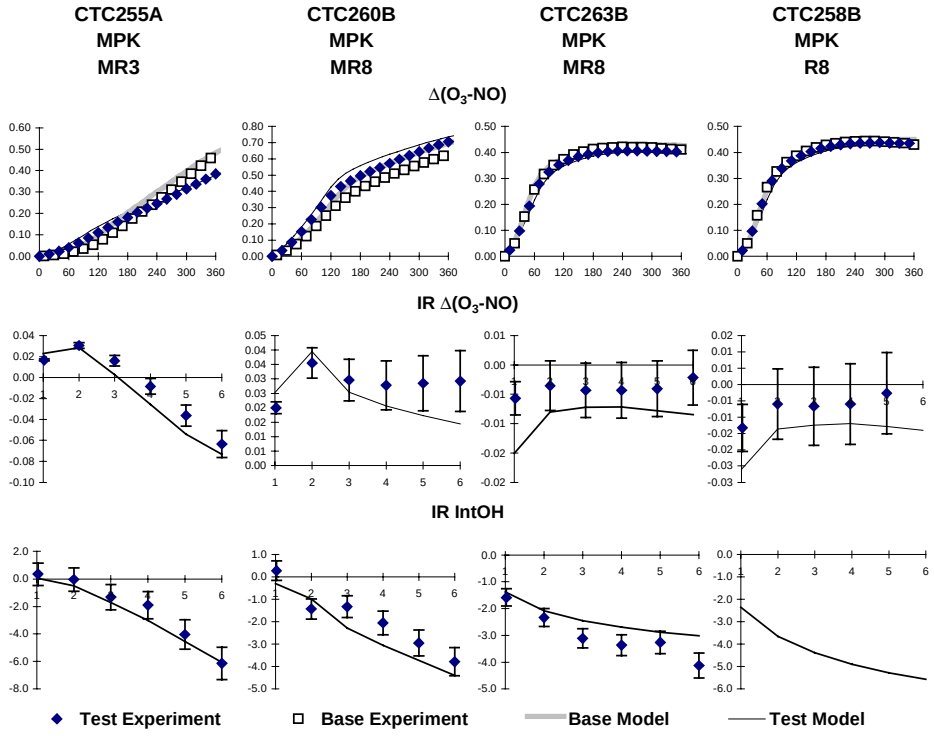

Figure B-37. Plots of experimental and calculated results of the incremental reactivity experiments with methyl propyl ketone.

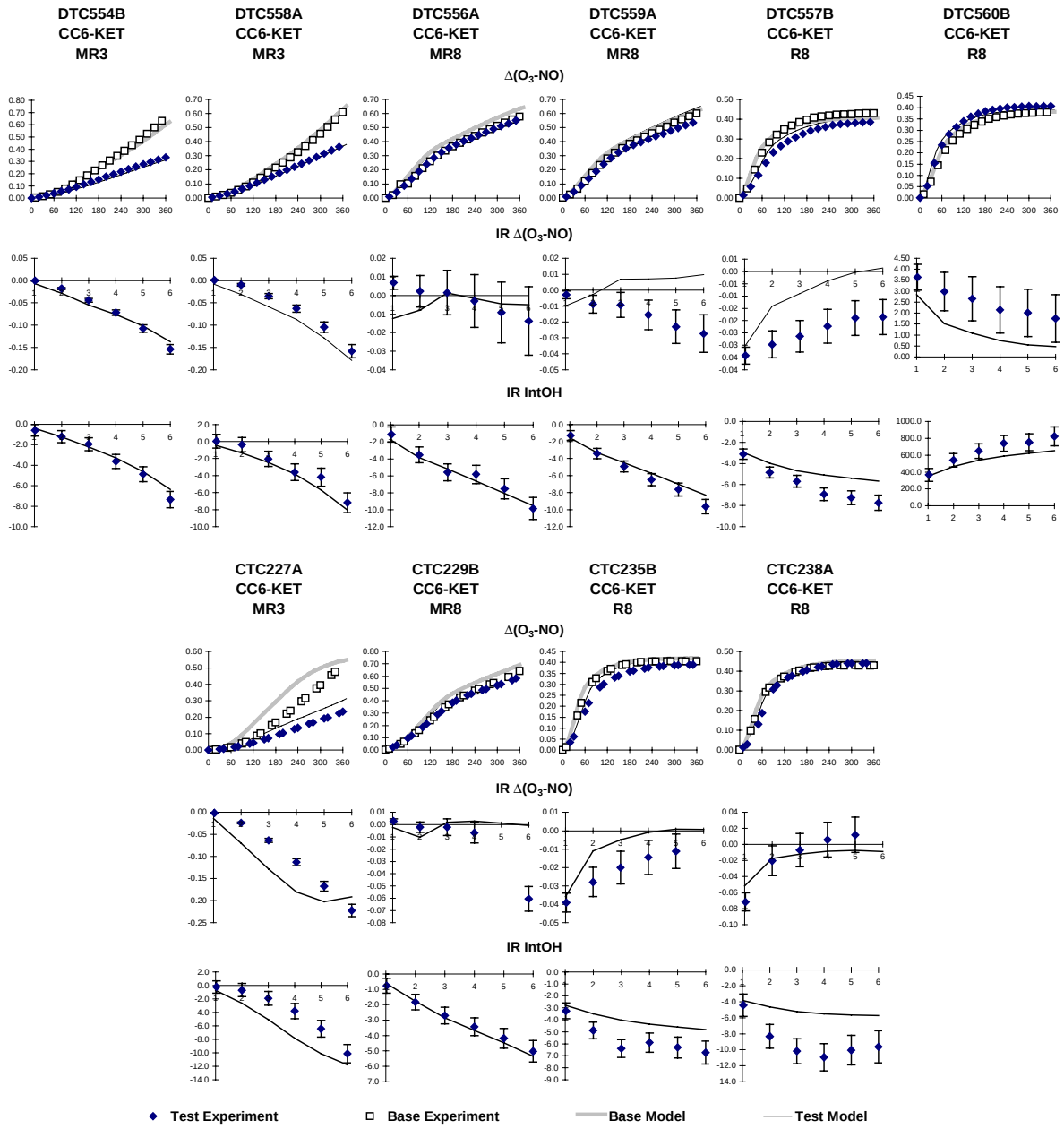

Figure B-38. Plots of experimental and calculated results of the incremental reactivity experiments with cyclohexanone.

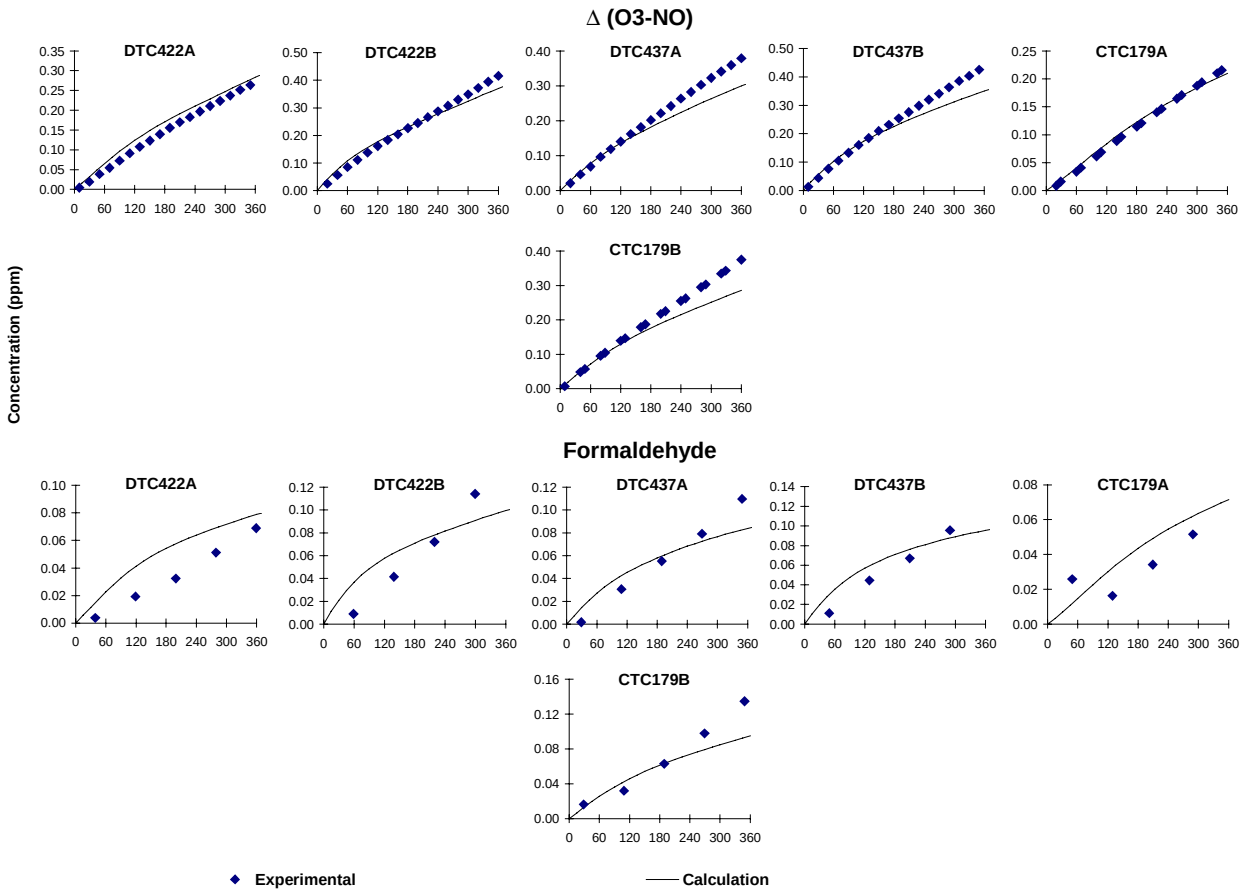

Figure B-39. Plots of experimental and calculated $\Delta([O_3]-[NO])$ and formaldehyde data for the methyl isobutyl ketone - NO_x experiments.

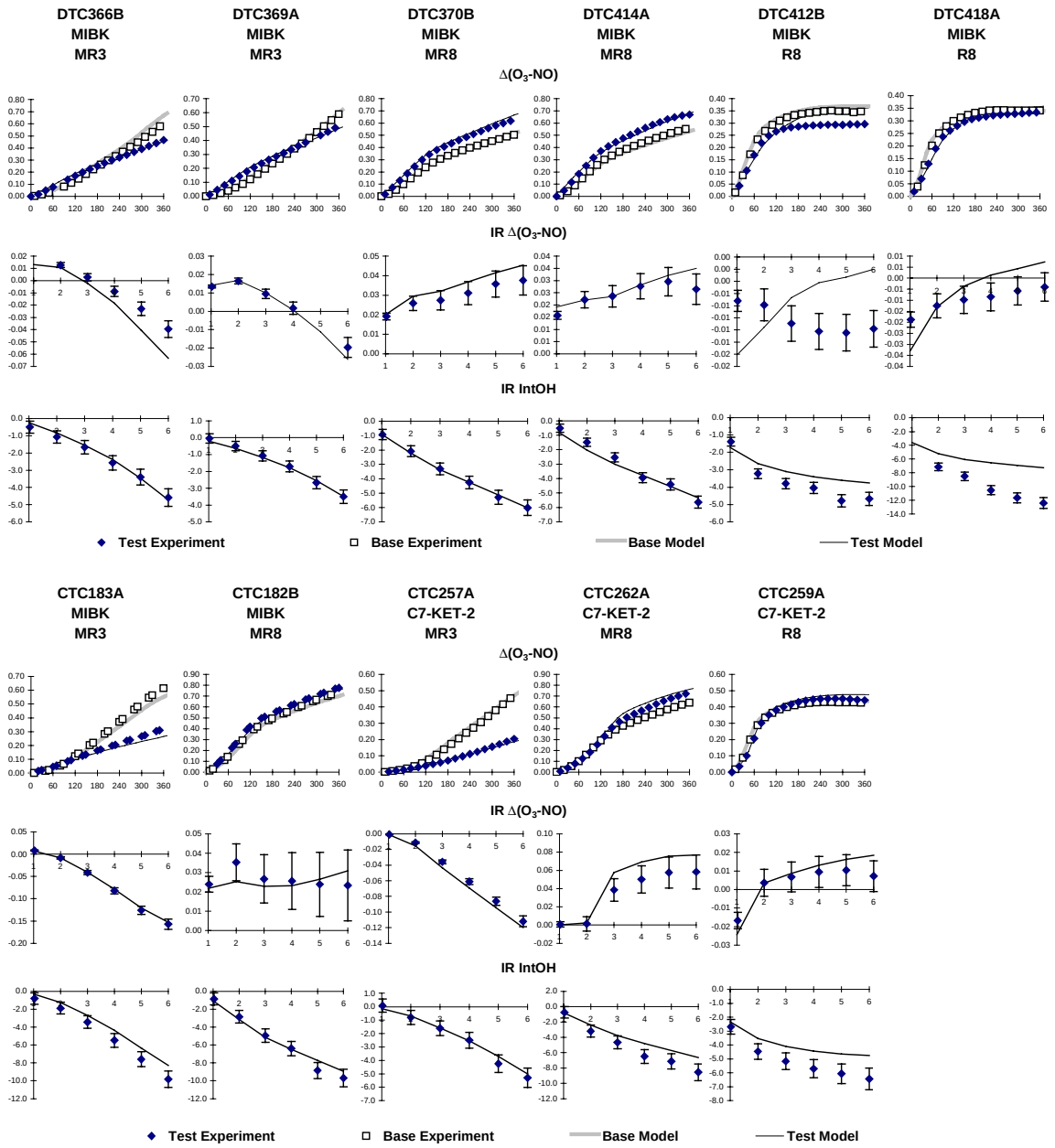

Figure B-40. Plots of experimental and calculated results of the incremental reactivity experiments with methyl isobutyl ketone and 2-heptanone.

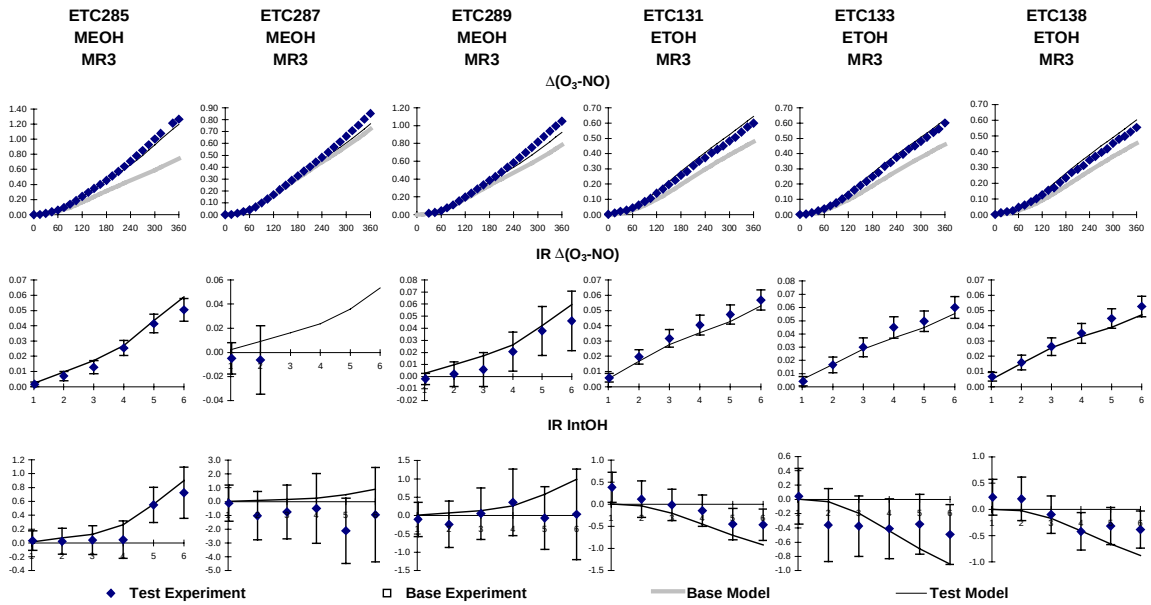

Figure B-41. Plots of experimental and calculated results of the incremental reactivity experiments with methanol and ethanol.

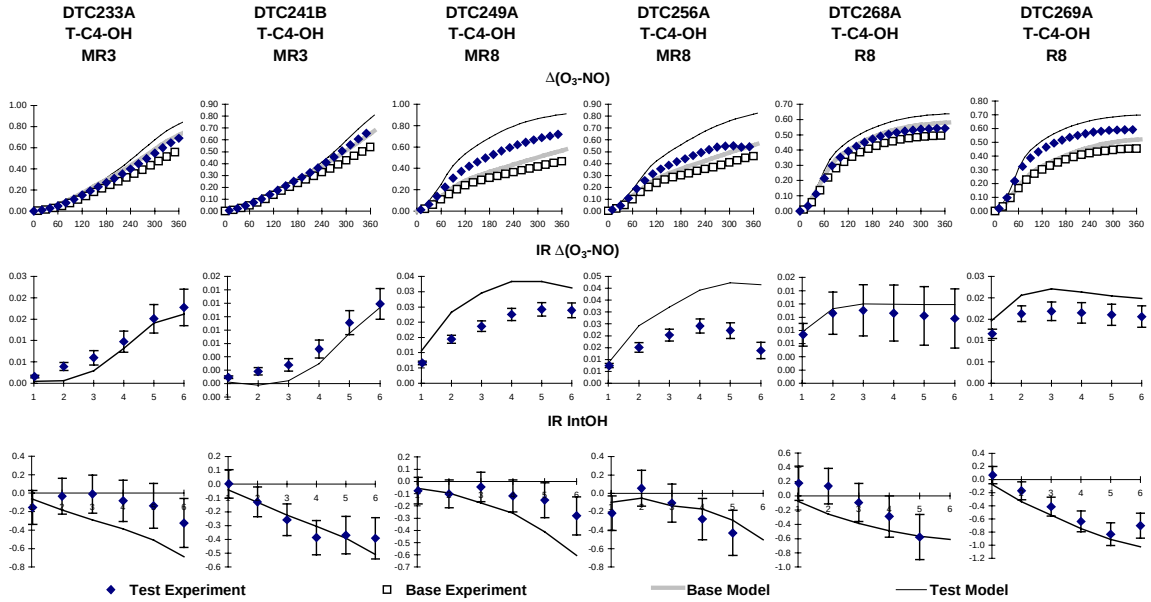

Figure B-42. Plots of experimental and calculated results of the incremental reactivity experiments with t-butyl alcohol. (Run DTC259A, whose results are very similar to those for run DTC269A, is not shown.)

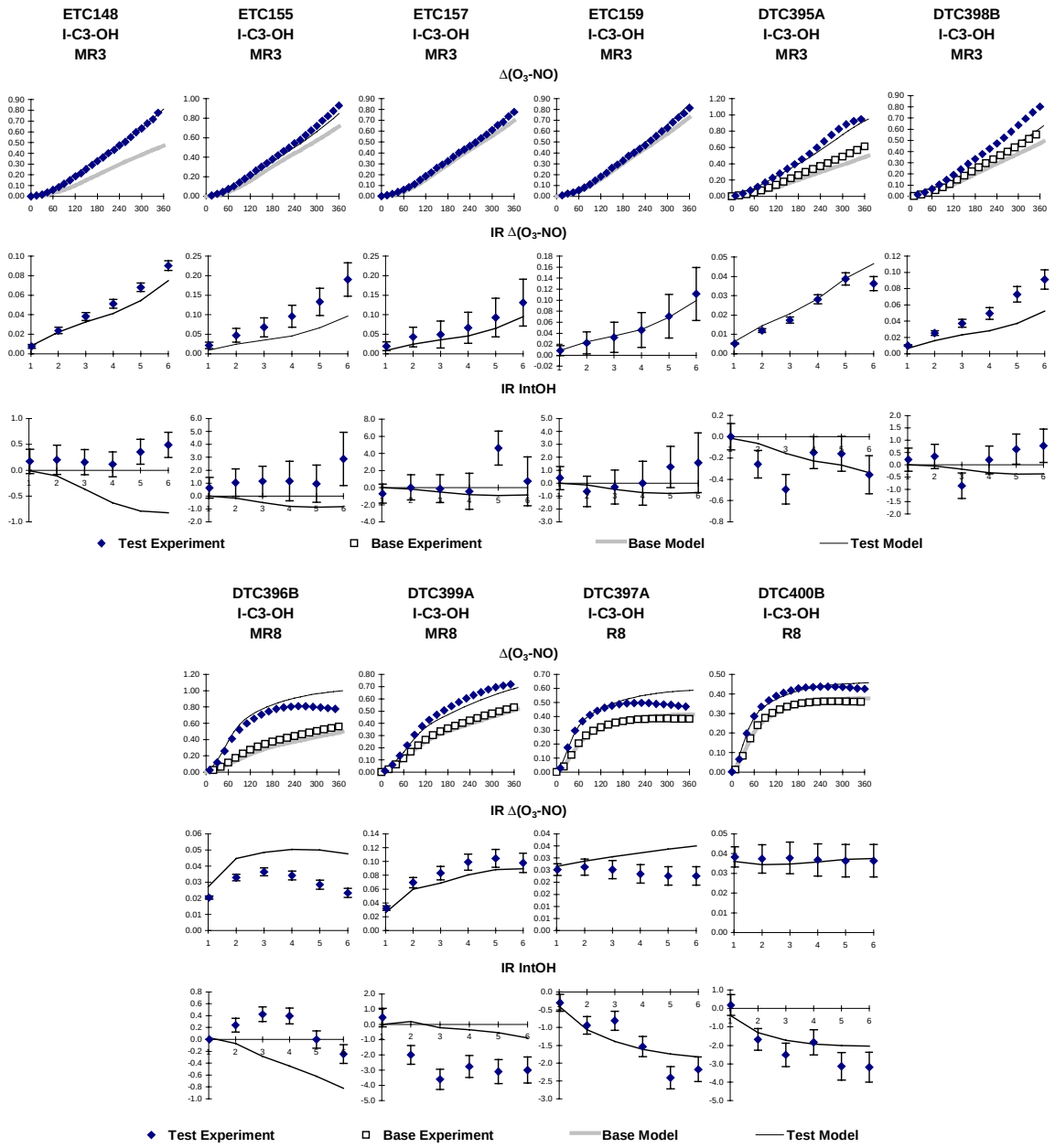

Figure B-43. Plots of experimental and calculated results of the incremental reactivity experiments with isopropyl alcohol.

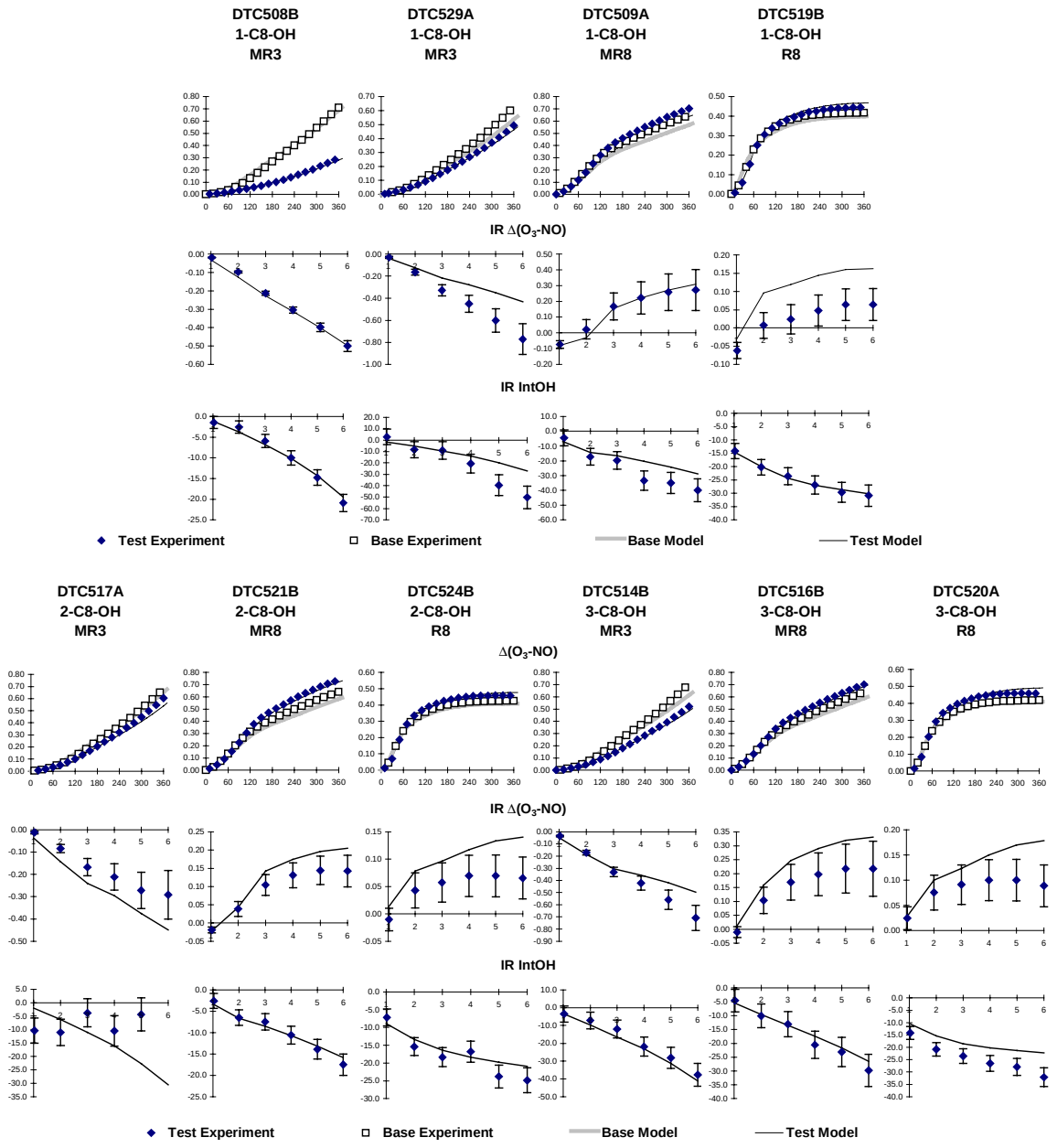

Figure B-44. Plots of experimental and calculated results of the incremental reactivity experiments with 1-, 2-, and 3-octanols.

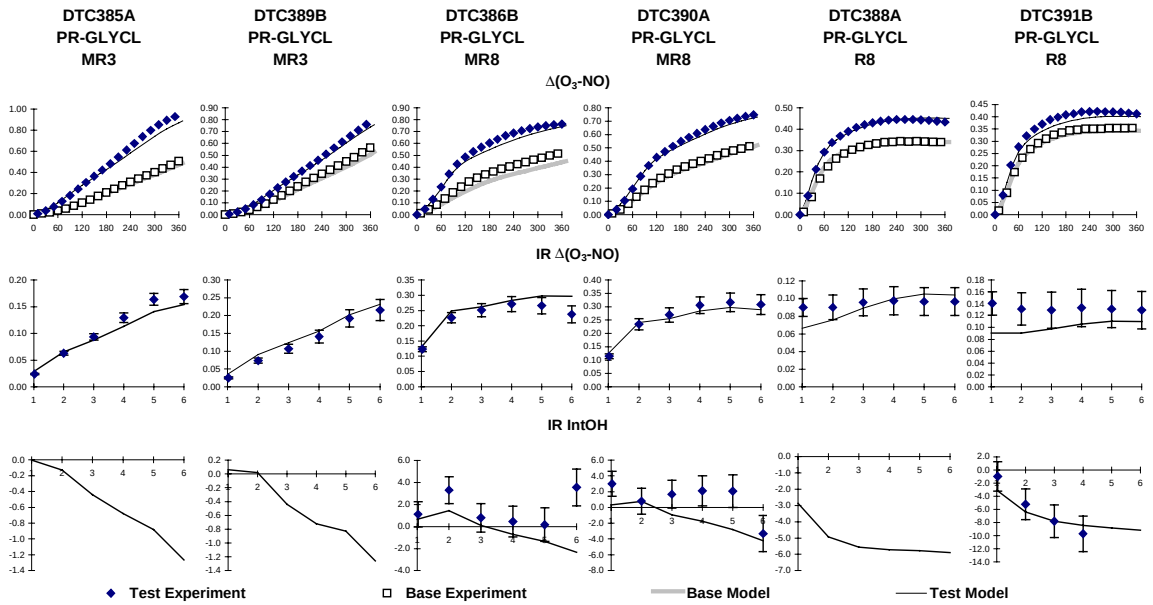

Figure B-45. Plots of experimental and calculated results of the incremental reactivity experiments with propylene glycol.

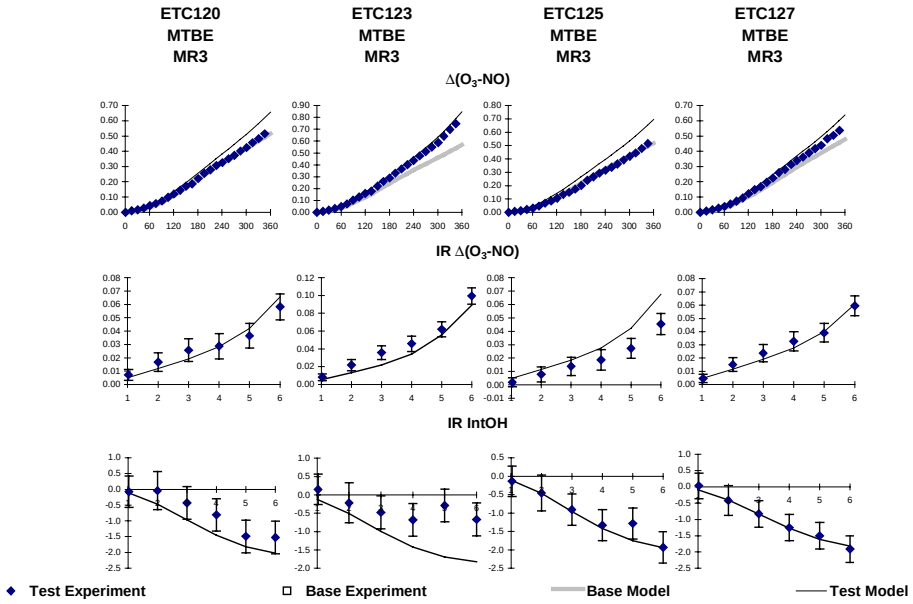

Figure B-46. Plots of experimental and calculated results of the incremental reactivity experiments with methyl t-butyl ether.

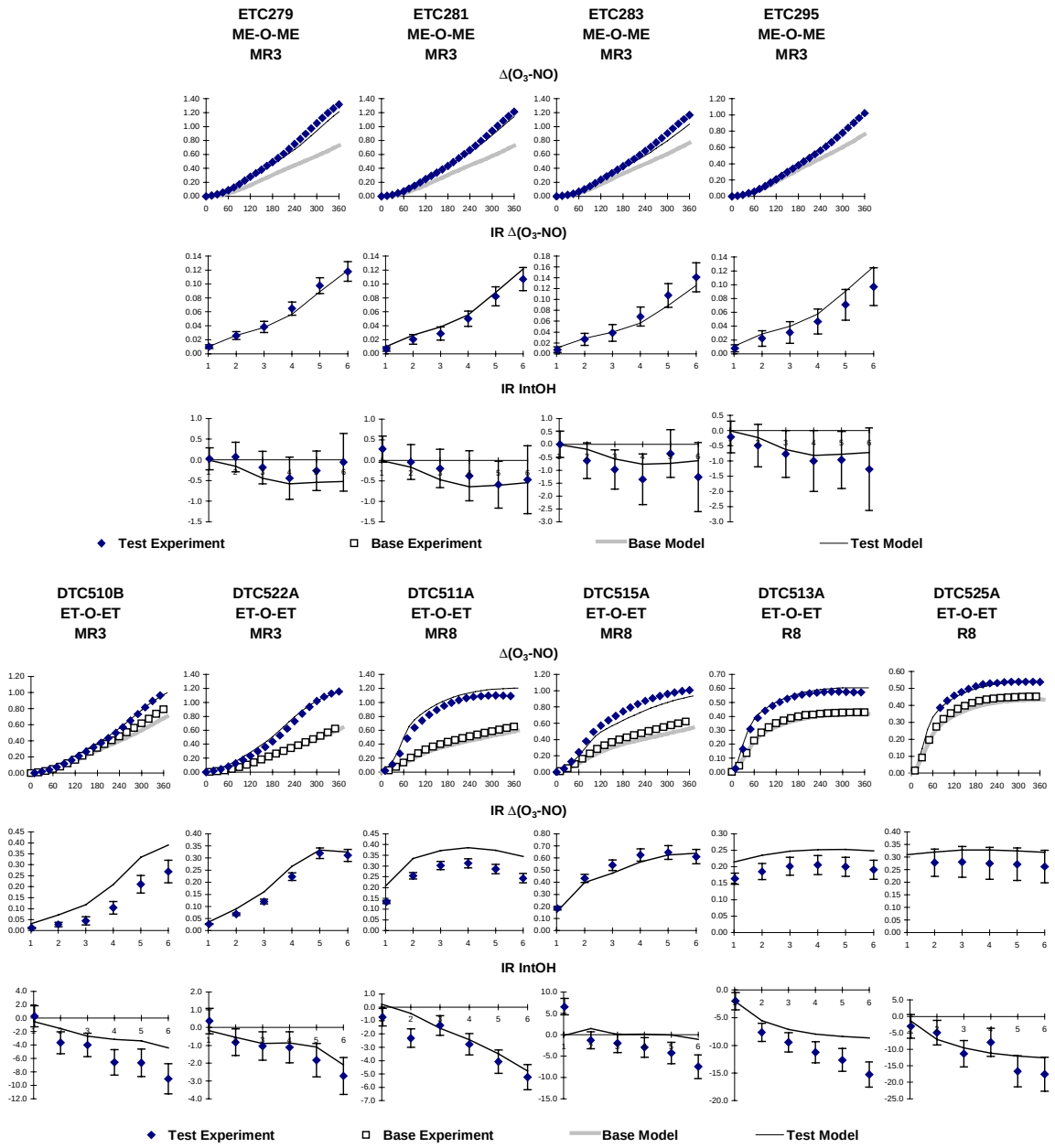

Figure B-47. Plots of experimental and calculated results of the incremental reactivity experiments with dimethyl ether and diethyl ether.

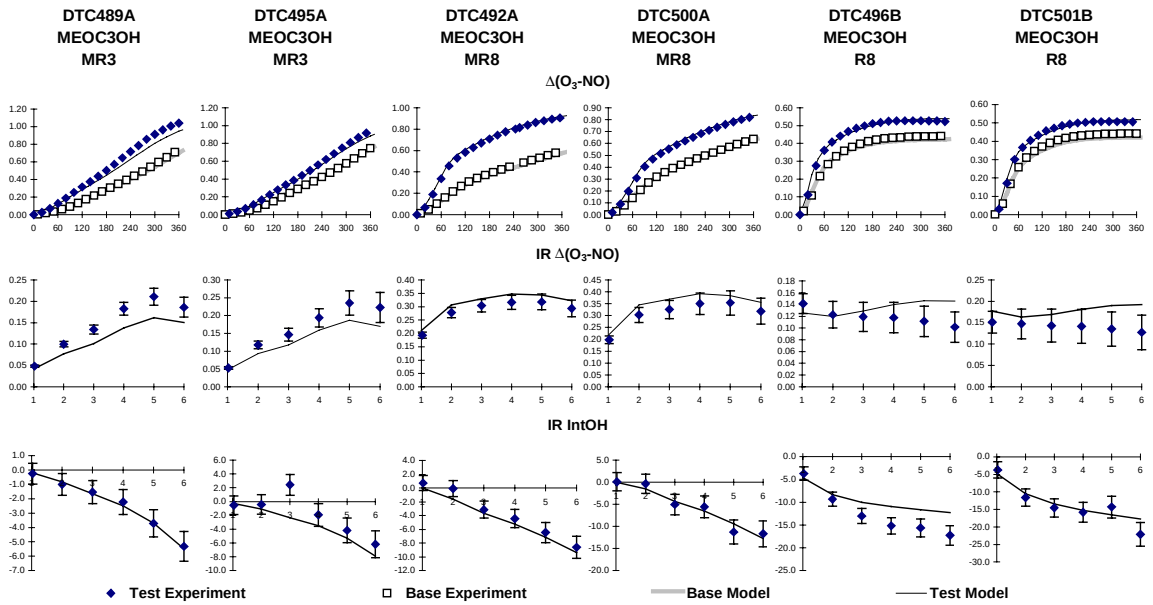

Figure B-48. Plots of experimental and calculated results of the incremental reactivity experiments with 1-Methoxy-2-Propanol

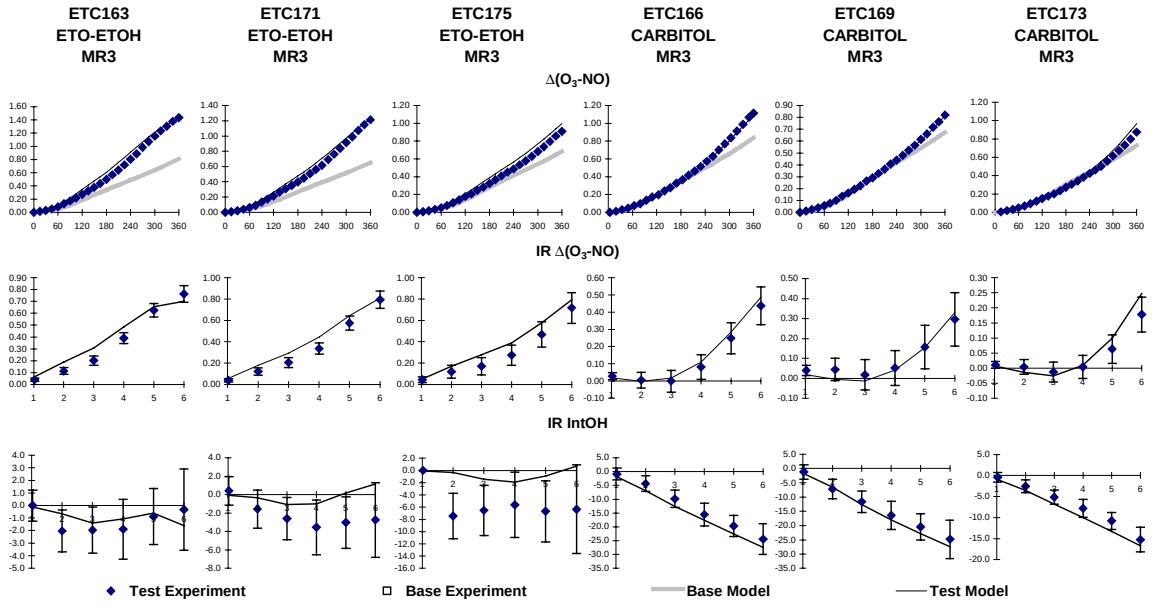

Figure B-49. Plots of experimental and calculated results of the incremental reactivity experiments with ethoxy ethanol and carbitol.

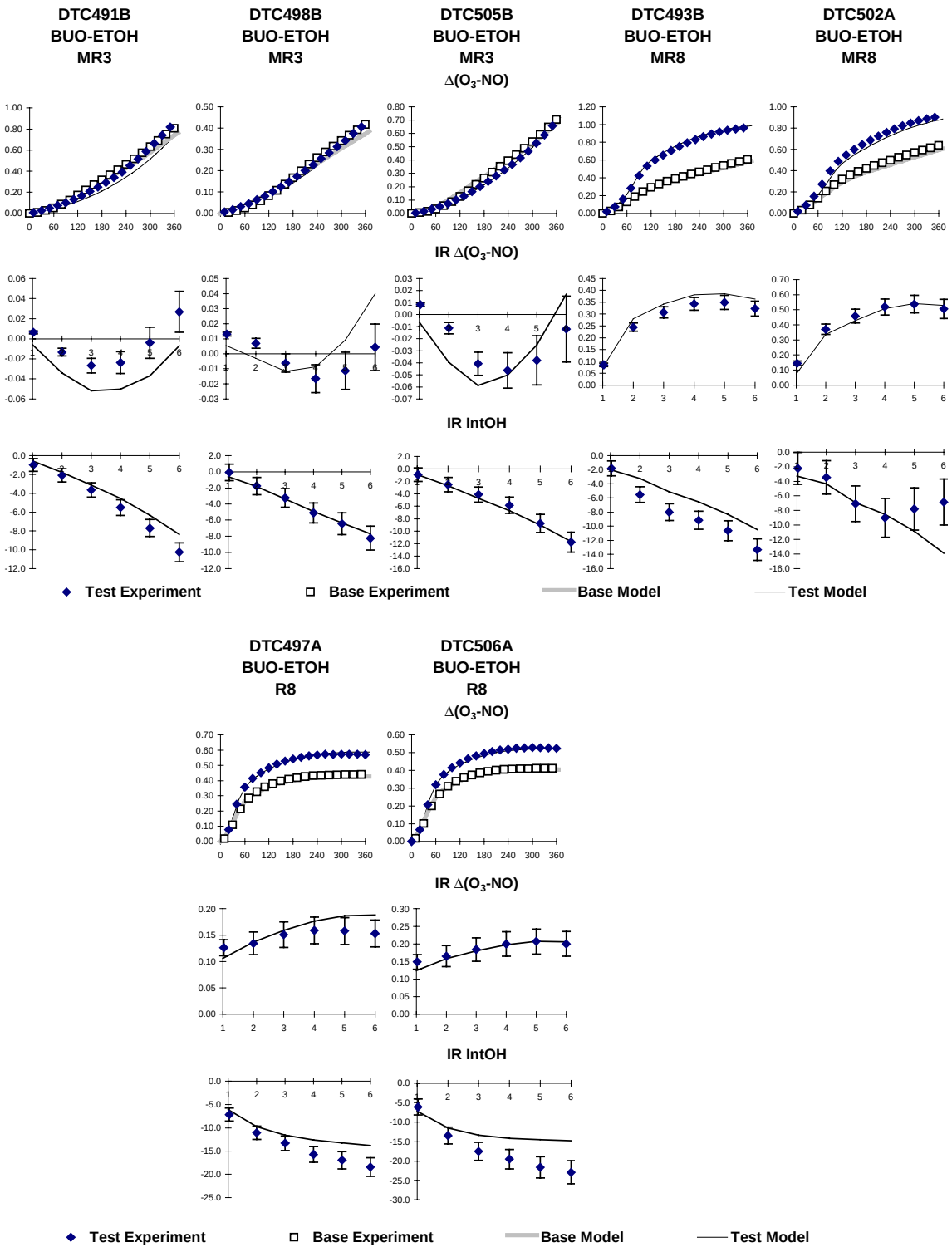

Figure B-50. Plots of experimental and calculated results of the incremental reactivity experiments with butoxy ethanol.

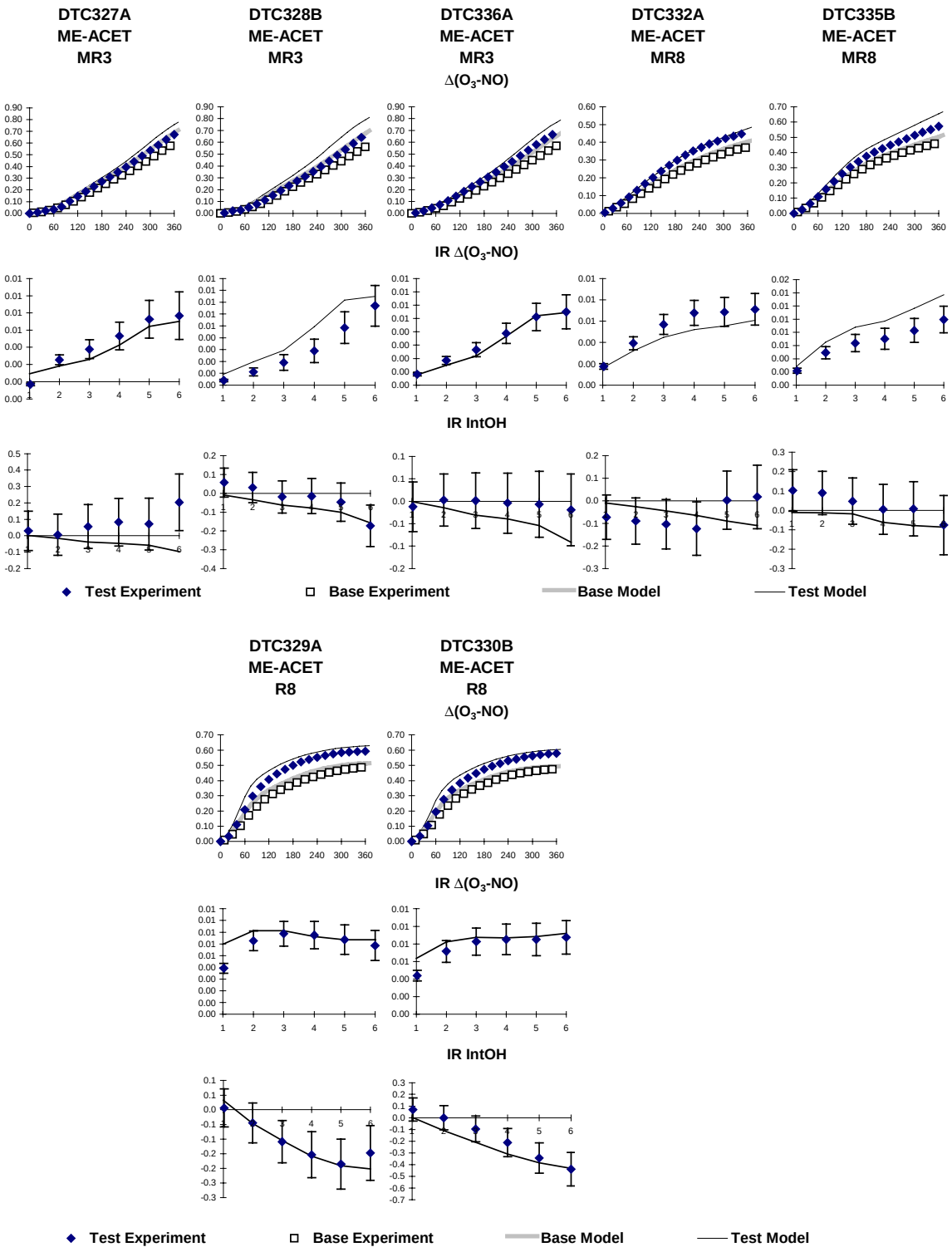

Figure B-51. Plots of experimental and calculated results of the incremental reactivity experiments with methyl acetate.

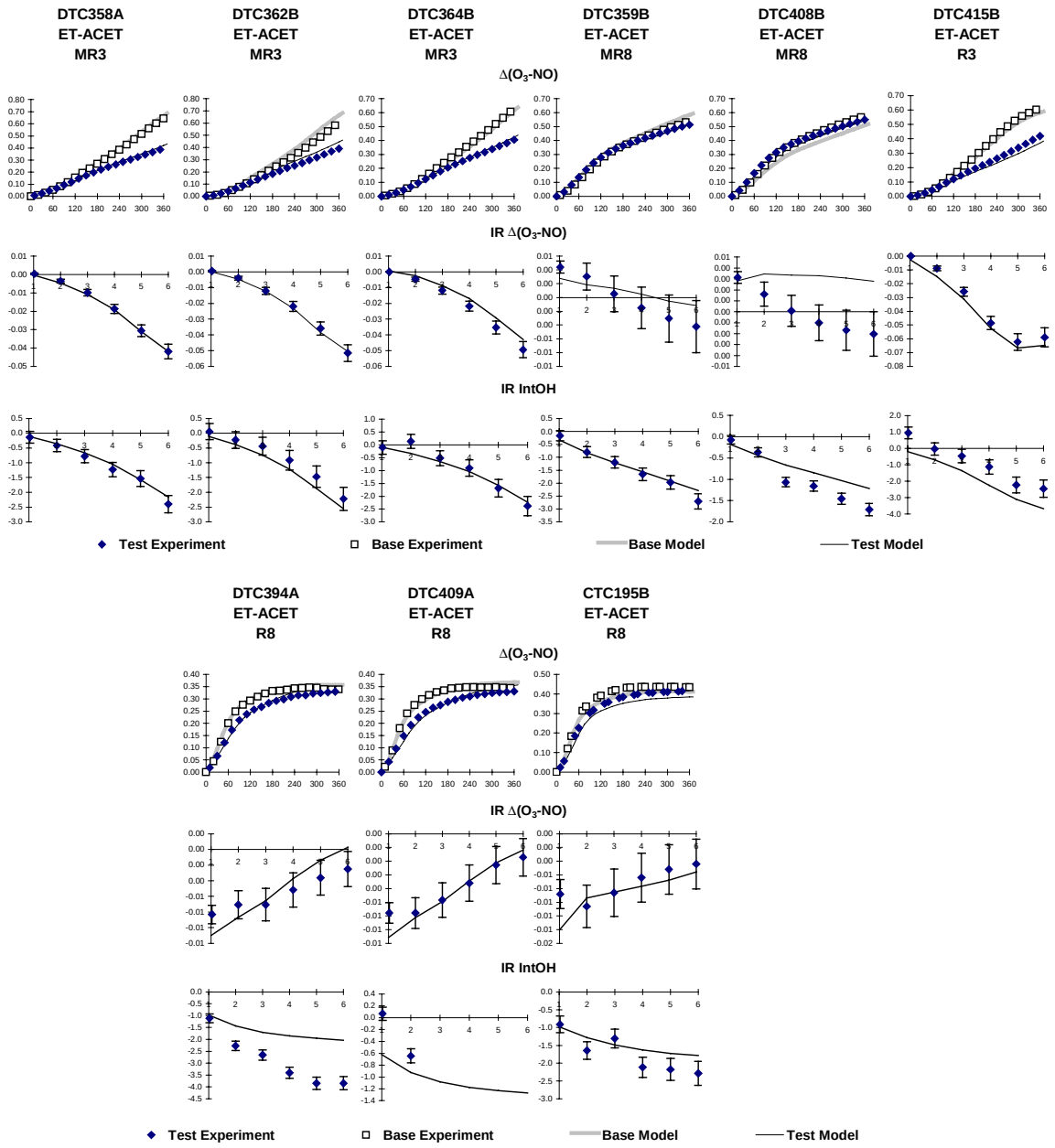

Figure B-52. Plots of experimental and calculated results of the incremental reactivity experiments with ethyl acetate.

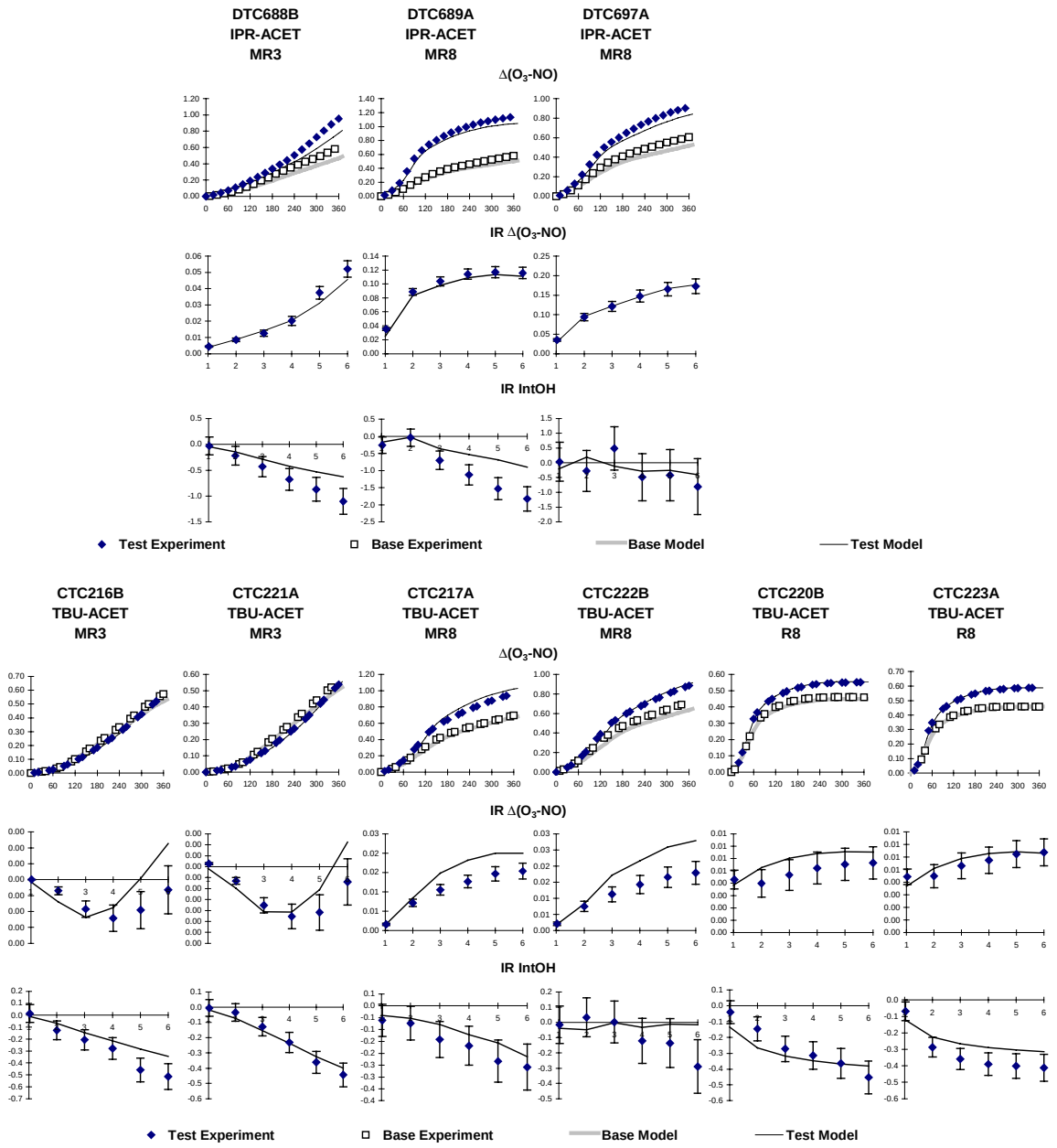

Figure B-53. Plots of experimental and calculated results of the incremental reactivity experiments with isopropyl and t-butyl acetates.

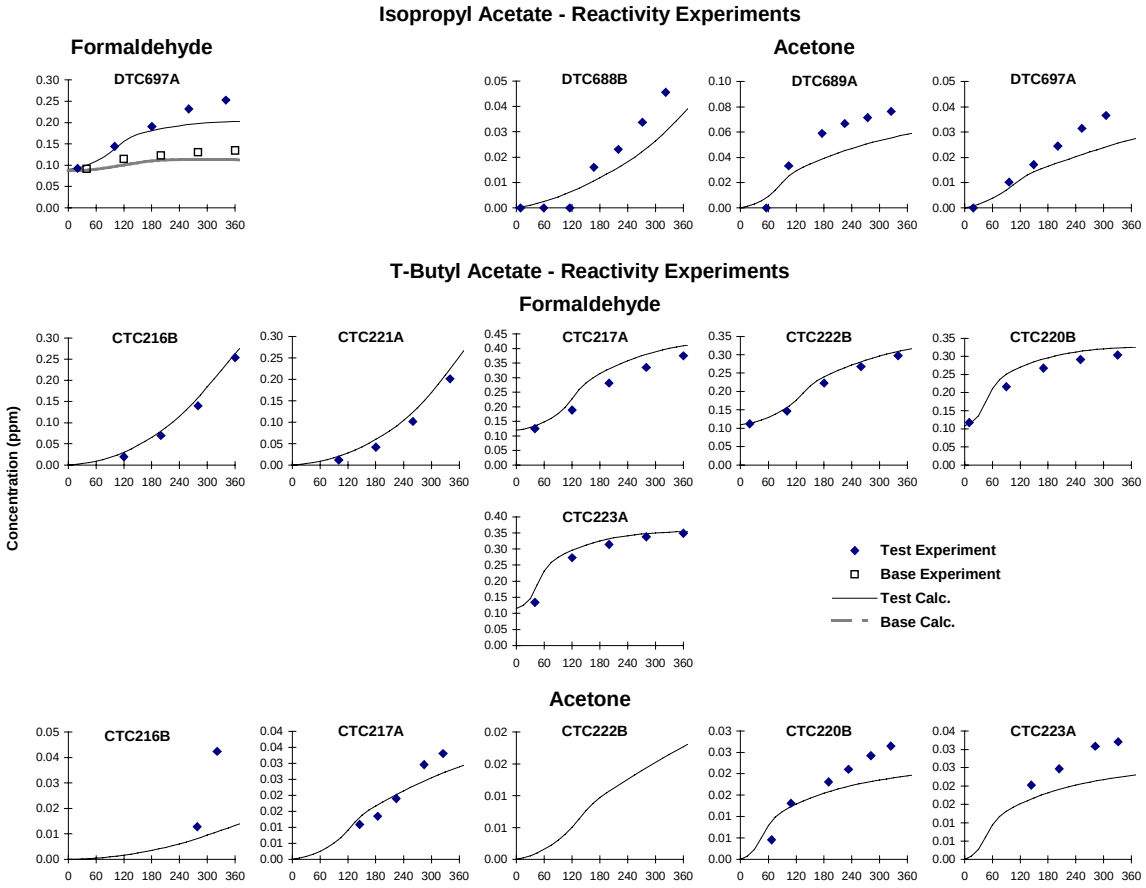

Figure B-54. Plots of experimental and calculated formaldehyde and acetone data for the isopropyl acetate and t-butyl acetate incremental reactivity experiments.

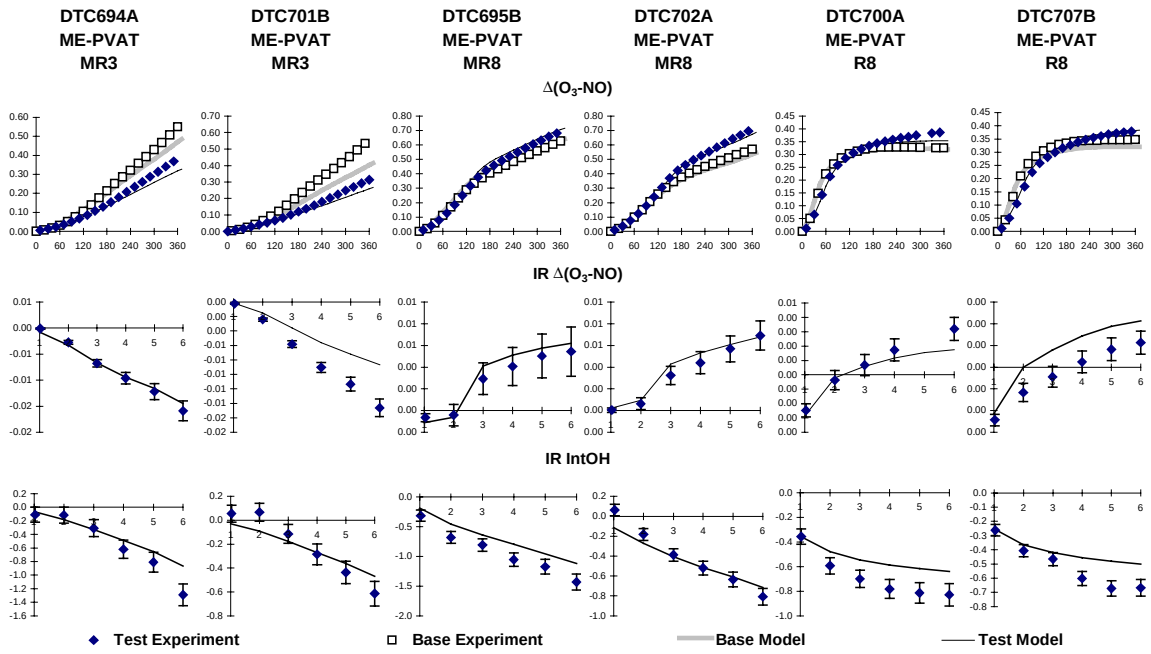

Figure B-55. Plots of experimental and calculated results of the incremental reactivity experiments with methyl pivalate.

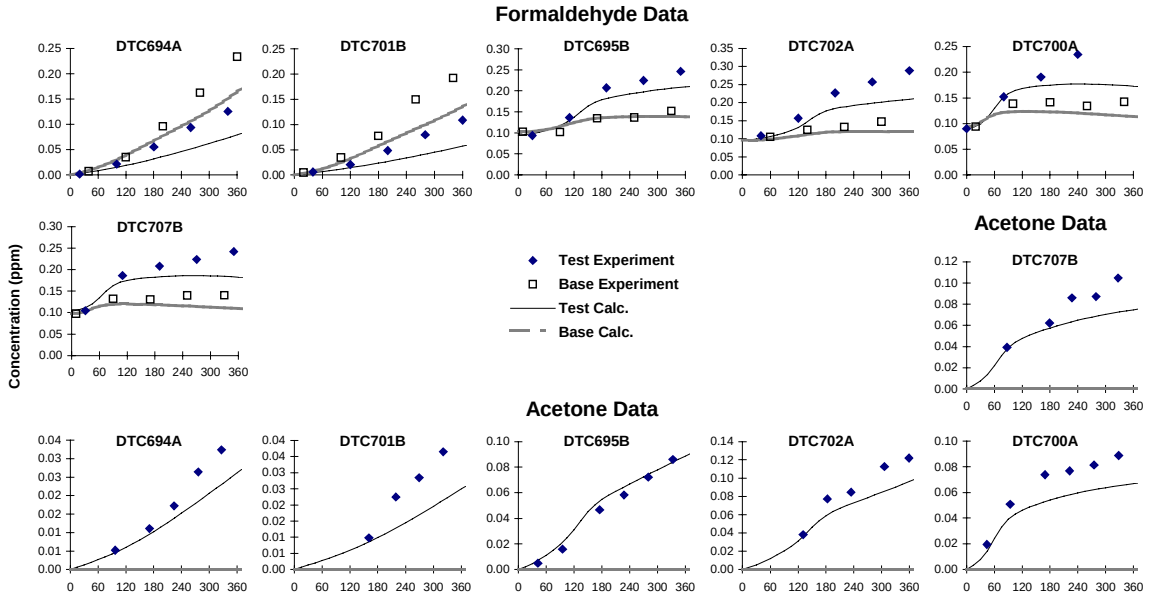

Figure B-56. Plots of experimental and calculated formaldehyde and acetone data for the methyl pivalate incremental reactivity experiments.

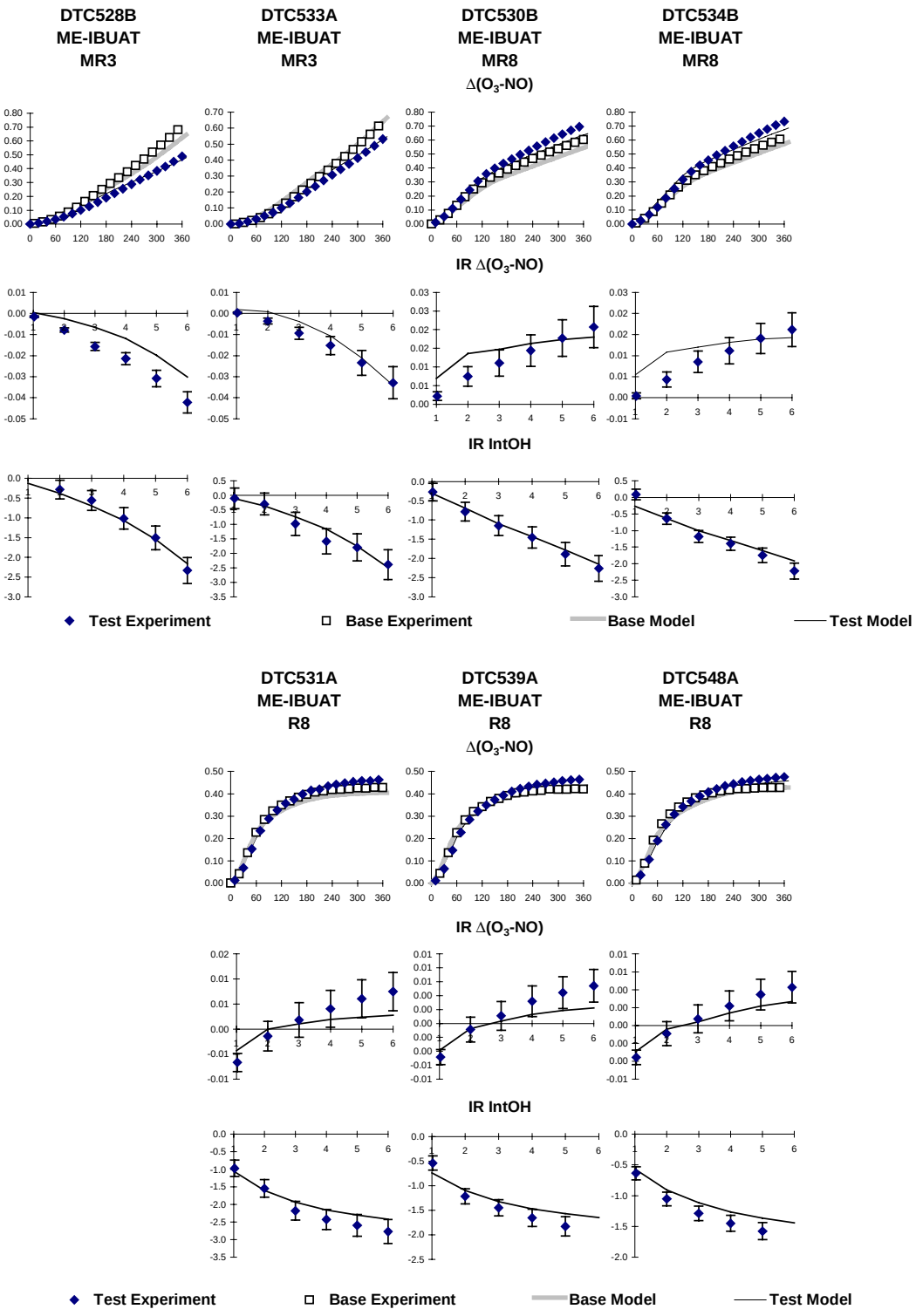

Figure B-57. Plots of experimental and calculated results of the incremental reactivity experiments with methyl isobutyrate.

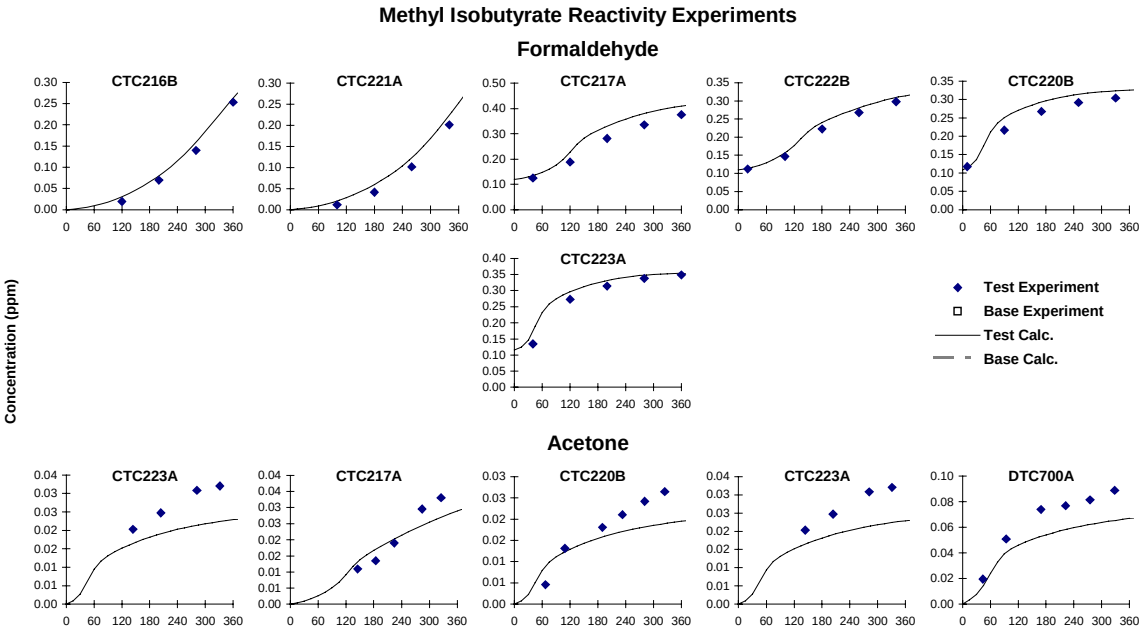

Figure B-58. Plots of experimental and calculated formaldehyde and acetone data for the methyl isobutyrate incremental reactivity experiments.

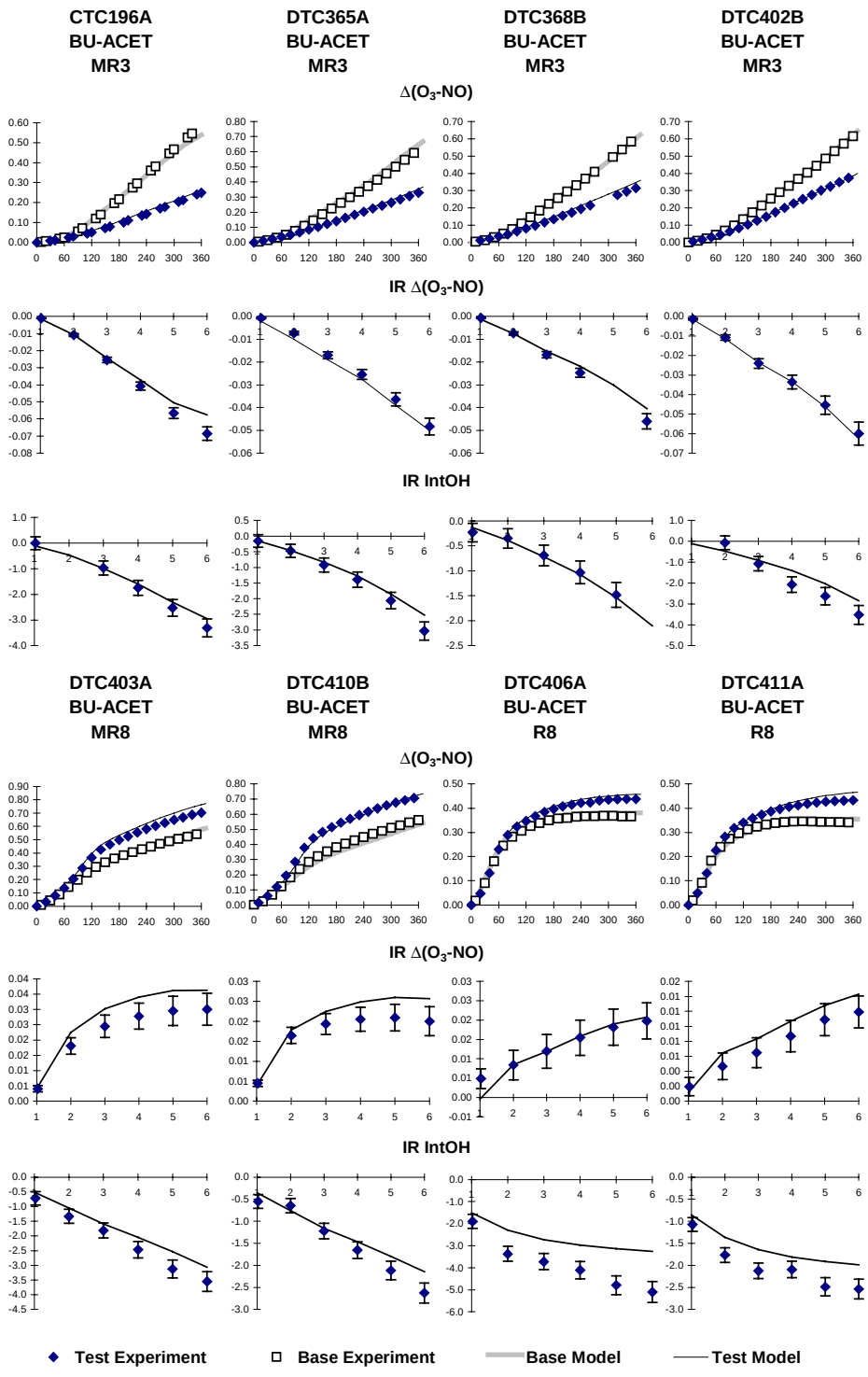

Figure B-59. Plots of experimental and calculated results of the incremental reactivity experiments with butyl acetate.

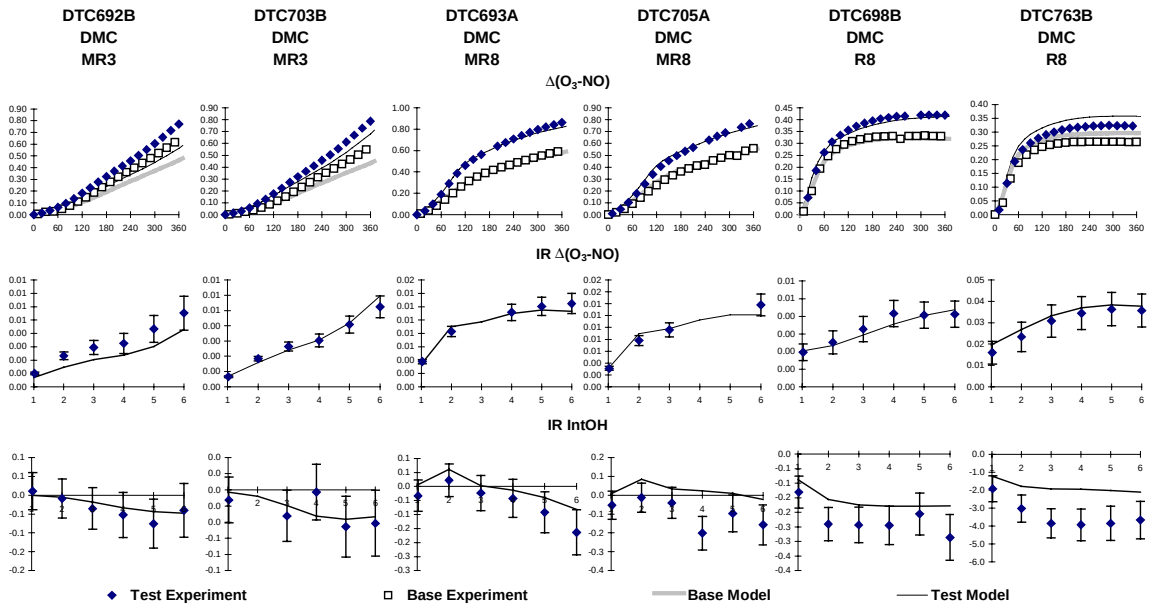

Figure B-60. Plots of experimental and calculated results of the incremental reactivity experiments with dimethyl carbonate.

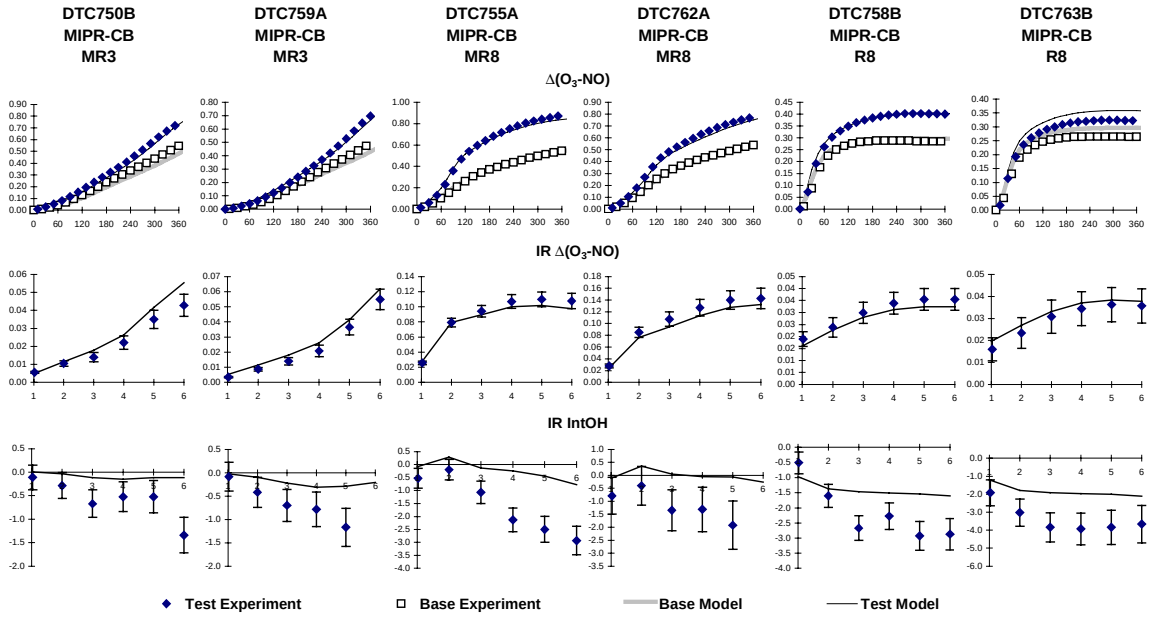

Figure B-61. Plots of experimental and calculated results of the incremental reactivity experiments with methyl isopropyl carbonate.

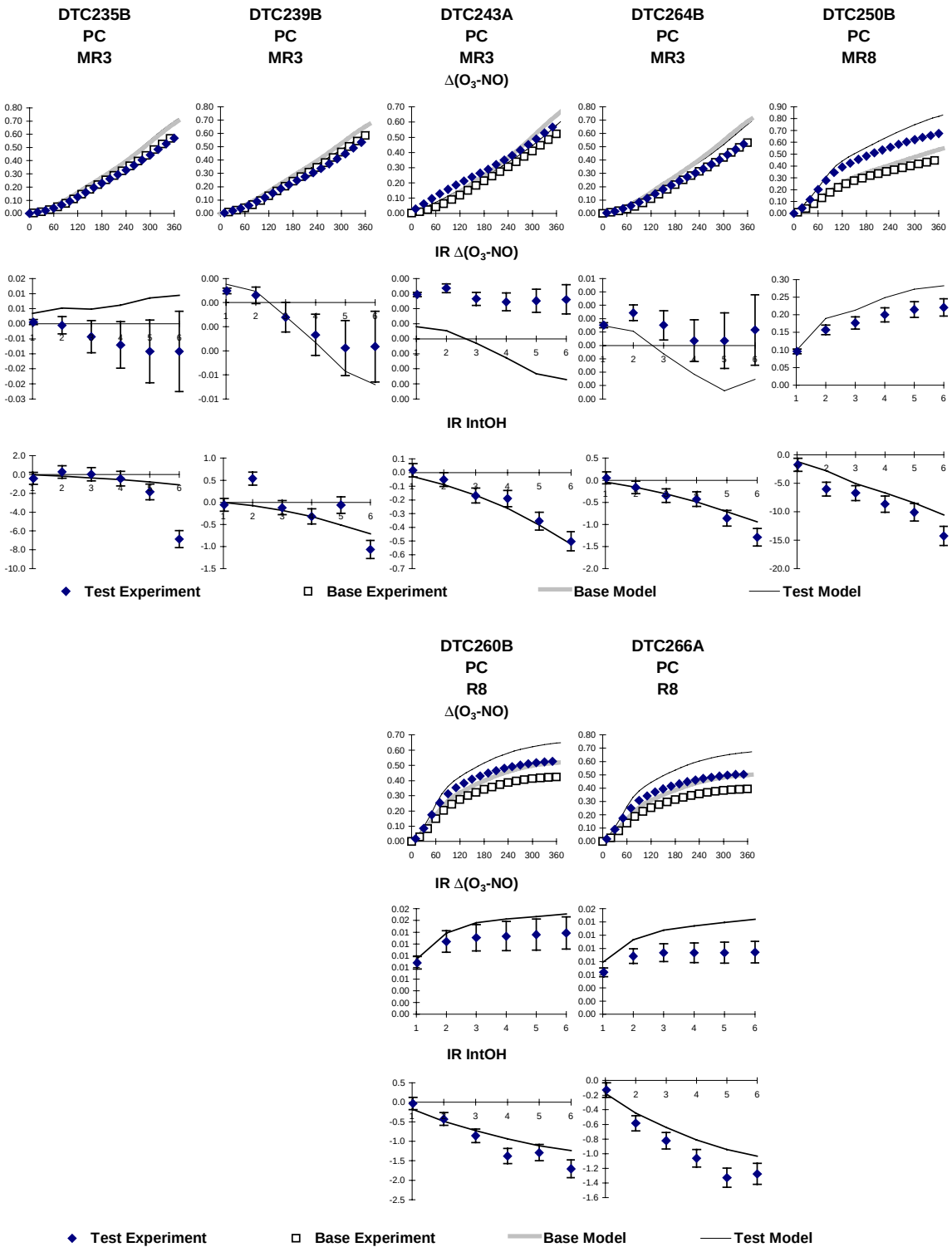

Figure B-62. Plots of experimental and calculated results of the incremental reactivity experiments with propylene carbonate.

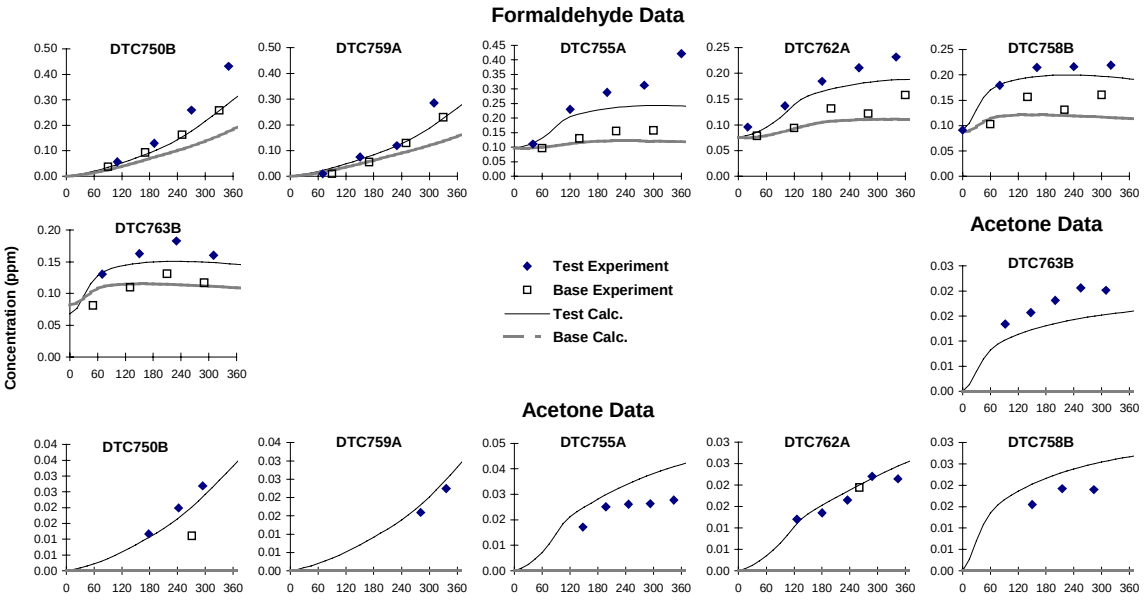

Figure B-63. Plots of experimental and calculated formaldehyde and acetone data for the methyl isopropyl carbonate incremental reactivity experiments.

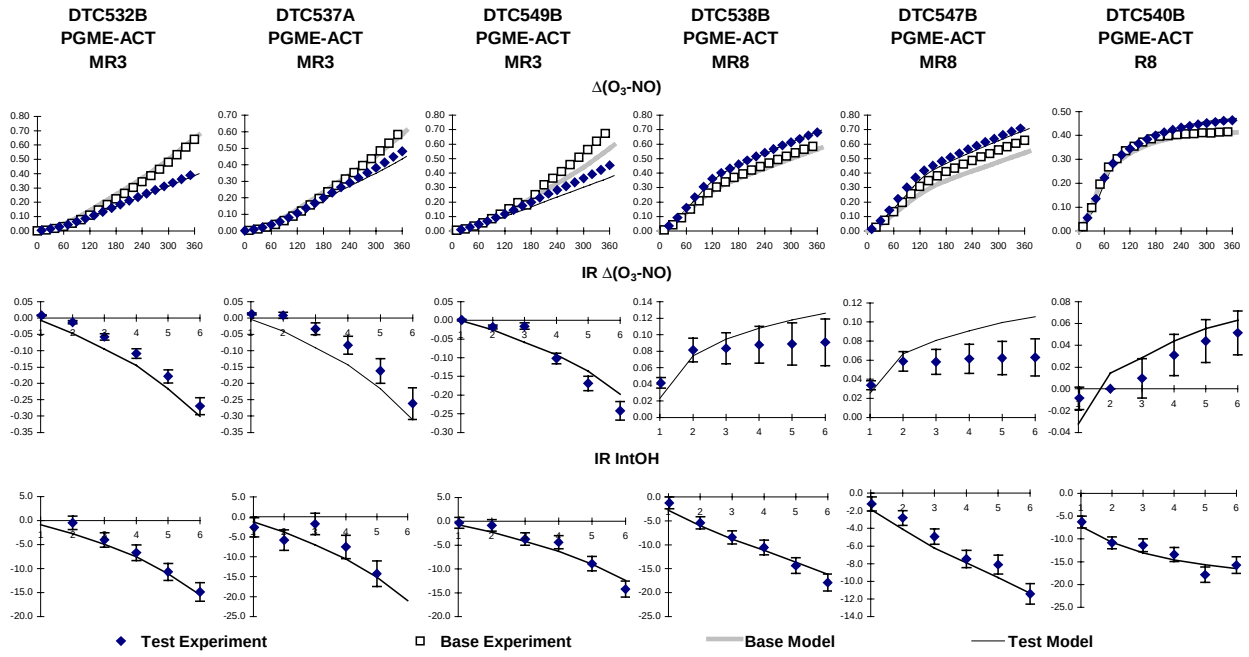

Figure B-64. Plots of experimental and calculated results of the incremental reactivity experiments with propylene glycol methyl ether acetate.

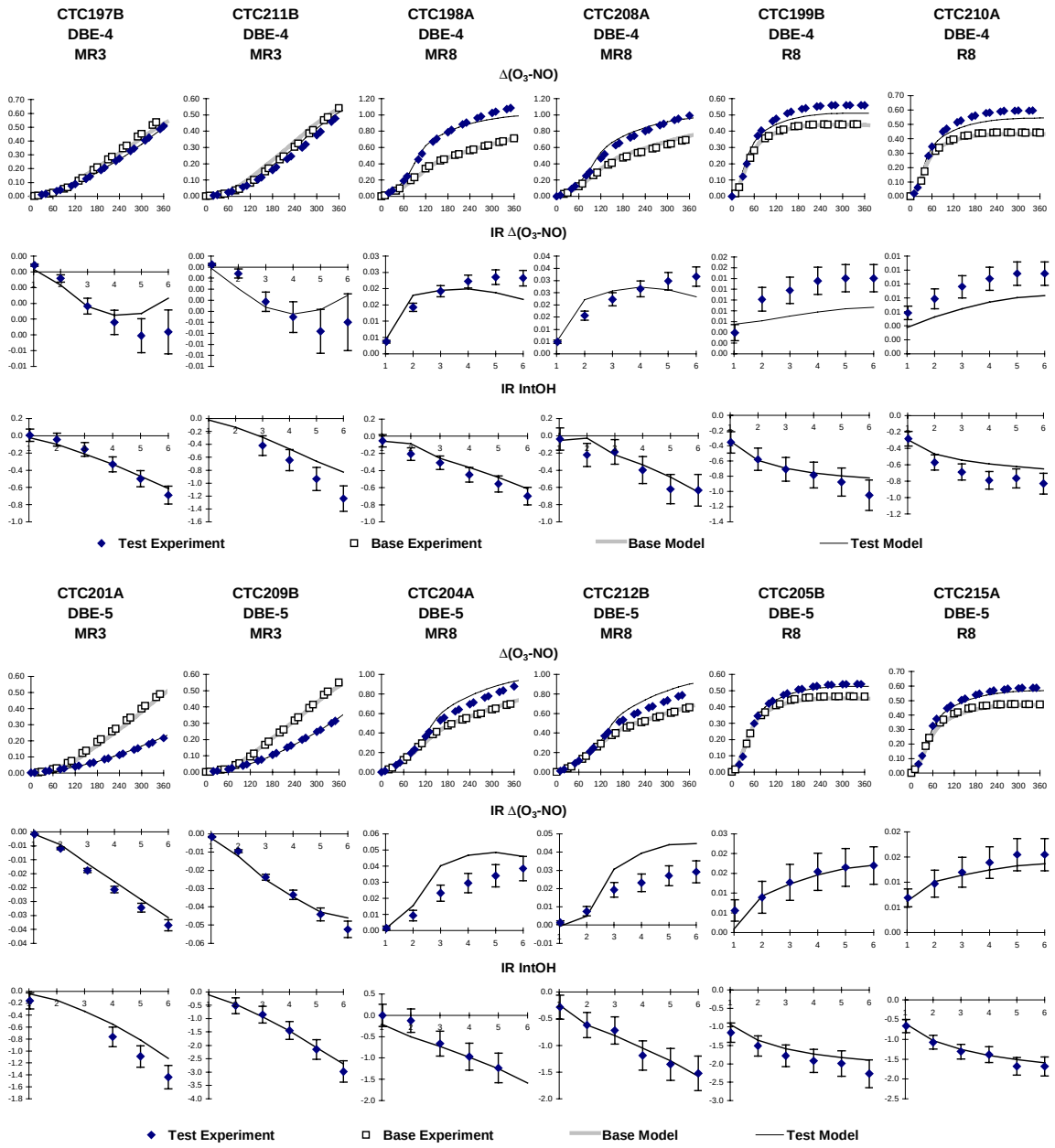

Figure B-65. Plots of experimental and calculated results of the incremental reactivity experiments with the dibasic esters Dimethyl Glutarate and Dimethyl Adipate.

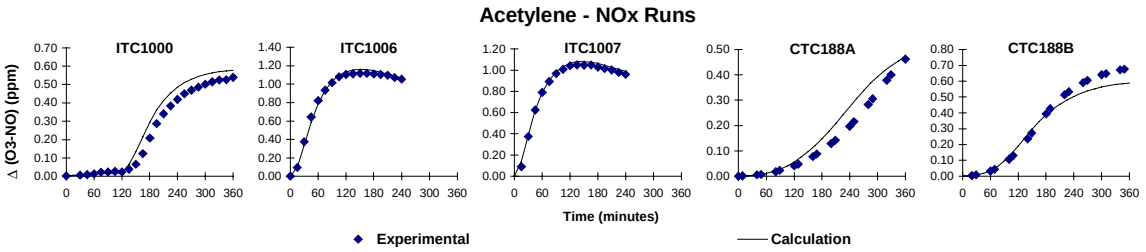

Figure B-66. Plots of experimental and calculated $\Delta([O_3]-[NO])$ data for the acetylene - NO_x experiments.

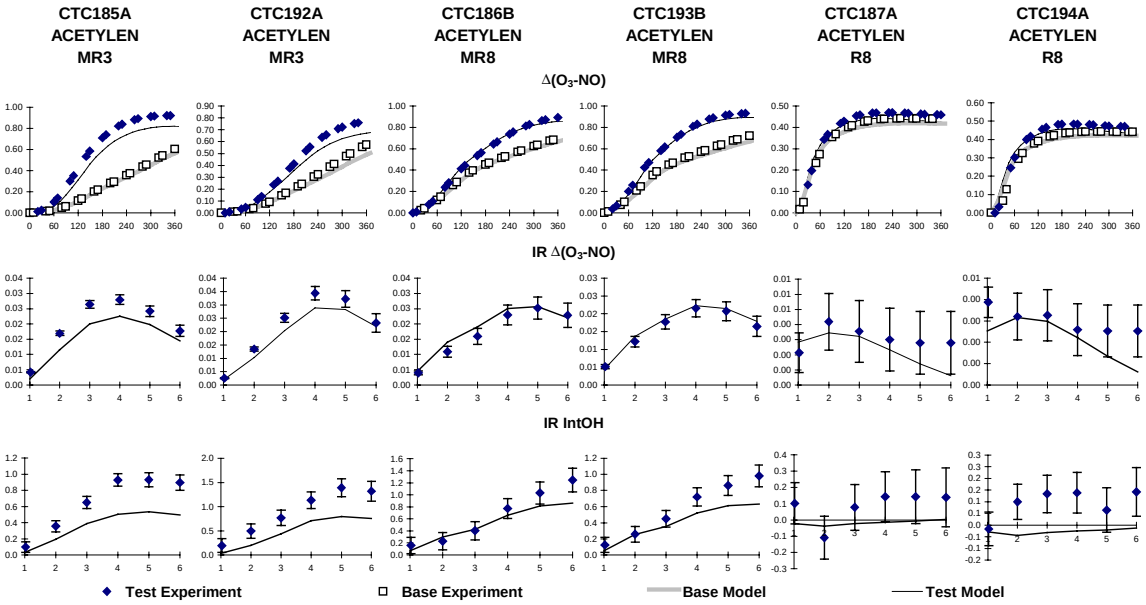

Figure B-67. Plots of experimental and calculated results of the incremental reactivity experiments with acetylene. (Run CTC184B, which has similar results as run CTC185A, is not shown.)

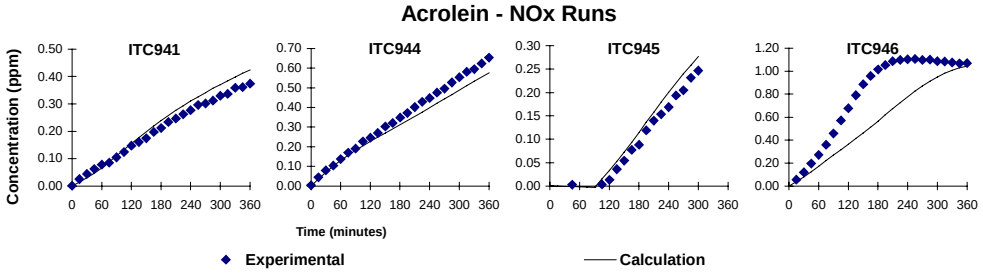

Figure B-68. Plots of experimental and calculated $\Delta([O_3]-[NO])$ data for the acrolein - NO_x experiments.

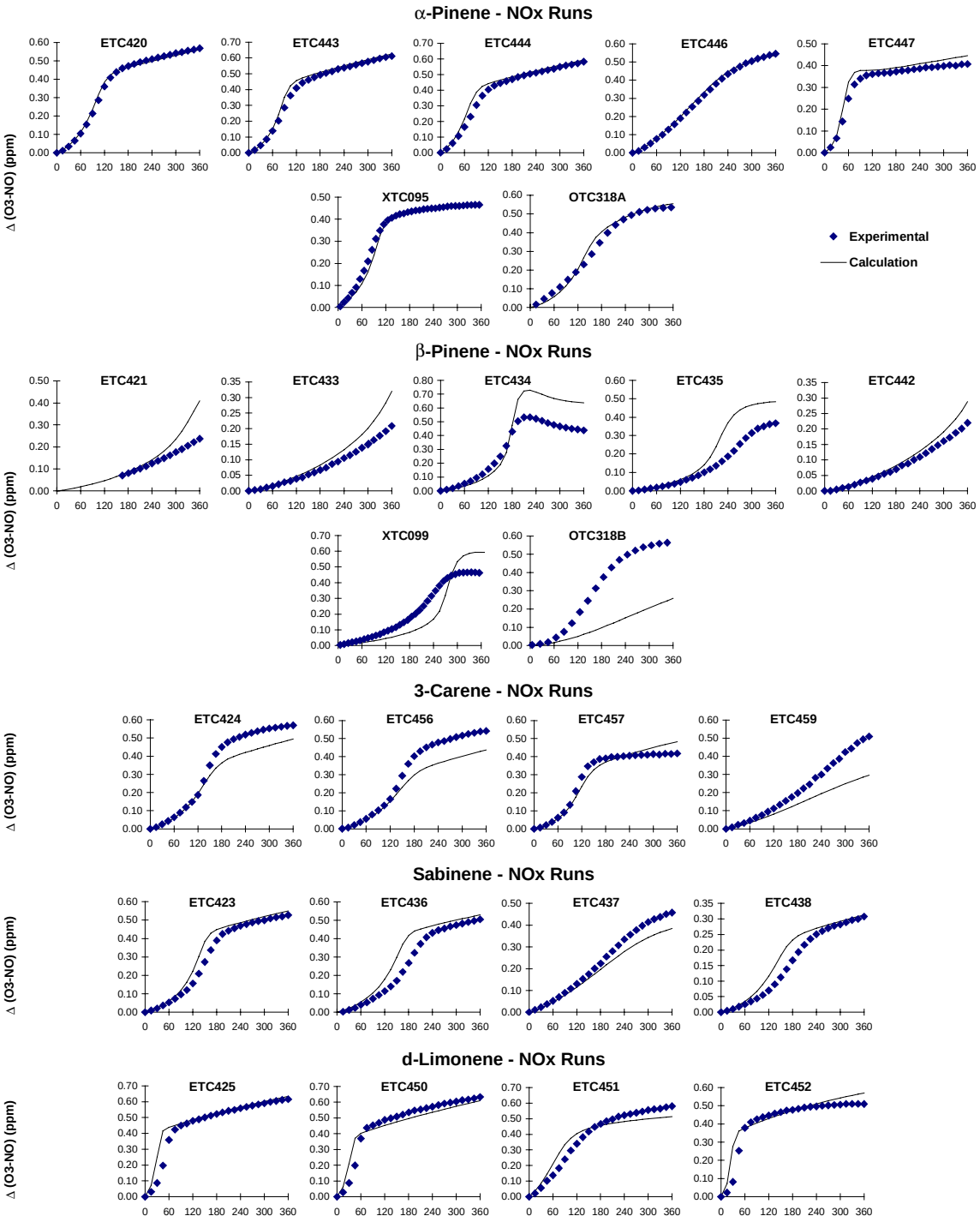

Figure B-69. Plots of experimental and calculated $\Delta([O_3]-[NO])$ data for the terpene - NO_x experiments.

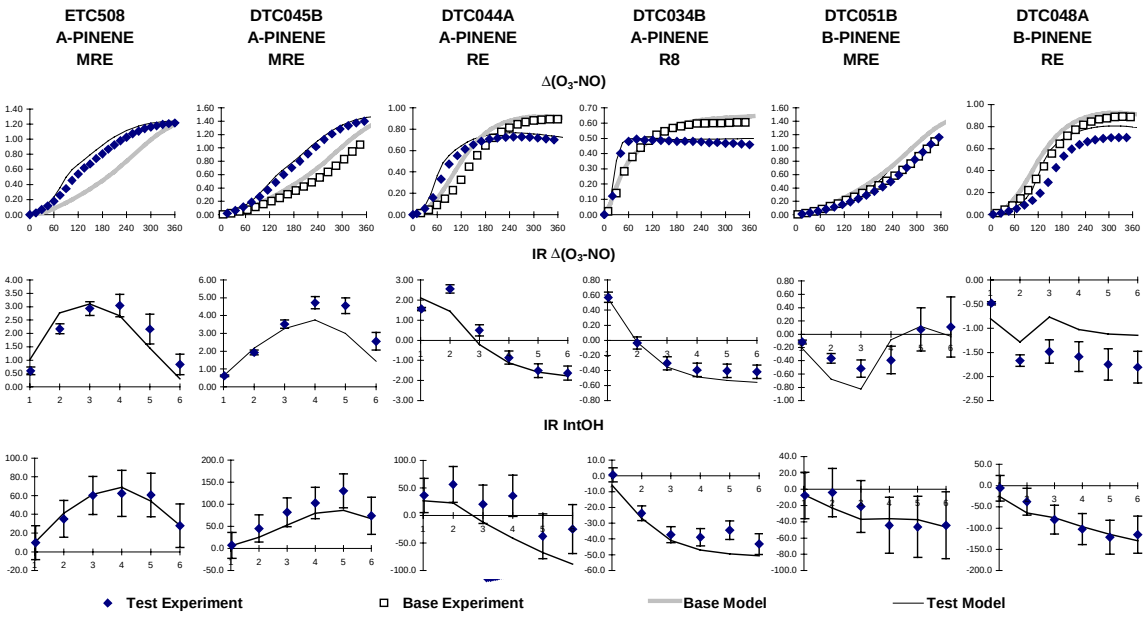

Figure B-70. Plots of experimental and calculated results of the incremental reactivity experiments with α- and β-pinenes.

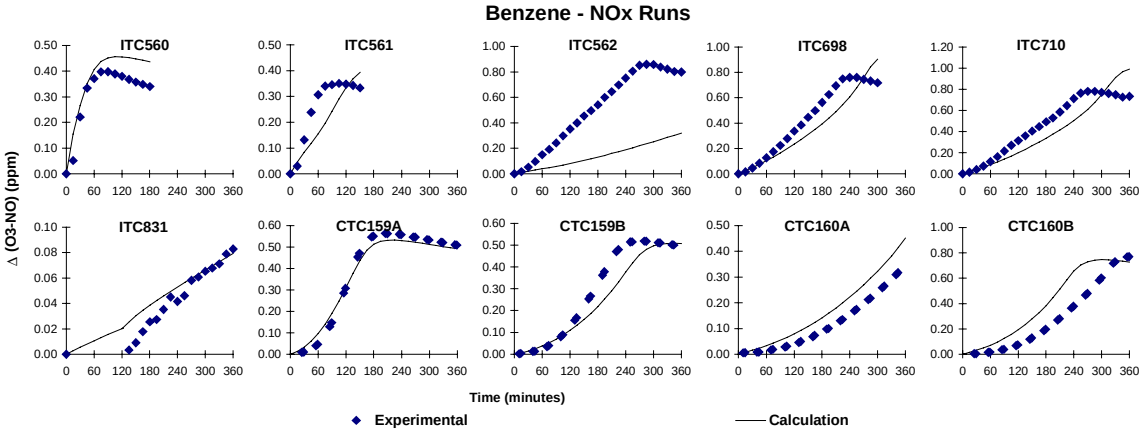

Figure B-71. Plots of experimental and calculated $\Delta([O_3]-[NO])$ data for the benzene - NO_2 experiments.

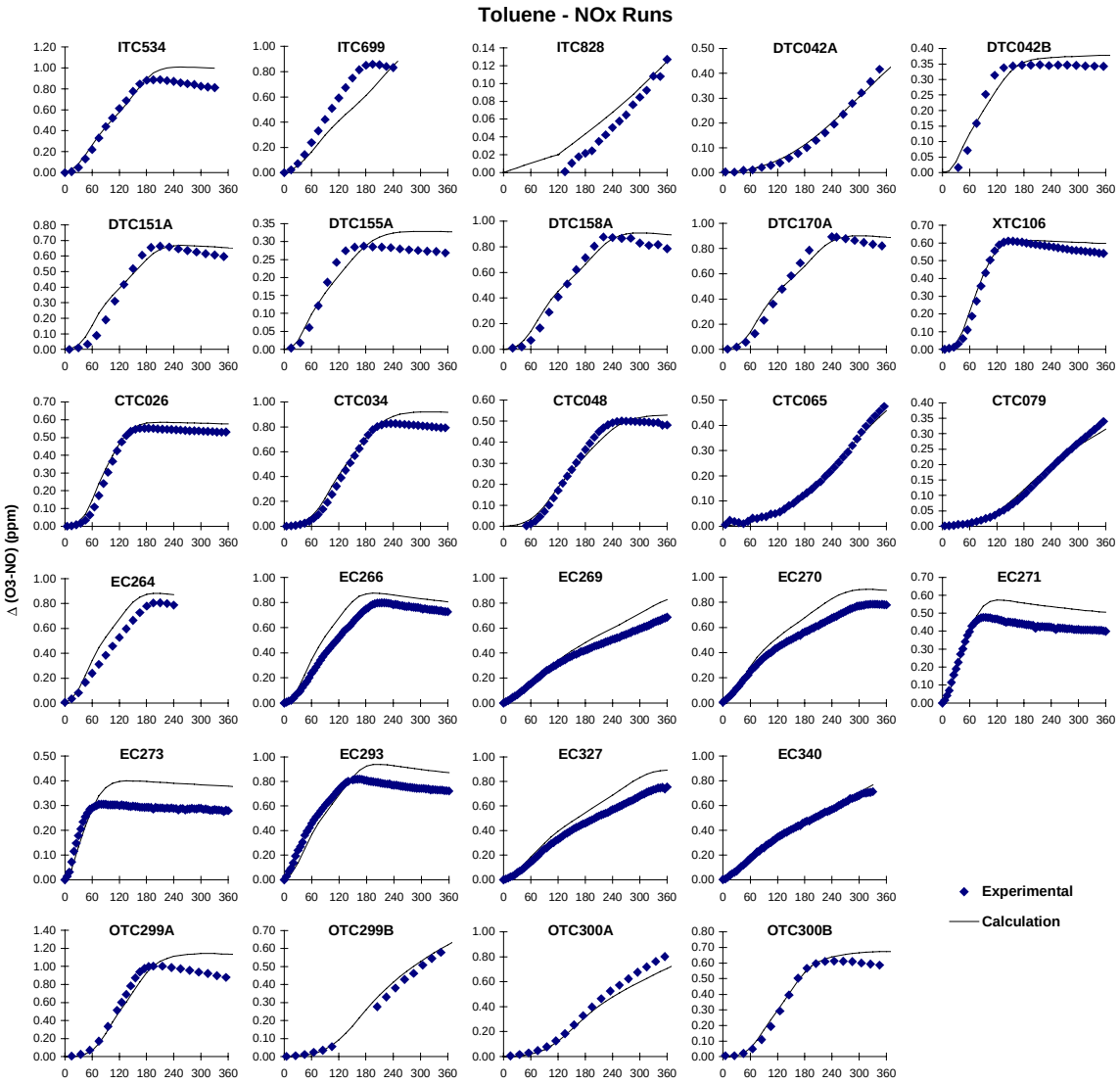

Figure B-72. Plots of experimental and calculated $\Delta([O_3]-[NO])$ data for the toluene - NO_x experiments.

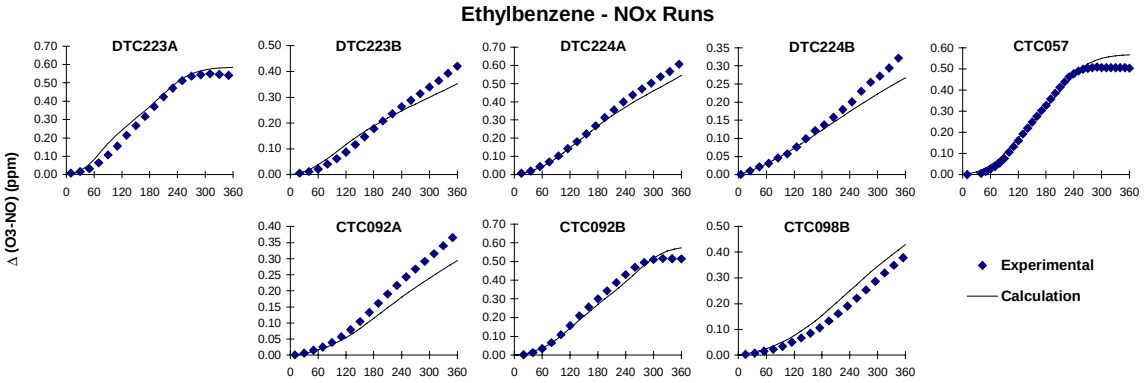

Figure B-73. Plots of experimental and calculated $\Delta([O_3]-[NO])$ data for the ethylbenzene - NO_x experiments.

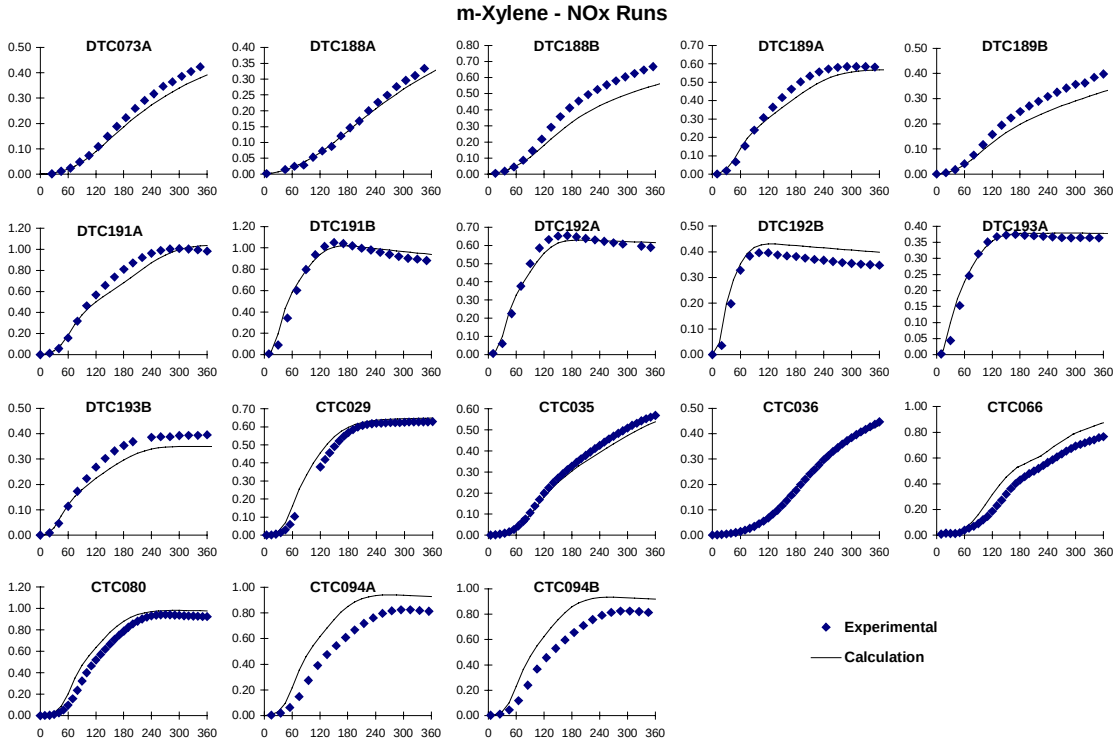

Figure B-74. Plots of experimental and calculated $\Delta([O_3]-[NO])$ data for the m-xylene - NO_2 experiments.

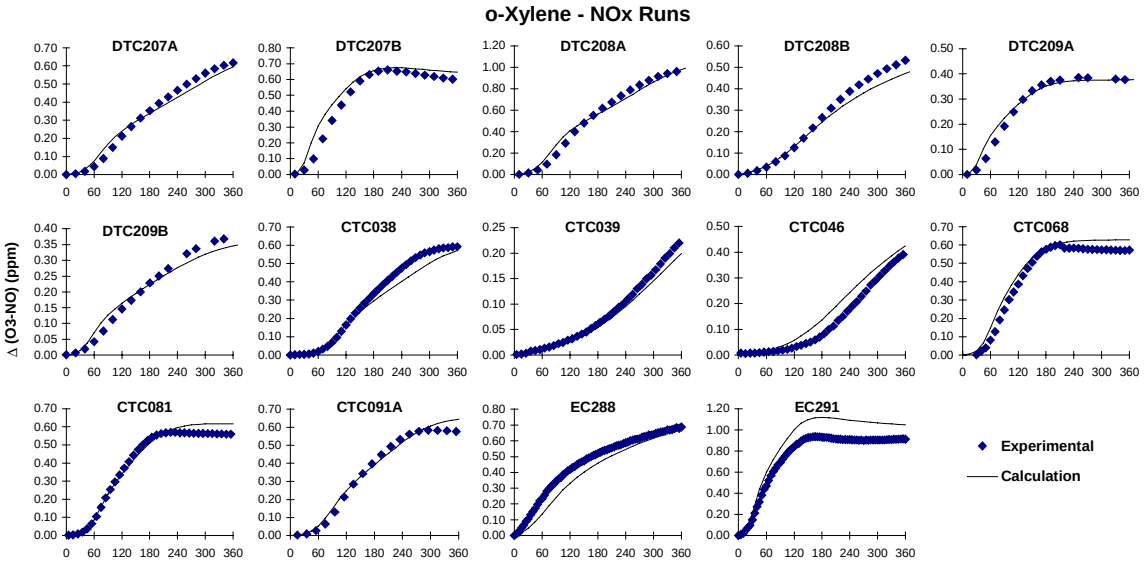

Figure B-75. Plots of experimental and calculated $\Delta([O_3]-[NO])$ data for the o-xylene - NO_2 experiments.

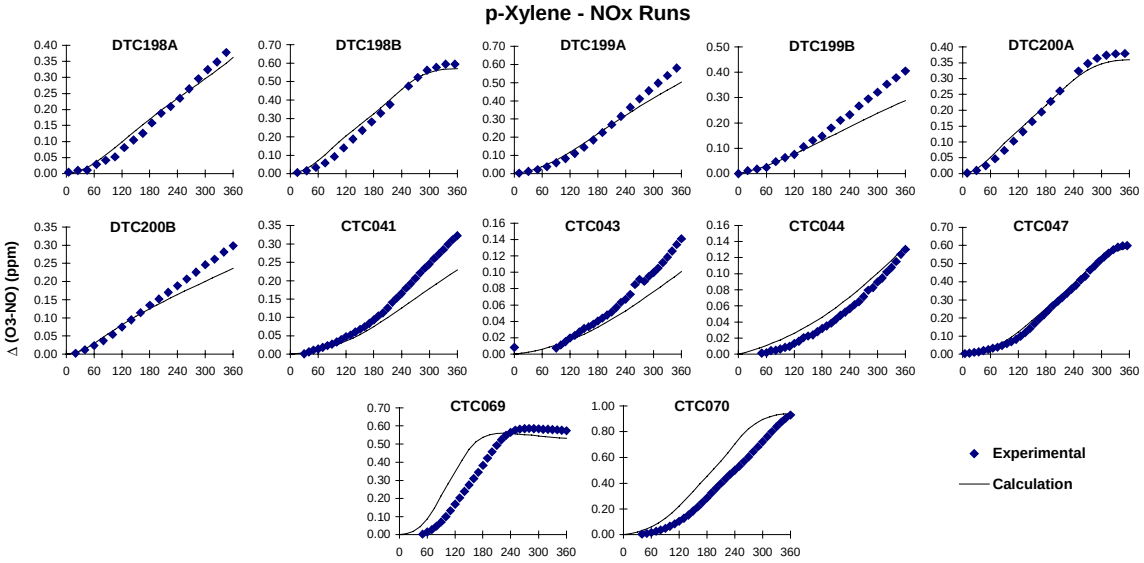

Figure B-76. Plots of experimental and calculated $\Delta([O_3]-[NO])$ data for the p-xylene - NO_x experiments.

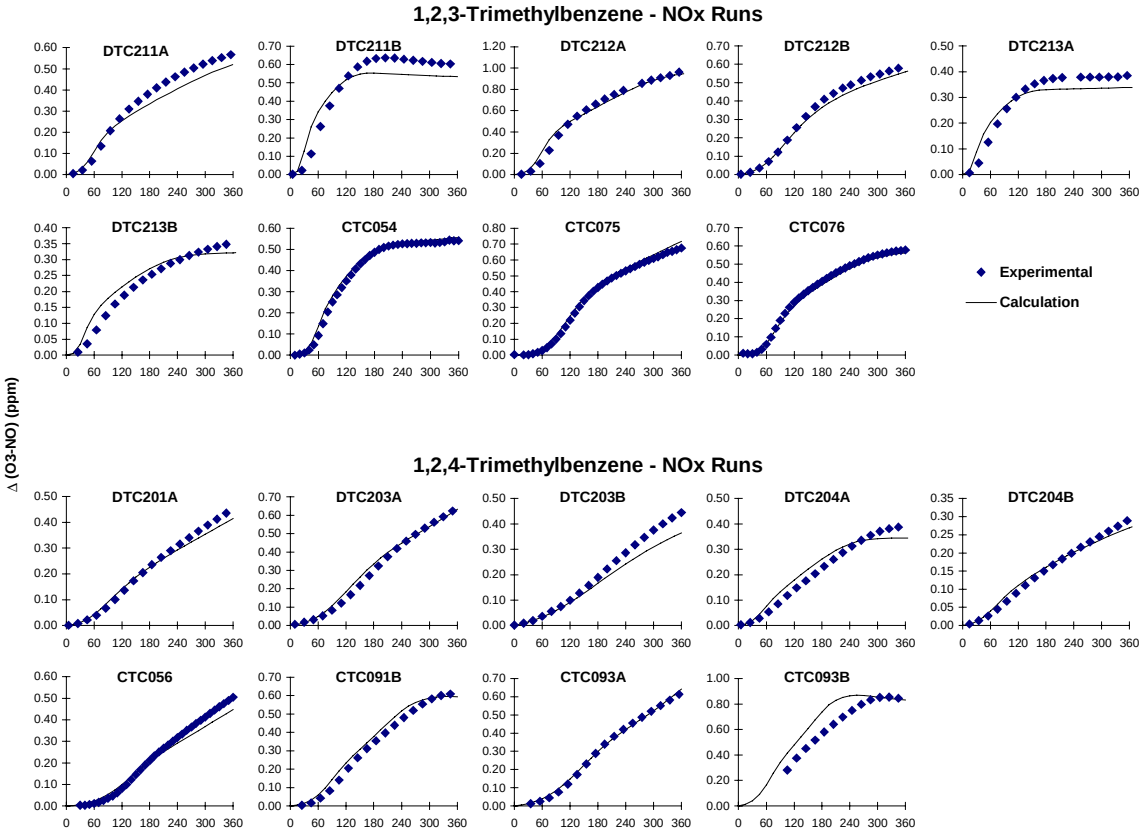

Figure B-77. Plots of experimental and calculated $\Delta([O_3]-[NO])$ data for the 1,2,3-trimethylbenzene and 1,2,4-trimethylbenzene - NO_x experiments.

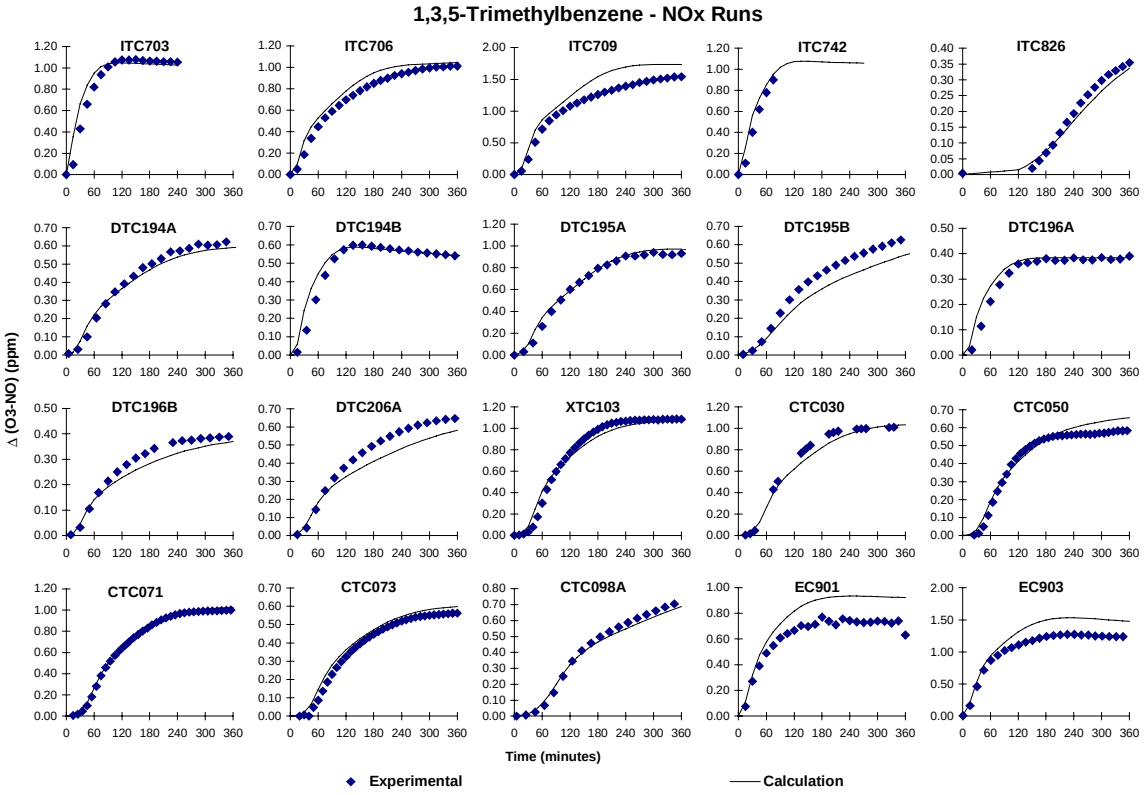

Figure B-78. Plots of experimental and calculated $\Delta([O_3]-[NO])$ data for the 1,3,5-trimethylbenzene - NO_x experiments.

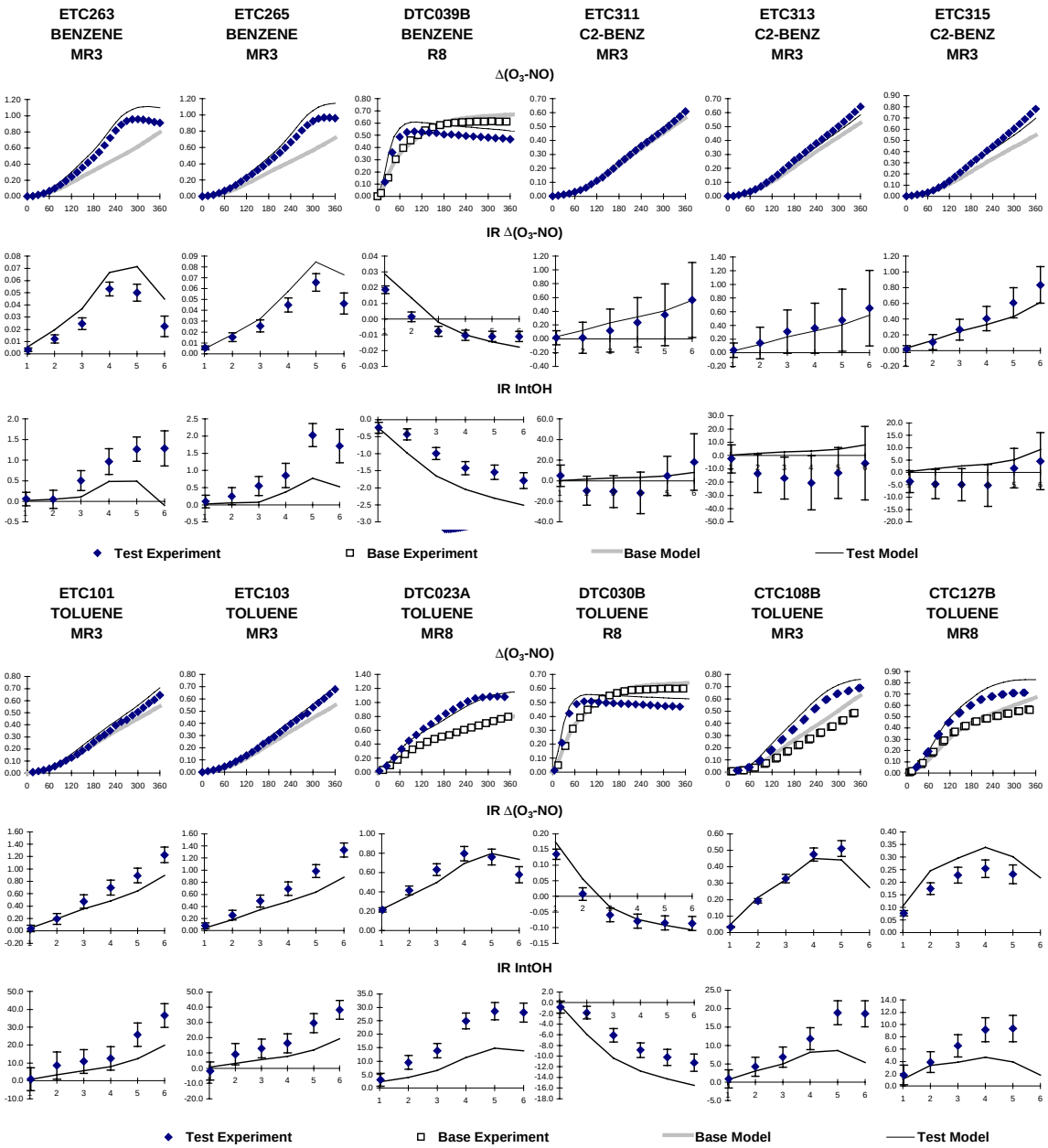

Figure B-79. Plots of experimental and calculated results of the incremental reactivity experiments with benzene, toluene, and ethylbenzene.

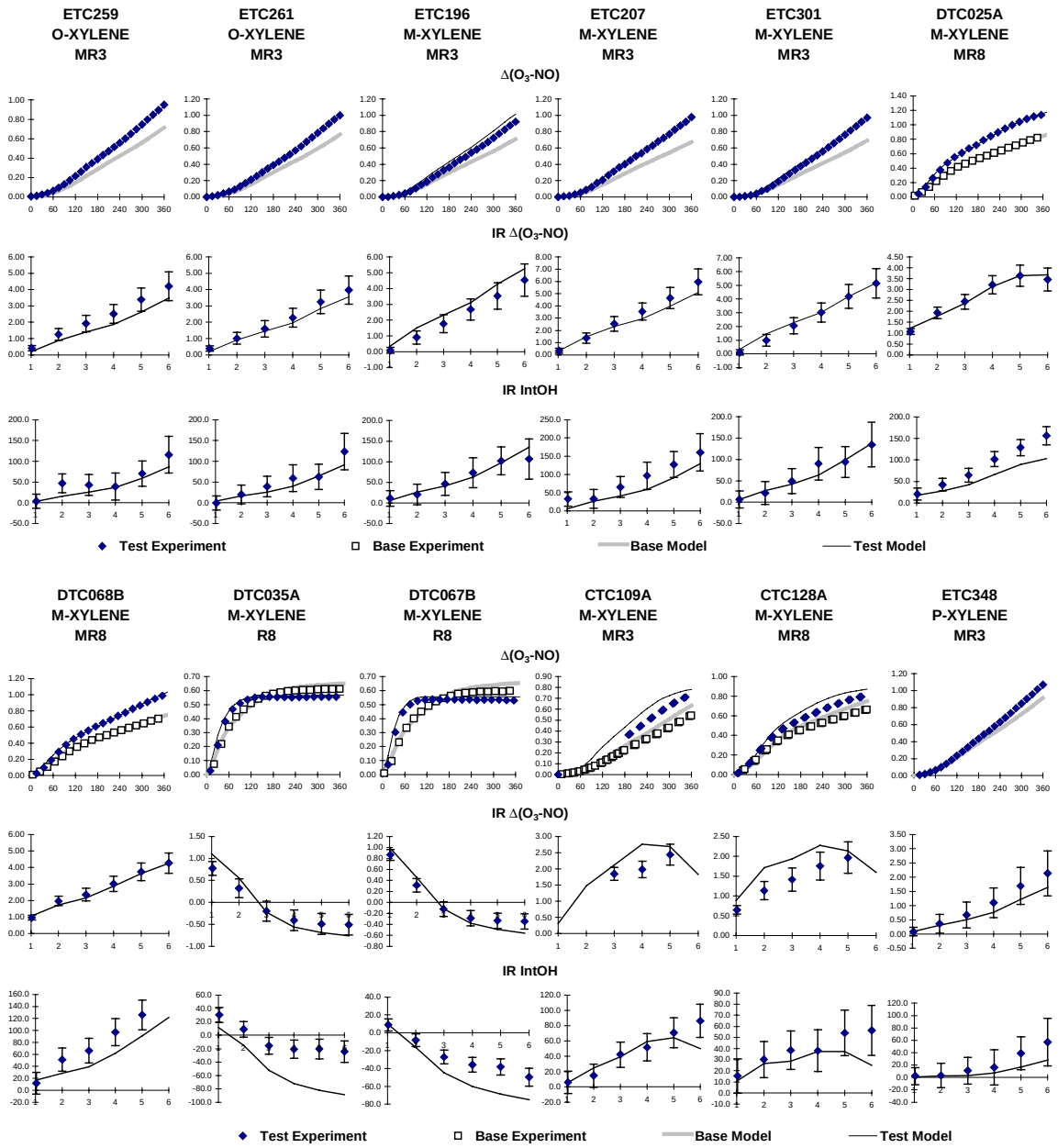

Figure B-80. Plots of experimental and calculated results of the incremental reactivity experiments with o-, m-, and p-xylenes.

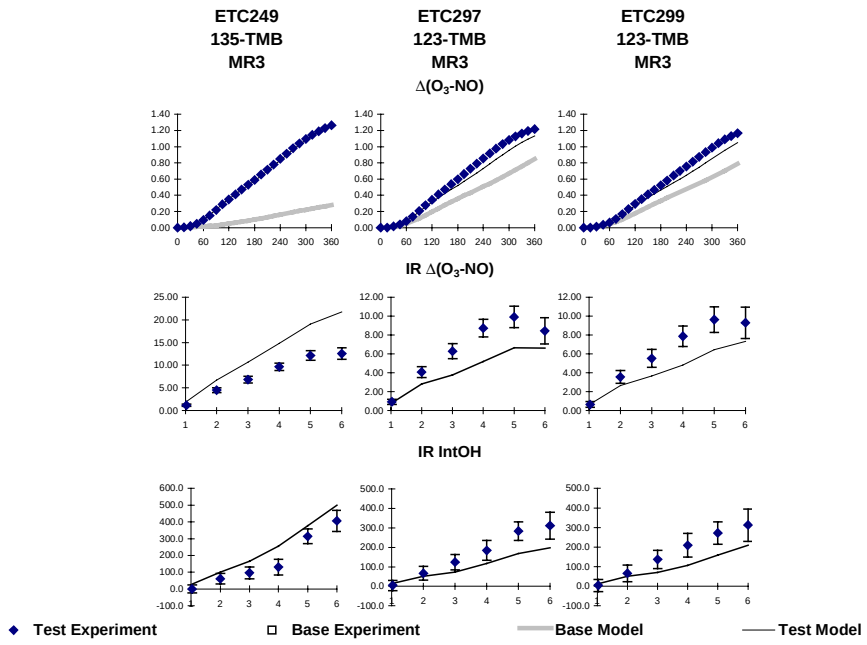

Figure B-81. Plots of experimental and calculated results of the incremental reactivity experiments with the trimethyl benzenes.

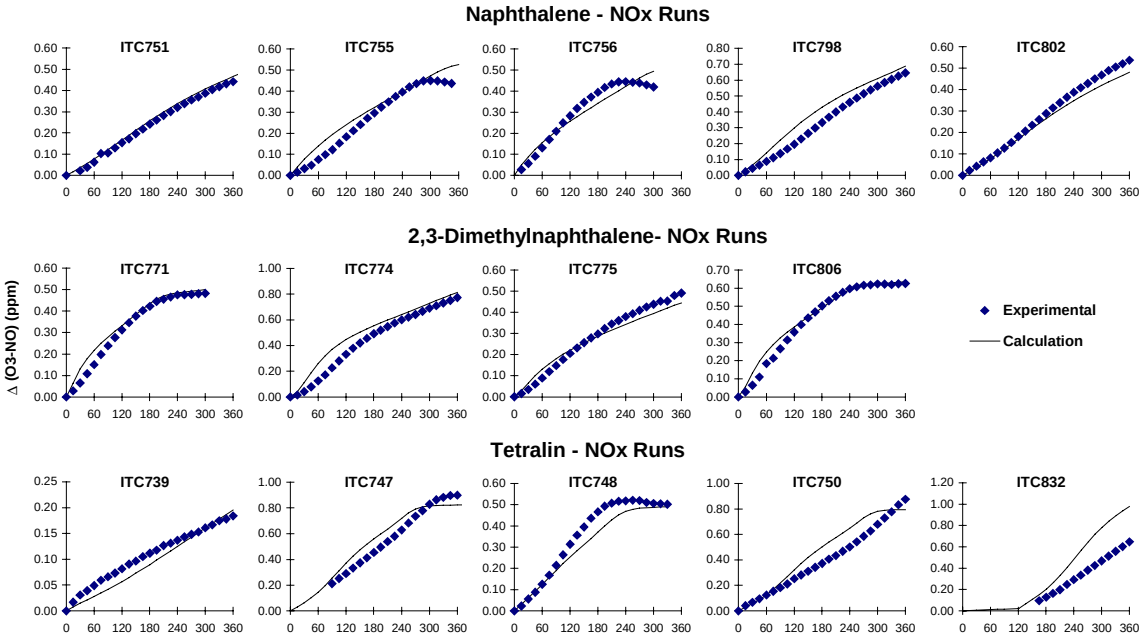

Figure B-82. Plots of experimental and calculated $\Delta([O_3]-[NO])$ data for the naphthalene - NO_x, 2,3-dimethylnaphthalene - NO_x and tetralin - NO_x experiments.

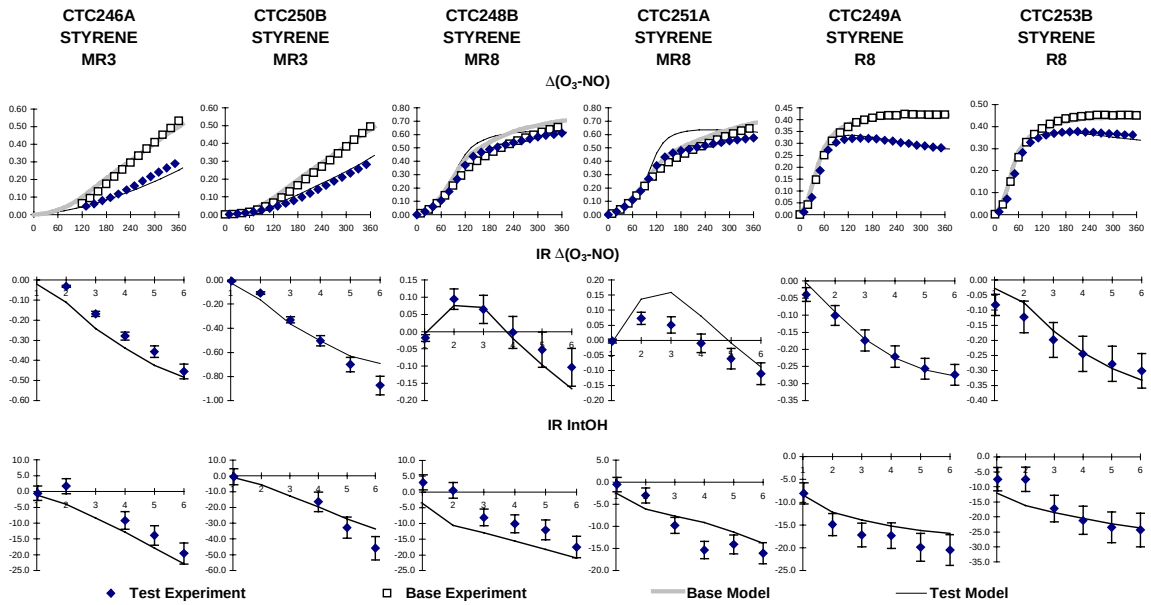

Figure B-83. Plots of experimental and calculated results of the incremental reactivity experiments with styrene.

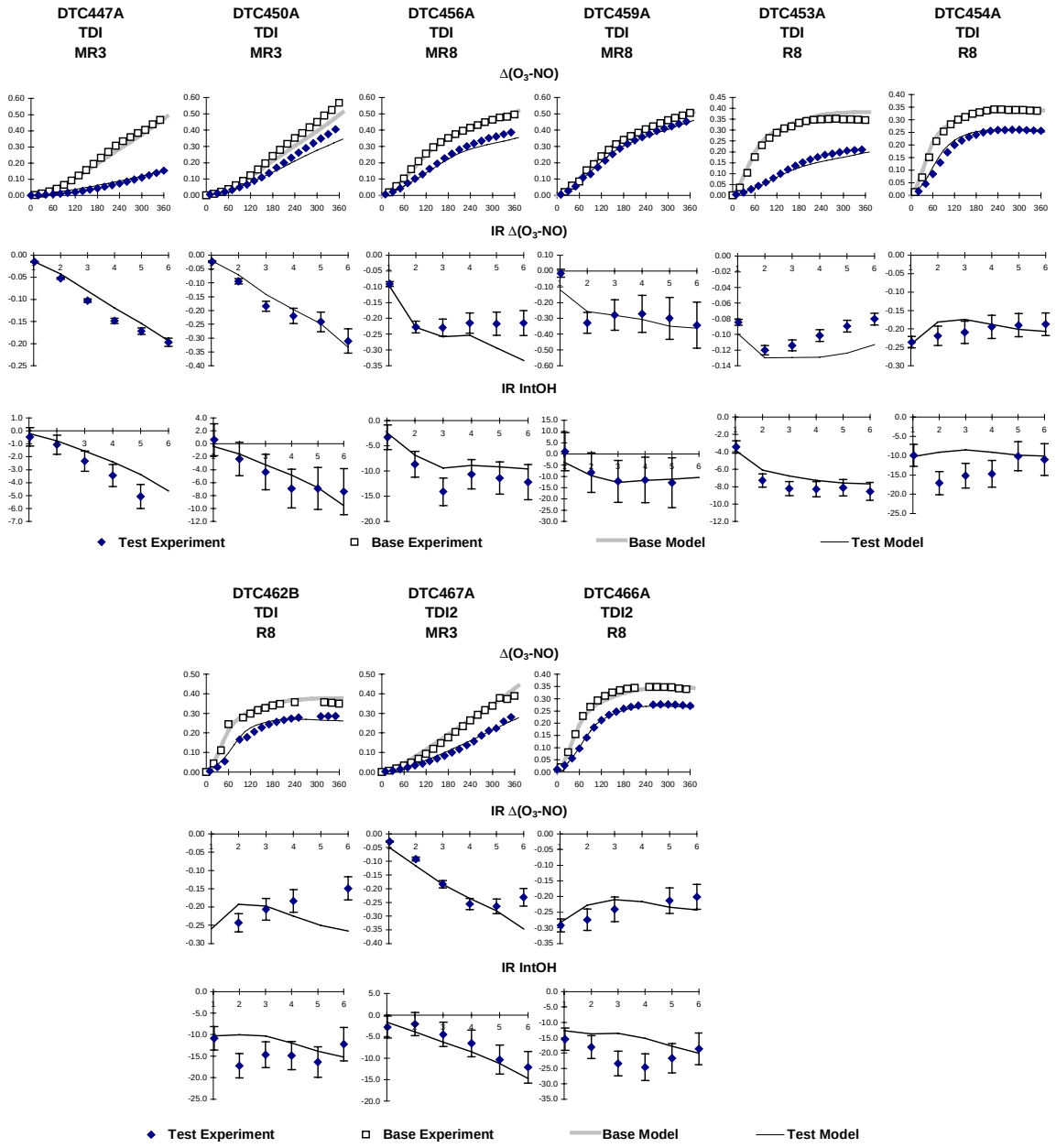

Figure B-84. Plots of experimental and calculated results of the incremental reactivity experiments with the toluene diisocyanate isomers (TDI and TDI2)

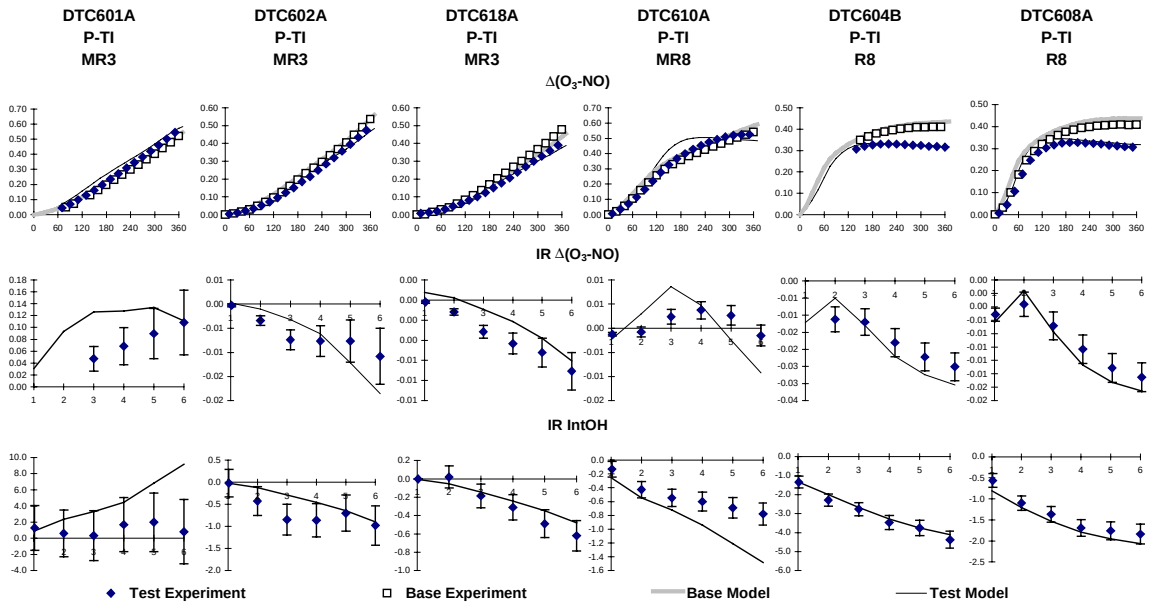

Figure B-85. Plots of experimental and calculated results of the incremental reactivity experiments with para toluene isocyanate.

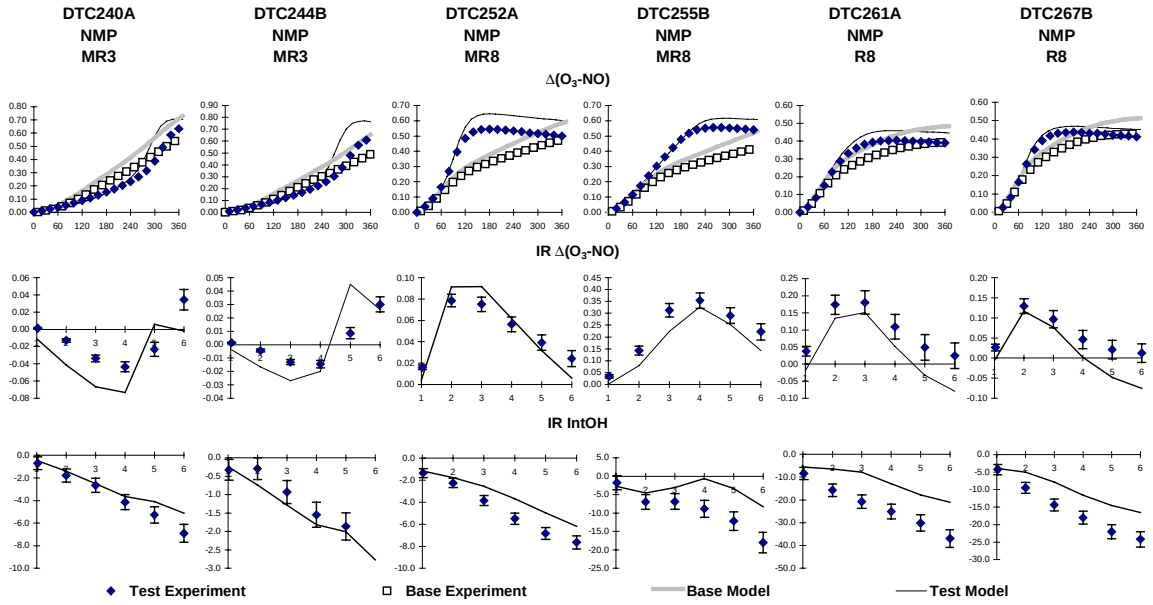

Figure B-86. Plots of experimental and calculated results of the incremental reactivity experiments with N-Methyl-2-Pyrrolidone.

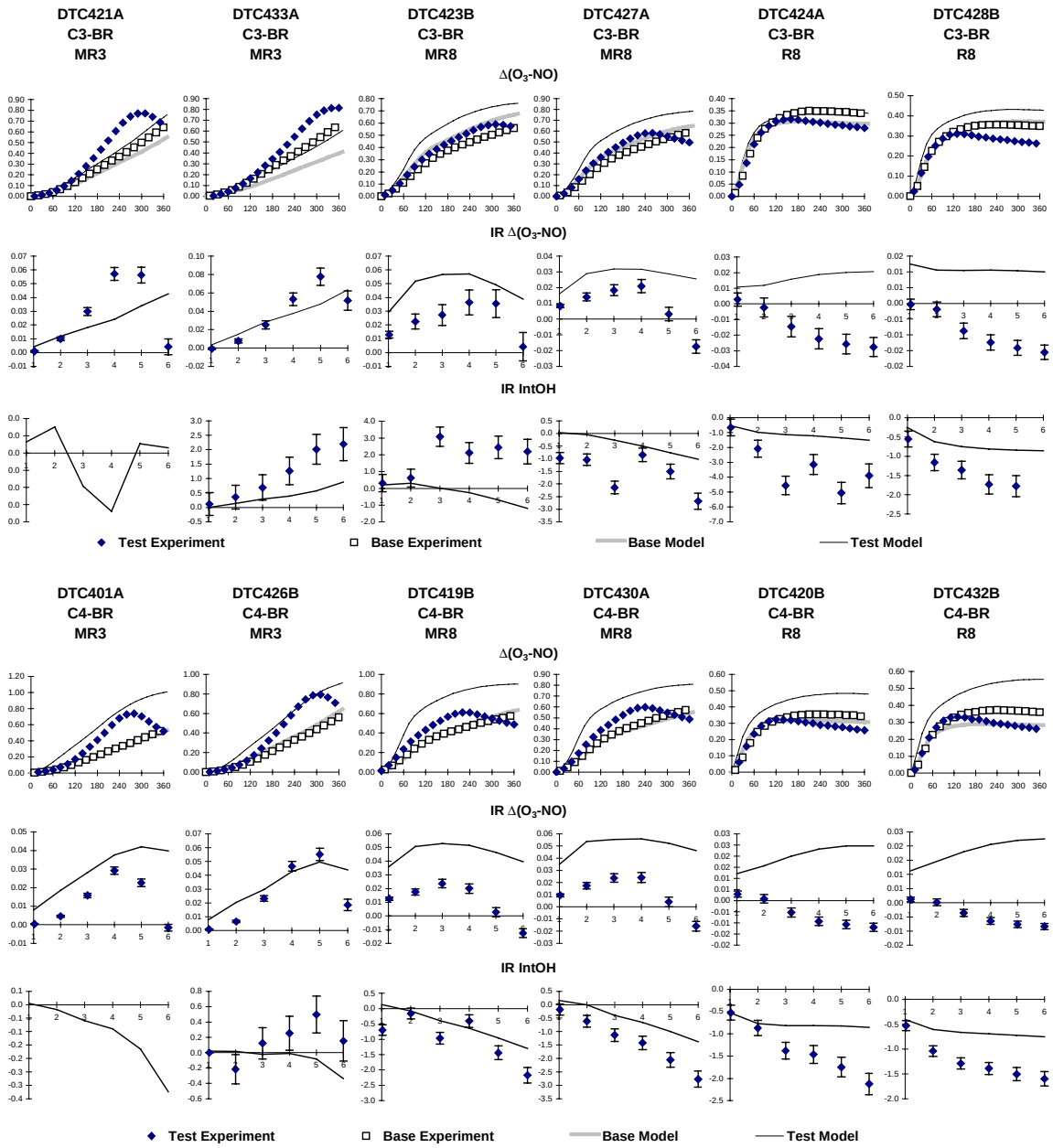

Figure B-87. Plots of experimental and calculated results of the incremental reactivity experiments with propyl and n-butyl bromides.

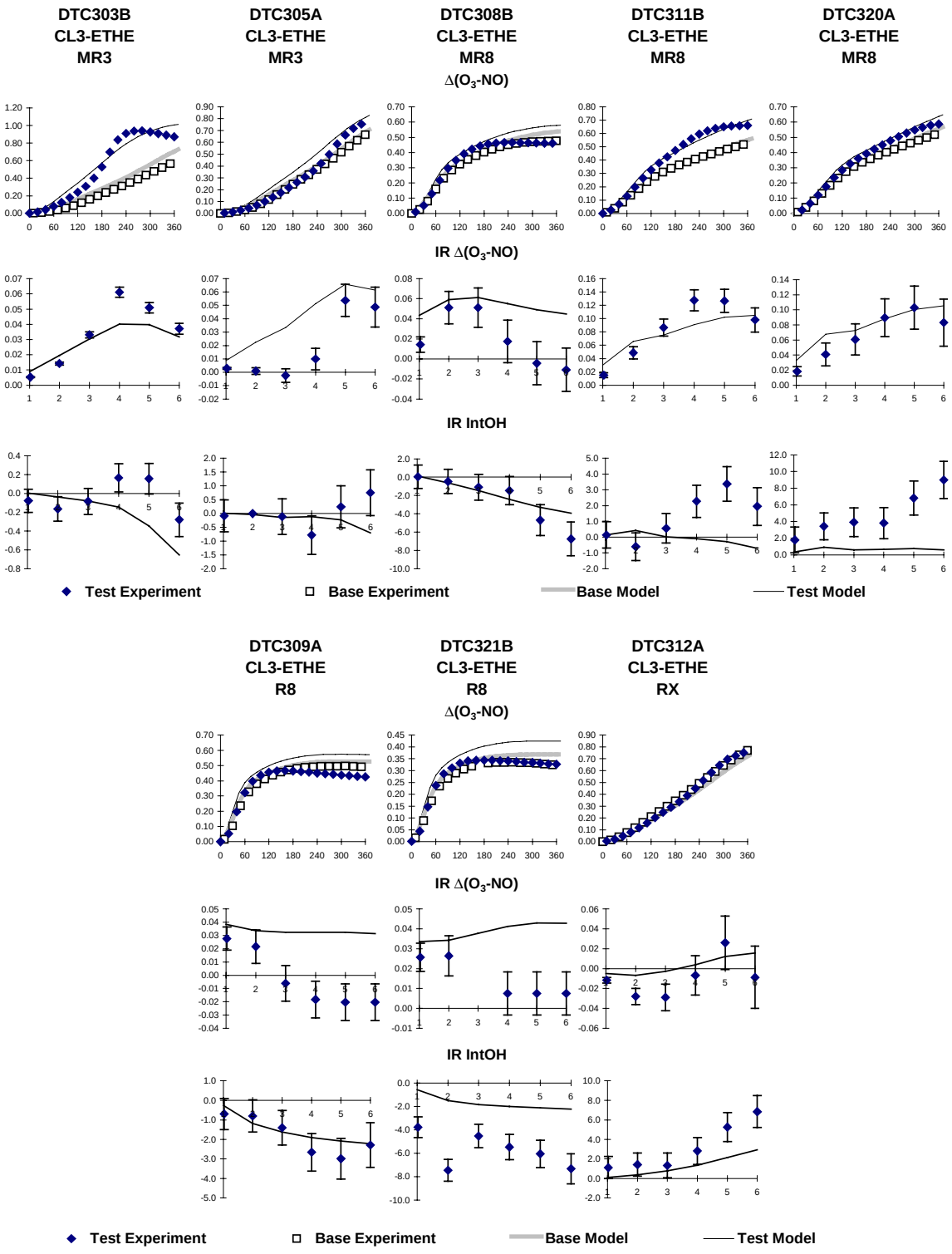

Figure B-88. Plots of experimental and calculated results of the incremental reactivity experiments with trichloroethylene.

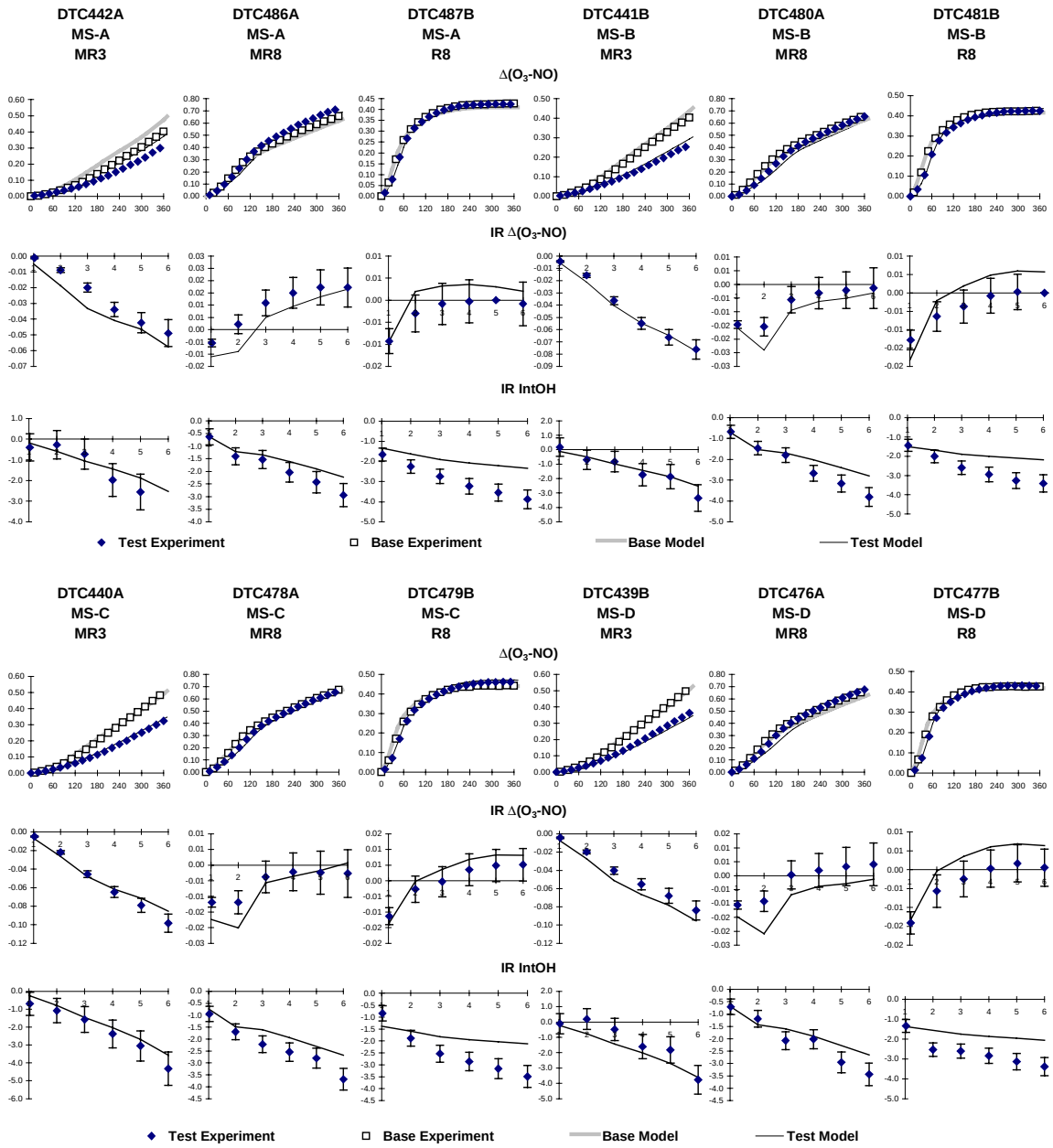

Figure B-89. Plots of experimental and calculated results of the incremental reactivity experiments with the mineral spirits samples used in the Safety-Kleen study (Carter et al, 1997f).

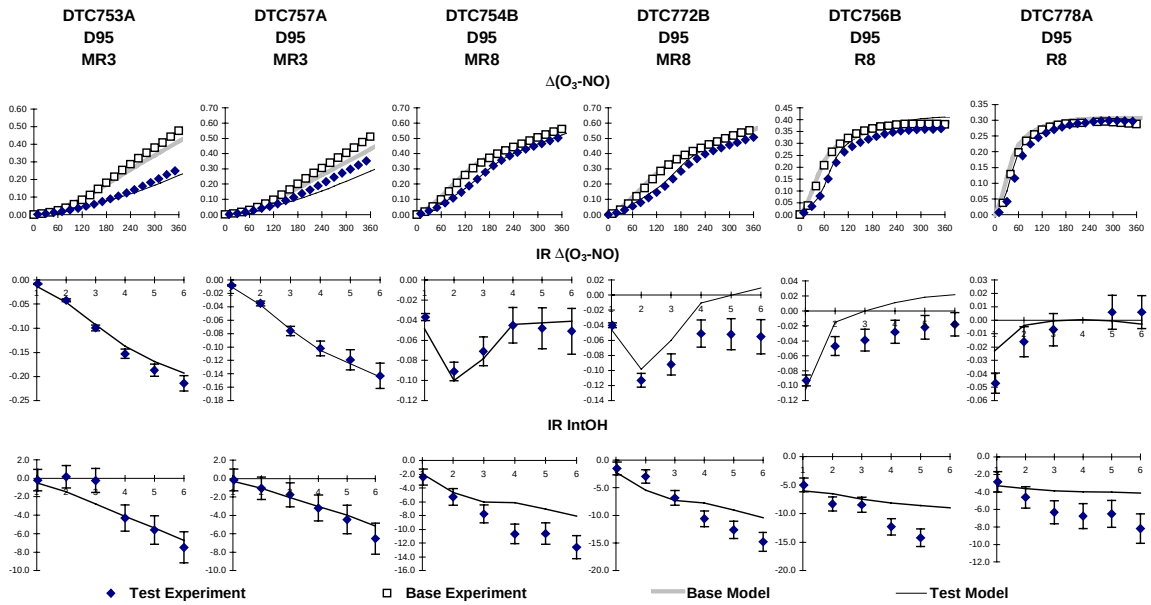

Figure B-90. Plots of experimental and calculated results of the incremental reactivity experiments with Exxon D95® fluid..

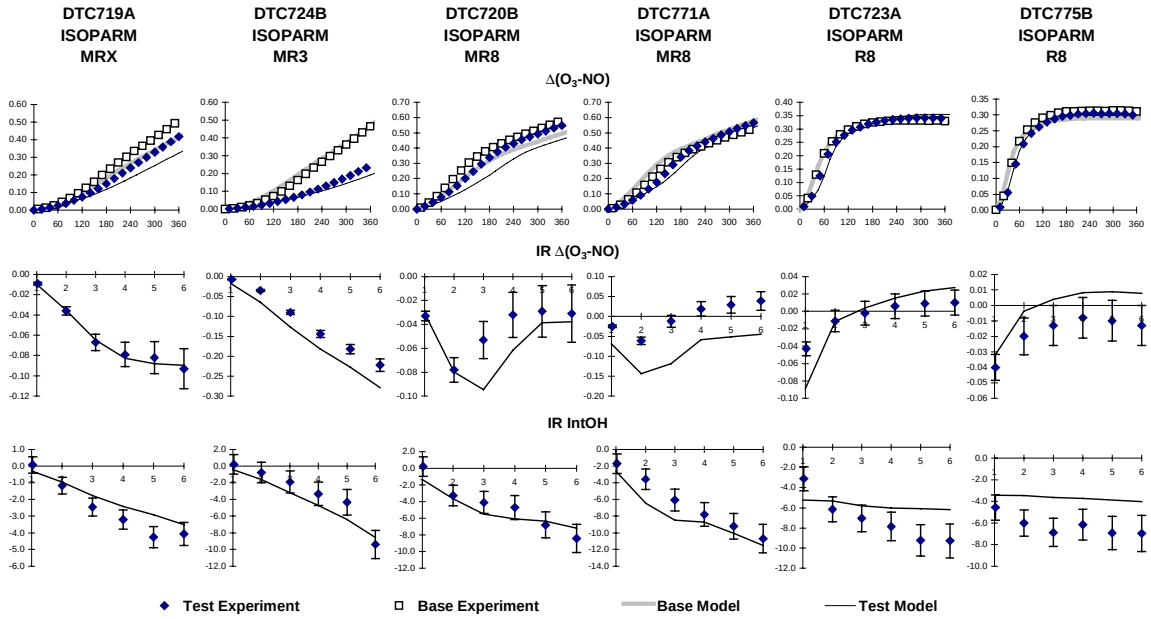

Figure B-91. Plots of experimental and calculated results of the incremental reactivity experiments with Exxon Isopar-M® Fluid.

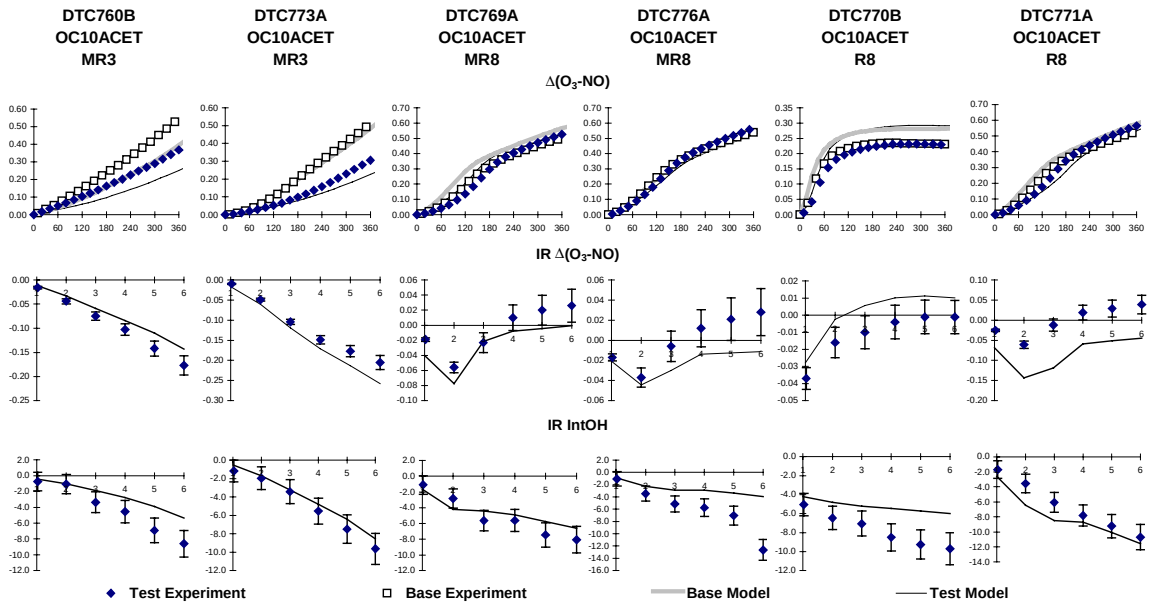

Figure B-92. Plots of experimental and calculated results of the incremental reactivity experiments with Exxon Exxate-1000 Fluid (used to derive the reactivities of "oxo-decyl acetate").

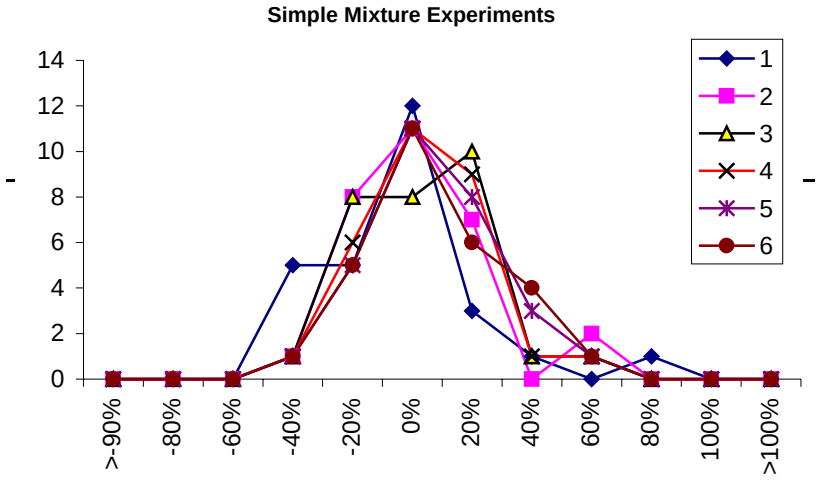

Figure B-93. Distribution plots of percentage errors of fits of calculated to experimental hourly $\Delta([O_3]-[NO])$ data for the simple mixture experiments (most carried out in the SAPRC EC).

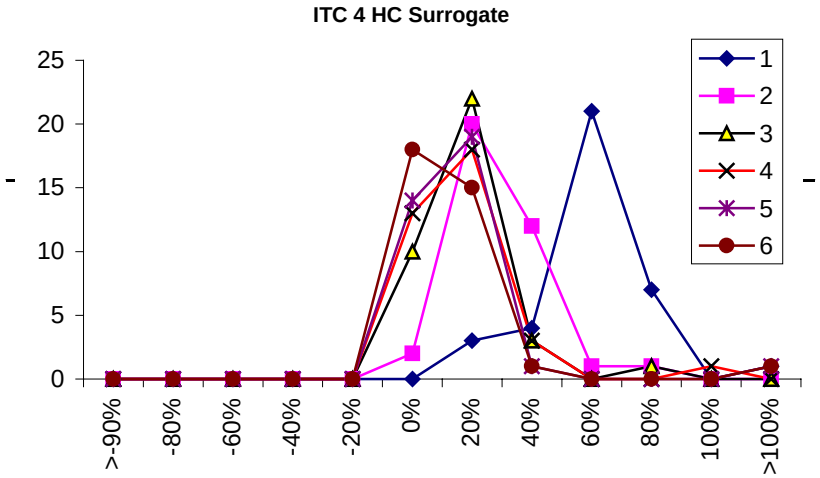

Figure B-94. Distribution plots of percentage errors of fits of calculated to experimental hourly $\Delta([O_3]-[NO])$ data for the four hydrocarbon surrogate experiments carried out in the ITC.

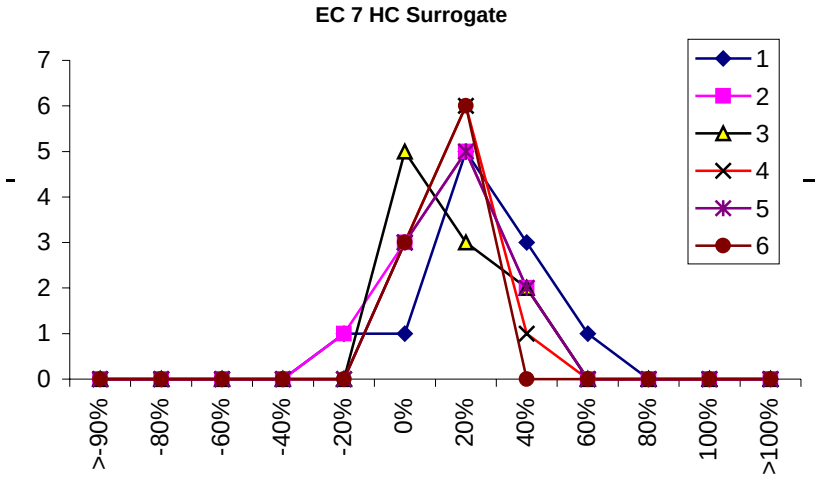

Figure B-95. Distribution plots of percentage errors of fits of calculated to experimental hourly $\Delta([O_3]-[NO])$ data for the seven hydrocarbon surrogate experiments carried out in the SAPRC EC.

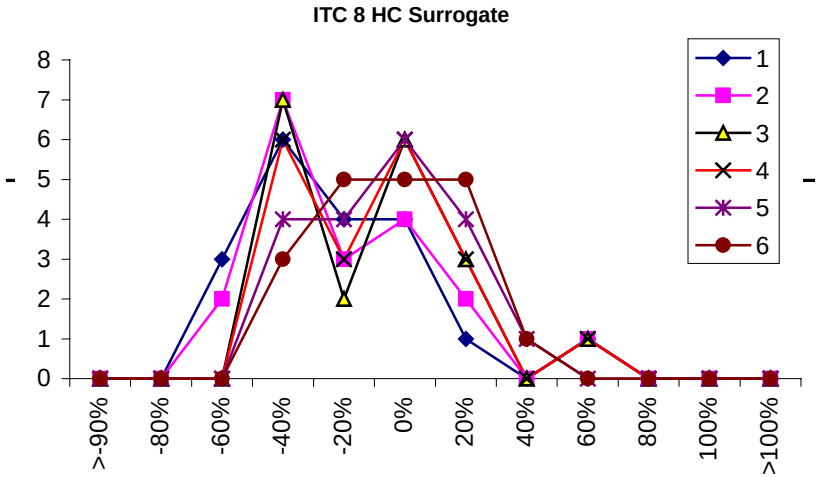

Figure B-96. Distribution plots of percentage errors of fits of calculated to experimental hourly $\Delta([O_3]-[NO])$ data for the eight hydrocarbon surrogate experiments carried out in the ITC.

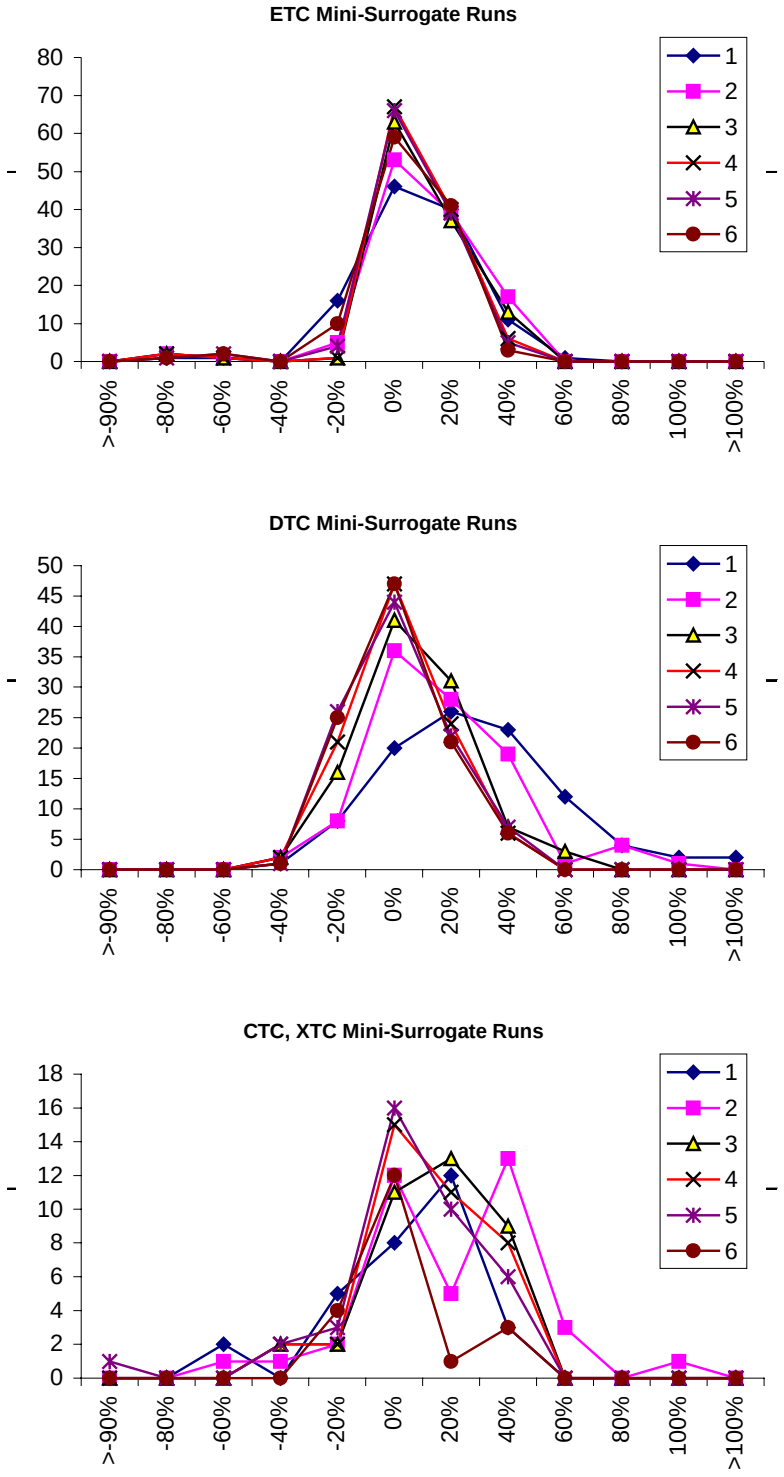

Figure B-97. Distribution plots of percentage errors of fits of calculated to experimental hourly $\Delta([O_3]-[NO])$ data for the base-case mini-surrogate experiments carried out in various chambers.

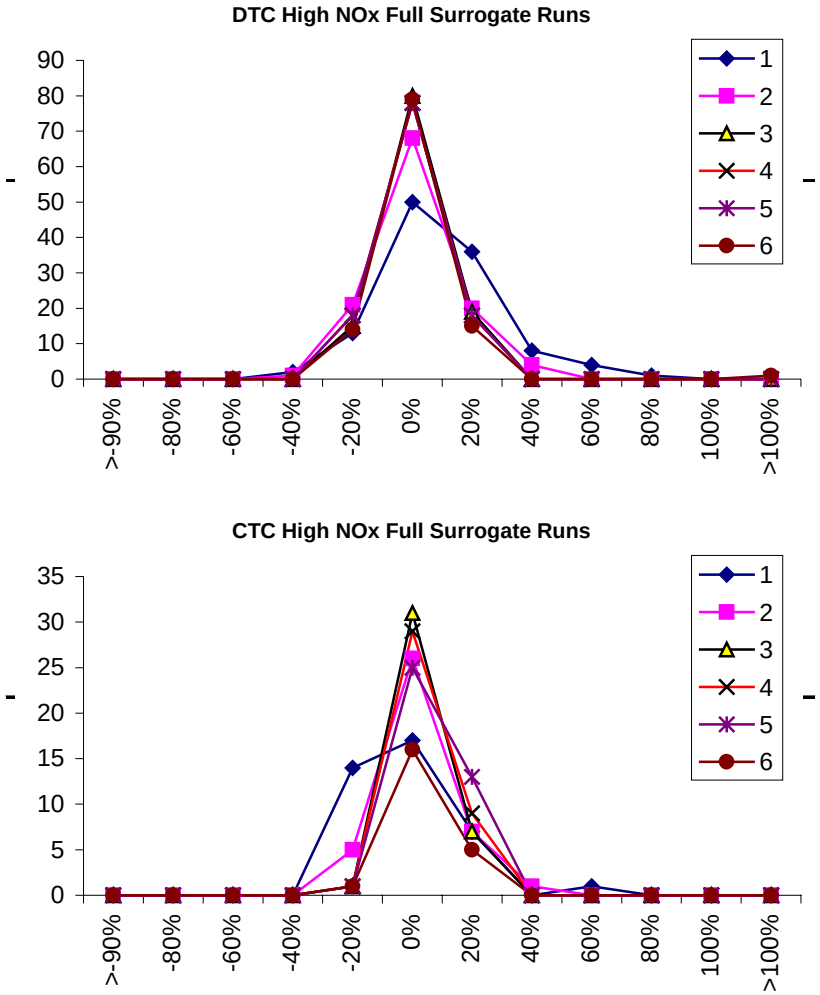

Figure B-98. Distribution plots of percentage errors of fits of calculated to experimental hourly $\Delta([O_3]-[NO])$ data for the base-case high NO_x full surrogate experiments carried out in various chambers.

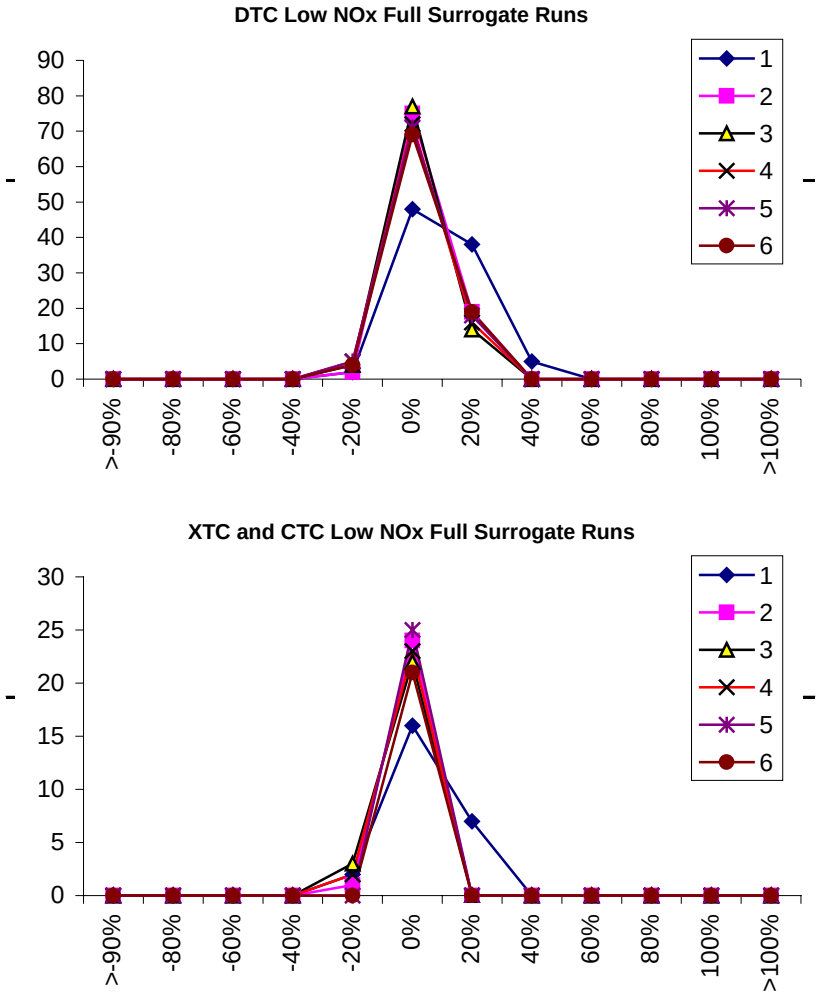

Figure B-99. Distribution plots of percentage errors of fits of calculated to experimental hourly $\Delta([O_3]-[NO])$ data for the base-case low NO_x full surrogate experiments.

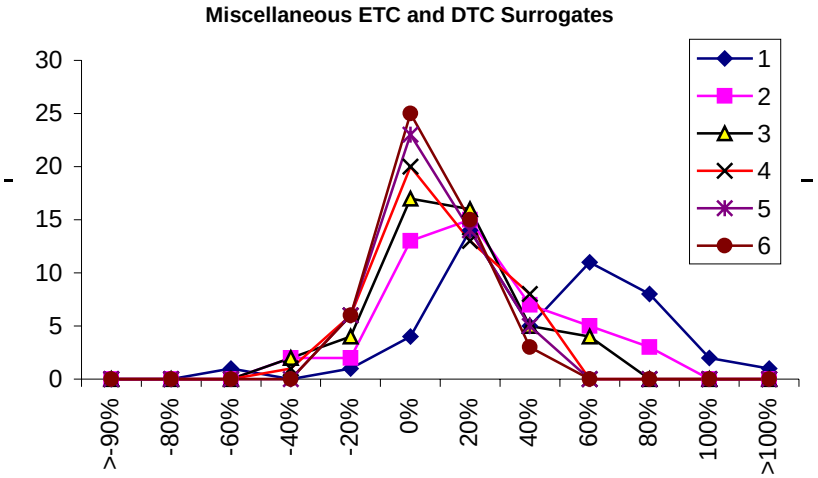

Figure B-100. Distribution plots of percentage errors of fits of calculated to experimental hourly $\Delta([O_3]-[NO])$ data for the miscellaneous non-standard surrogates used in various incremental reactivity experiments in the ETC and DTC.