

## Excited State Evolution towards Ligand Loss and Ligand Chelation at Group 6 Metal Carbonyl Centres

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### Supporting Information

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Analysis of excited states and orbital compositions

(eta-6-Benzophenone)Cr(CO)3

Molecule: C16H10CrO4  
 Details: #p b3lyp/Tzvp Geom=Check SCF=Tight Pop=Full IOp(3/33=1)  
 Source file: benzphenonePt0AOMix.log  
 Population analysis: MPA  
 473 orbitals( 473 canonical) 81 alpha + 81 beta electrons  
 Number of fragments: 3  
 Fragment 1 ( 24 atoms, 326 orbitals): Benzophenone  
 Fragment 2 ( 6 atoms, 114 orbitals): CO Ligands  
 Fragment 3 ( 1 atoms, 33 orbitals): Cr

COMPOSITIONS OF MOLECULAR ORBITALS (GROSS CONTRIBUTIONS, %)  
 AND OVERLAP POPULATIONS (OP) BETWEEN FRAGMENTS

Alpha MO:	71	72	73	74	75	76	77	78	79	80
Energy(eV):	HOMO-10	HOMO-9	HOMO-8	HOMO-7	HOMO-6	HOMO-5	HOMO-4	HOMO-3	HOMO-2	HOMO-1
Symmetry:	na	na	na	na	na	na	na	na	na	na
=====										
FRAG# 1:	97.87	99.07	99.62	85.21	86.90	99.46	99.92	99.67	3.84	15.14
FRAG# 2:	1.09	0.47	0.15	2.12	1.92	0.09	0.02	0.04	24.06	23.77
FRAG# 3:	1.04	0.46	0.23	12.68	11.18	0.46	0.07	0.28	72.10	61.10
OP( 1 & 2 )	-0.004	-0.001	0.000	-0.002	0.002	0.000	0.000	-0.001	0.006	0.014
OP( 1 & 3 )	0.004	0.002	0.001	0.094	0.079	0.001	-0.001	0.001	-0.075	0.030
OP( 2 & 3 )	0.002	0.000	0.000	-0.004	-0.004	0.000	0.000	0.000	0.085	0.081
=====										
Alpha MO:	81	82	83	84	85	86	87	88	89	90
Energy(eV):	HOMO	LUMO	LUMO+1	LUMO+2	LUMO+3	LUMO+4	LUMO+5	LUMO+6	LUMO+7	LUMO+8
Symmetry:	na	na	na	na	na	na	na	na	na	na
=====										
FRAG# 1:	20.44	84.40	83.68	89.48	96.48	17.22	14.54	14.76	50.85	6.78
FRAG# 2:	22.01	7.43	11.58	7.39	2.30	39.36	43.44	54.99	11.16	57.43
FRAG# 3:	57.55	8.17	4.74	3.13	1.22	43.42	42.01	30.25	37.99	35.79
OP( 1 & 2 )	0.013	-0.036	-0.113	-0.090	-0.008	-0.273	-0.262	-0.510	0.269	0.211
OP( 1 & 3 )	0.036	-0.106	-0.058	-0.045	-0.014	-0.494	-0.393	-0.722	-1.124	-0.499
OP( 2 & 3 )	0.075	0.039	-0.004	-0.022	-0.001	0.094	0.126	0.039	-1.572	-1.051

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.5207 eV 491.86 nm f=0.0007 <S\*\*2>=0.000  
 80 -> 82 0.68655  
 This state for optimization and/or second-order correction.  
 Total Energy, E(TD-HF/TD-KS) = -1961.39734728  
 Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 2.6906 eV 460.80 nm f=0.0001 <S\*\*2>=0.000  
 79 -> 82 0.68920

Excited State 3: Singlet-A 2.8326 eV 437.71 nm f=0.0666 <S\*\*2>=0.000  
 80 -> 83 0.21390  
 81 -> 82 0.65005

Excited State 4: Singlet-A 3.4022 eV 364.42 nm f=0.0002 <S\*\*2>=0.000  
 79 -> 84 -0.13267  
 79 -> 86 -0.29986  
 79 -> 87 0.11347  
 80 -> 86 -0.12229  
 81 -> 83 0.47595  
 81 -> 84 0.18815  
 81 -> 86 0.16583  
 81 -> 87 0.19062

Excited State 5: Singlet-A 3.4463 eV 359.76 nm f=0.0012 <S\*\*2>=0.000  
 79 -> 83 0.19387  
 79 -> 84 0.14587  
 79 -> 86 0.29752  
 79 -> 87 0.35630  
 79 -> 94 -0.15815  
 80 -> 83 0.12305  
 80 -> 86 0.11838  
 81 -> 83 0.28892  
 81 -> 86 -0.14947

Excited State	6:	Singlet-A	3.4533 eV	359.03 nm	f=0.0007	<S**2>=0.000
	79 ->	84	-0.14347			
	79 ->	86	-0.28850			
	79 ->	87	0.21465			
	80 ->	84	0.21471			
	80 ->	86	0.41098			
	80 ->	87	-0.16558			
	81 ->	87	-0.18188			
Excited State	7:	Singlet-A	3.5535 eV	348.91 nm	f=0.0011	<S**2>=0.000
	79 ->	83	0.12029			
	79 ->	87	0.30706			
	79 ->	94	-0.13376			
	80 ->	86	-0.14962			
	81 ->	83	-0.33790			
	81 ->	84	-0.11313			
	81 ->	87	0.37688			
	81 ->	94	-0.15733			
Excited State	8:	Singlet-A	3.5822 eV	346.11 nm	f=0.0005	<S**2>=0.000
	79 ->	83	0.14542			
	79 ->	88	0.15342			
	80 ->	83	-0.14051			
	80 ->	86	0.13203			
	80 ->	87	0.39481			
	80 ->	94	-0.13647			
	81 ->	83	-0.12785			
	81 ->	84	0.16663			
	81 ->	86	0.38172			
	81 ->	87	-0.10333			
Excited State	9:	Singlet-A	3.6388 eV	340.73 nm	f=0.0004	<S**2>=0.000
	79 ->	83	0.60751			
	79 ->	84	0.12473			
	79 ->	87	-0.12438			
	80 ->	87	-0.19170			
Excited State	10:	Singlet-A	3.6487 eV	339.80 nm	f=0.0039	<S**2>=0.000
	76 ->	82	-0.36329			
	78 ->	82	0.57793			

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(eta-6-AllylBenzene)Cr(CO)3

Molecule: C12H10CrO3  
 Details: #P b3lyp/Tzvp Pop=Full SCF=Tight IOp(3/33=1) Guess=Read Geom=Check  
 Source file: AllylB3LYPTzvpAOMix.log  
 Population analysis: MPA  
 378 orbitals( 378 canonical) 65 alpha + 65 beta electrons  
 Number of fragments: 3  
 Fragment 1 ( 1 atoms, 33 orbitals): Cr  
 Fragment 2 ( 6 atoms, 114 orbitals): (CO)3  
 Fragment 3 ( 19 atoms, 231 orbitals): Allylbenzene

Alpha MO:	61	62	63	64	65	66	67	68	69	70
	HOMO-4	HOMO-3	HOMO-2	HOMO-1	HOMO	LUMO	LUMO+1	LUMO+2	LUMO+3	LUMO+4
Energy (eV):	-8.68	-7.72	-5.98	-5.77	-5.76	-1.27	-1.20	-0.43	-0.38	-0.35
Symmetry:	na	na	na	na	na	na	na	na	na	na
=====										
FRAG# 1:	11.03	0.59	71.61	59.84	60.73	5.63	5.17	18.70	40.15	31.50
FRAG# 2:	1.94	0.08	25.16	24.48	24.87	11.63	11.26	13.51	44.38	38.76
FRAG# 3:	87.03	99.32	3.24	15.69	14.40	82.74	83.58	67.79	15.47	29.74
OP( 1 & 2 )	-0.005	-0.001	0.085	0.083	0.087	-0.005	0.000	0.006	0.144	0.121
OP( 1 & 3 )	0.080	0.004	-0.066	0.034	0.028	-0.072	-0.076	-0.273	-0.411	-0.282
OP( 2 & 3 )	0.005	-0.001	0.008	0.014	0.014	-0.141	-0.137	-0.131	-0.187	-0.171
=====										
Alpha MO:	71	72	73	74	75	76	77	78	79	80
	LUMO+5	LUMO+6	LUMO+7	LUMO+8	LUMO+9	LUMO+10	LUMO+11	LUMO+12	LUMO+13	LUMO+14
Energy (eV):	-0.08	0.46	0.53	0.56	0.64	0.94	0.97	1.23	1.53	1.61
Symmetry:	na	na	na	na	na	na	na	na	na	na
=====										
FRAG# 1:	33.22	89.99	26.77	35.73	1.02	21.90	26.61	6.94	6.88	11.01
FRAG# 2:	47.66	-0.84	65.84	57.65	83.75	58.40	61.95	8.27	7.13	8.91
FRAG# 3:	19.12	10.85	7.39	6.62	15.22	19.70	11.44	84.78	85.99	80.09
OP( 1 & 2 )	0.102	-5.735	-0.506	-1.188	-0.028	-0.251	-0.313	-0.187	-0.453	-2.493
OP( 1 & 3 )	-1.265	-2.917	-0.253	-0.562	-0.024	-0.123	-0.161	-0.075	-0.097	0.262
OP( 2 & 3 )	-0.584	1.057	0.130	0.236	0.075	0.048	0.019	-0.015	0.092	-0.588

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 3.2814 eV 377.84 nm f=0.0000 <S\*\*2>=0.000  
 64 -> 66 0.10435  
 64 -> 67 -0.27280  
 65 -> 66 0.57622  
 65 -> 68 -0.10468  
 65 -> 69 0.11827

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-KS) = -1733.62655260

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.3635 eV 368.61 nm f=0.0003 <S\*\*2>=0.000  
 63 -> 66 0.17334  
 63 -> 68 -0.20217  
 63 -> 70 0.28701  
 63 -> 77 0.12136  
 64 -> 66 -0.35026  
 65 -> 67 0.38605

Excited State 3: Singlet-A 3.3715 eV 367.75 nm f=0.0006 <S\*\*2>=0.000  
 63 -> 67 0.17145  
 63 -> 69 0.32008  
 63 -> 70 -0.11445  
 63 -> 76 0.10391  
 64 -> 67 0.45597  
 64 -> 69 0.15003  
 64 -> 70 -0.13439  
 65 -> 66 0.23906

Excited State	4:	Singlet-A	3.4710 eV	357.20 nm	f=0.0005	<S**2>=0.000
	63 ->	66	0.38937			
	63 ->	67	0.18898			
	63 ->	69	0.22602			
	64 ->	66	0.10703			
	64 ->	69	-0.16020			
	65 ->	66	-0.21116			
	65 ->	67	-0.15145			
	65 ->	68	-0.15558			
	65 ->	69	0.18973			
	65 ->	70	0.18783			
	65 ->	77	0.10633			
Excited State	5:	Singlet-A	3.4869 eV	355.58 nm	f=0.0008	<S**2>=0.000
	63 ->	66	0.36252			
	63 ->	67	-0.19823			
	63 ->	68	-0.10601			
	63 ->	70	0.14907			
	64 ->	66	0.26628			
	64 ->	70	-0.16696			
	65 ->	66	0.15221			
	65 ->	67	-0.19903			
	65 ->	68	0.13403			
	65 ->	69	-0.18769			
	65 ->	70	-0.16025			
	65 ->	77	-0.10221			
Excited State	6:	Singlet-A	3.5297 eV	351.26 nm	f=0.0006	<S**2>=0.000
	63 ->	67	-0.33550			
	64 ->	67	0.33636			
	64 ->	69	-0.32849			
	64 ->	76	-0.10621			
	65 ->	68	-0.15130			
	65 ->	70	0.22968			
Excited State	7:	Singlet-A	3.5393 eV	350.31 nm	f=0.0006	<S**2>=0.000
	63 ->	67	-0.15544			
	63 ->	71	-0.13035			
	64 ->	66	0.13049			
	64 ->	67	0.20857			
	64 ->	68	-0.20867			
	64 ->	69	0.18149			
	64 ->	70	0.26984			
	65 ->	69	0.38285			
	65 ->	70	-0.21478			
	65 ->	76	0.11837			
Excited State	8:	Singlet-A	3.6247 eV	342.05 nm	f=0.0021	<S**2>=0.000
	63 ->	66	0.40084			
	63 ->	68	0.17647			
	63 ->	69	-0.25412			
	63 ->	70	-0.21074			
	63 ->	77	-0.15001			
	64 ->	66	-0.16972			
	64 ->	68	-0.10205			
	64 ->	70	0.18993			
	64 ->	77	0.10362			
	65 ->	67	0.13734			
	65 ->	69	-0.13873			
Excited State	9:	Singlet-A	3.6868 eV	336.29 nm	f=0.0015	<S**2>=0.000
	63 ->	67	0.47167			
	63 ->	69	-0.22788			
	63 ->	70	0.18618			
	63 ->	76	-0.11463			
	64 ->	67	0.14142			
	64 ->	69	-0.23702			
	65 ->	68	0.12861			
	65 ->	70	-0.14148			
Excited State	10:	Singlet-A	3.9034 eV	317.63 nm	f=0.0001	<S**2>=0.000
	63 ->	68	0.12489			
	63 ->	69	-0.23918			
	63 ->	70	-0.14510			
	64 ->	68	0.23100			
	64 ->	70	-0.36353			
	65 ->	69	0.38874			

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(eta-6-Styrene)Cr(CO)3

Molecule: C11H8CrO3  
 Details: #P b3lyp/Tzvp SCF=Tight Pop=Full IOp(3/33=1) Guess=Read Geom=Check  
 Source file: StyreneB3LYPTzvpAOMix.log  
 Population analysis: MPA  
 347 orbitals( 347 canonical) 61 alpha + 61 beta electrons  
 Number of fragments: 3  
 Fragment 1 ( 16 atoms, 200 orbitals): Styrene  
 Fragment 2 ( 6 atoms, 114 orbitals): CO Ligands  
 Fragment 3 ( 1 atoms, 33 orbitals): Cr

Alpha MO:	51	52	53	54	55	56	57	58	59	60
	HOMO-10	HOMO-9	HOMO-8	HOMO-7	HOMO-6	HOMO-5	HOMO-4	HOMO-3	HOMO-2	HOMO-1
Energy(eV):	-10.96	-10.90	-10.87	-10.60	-10.31	-9.56	-9.00	-7.67	-6.03	-5.83
Symmetry:	na	na	na	na	na	na	na	na	na	na
=====										
FRAG# 1:	52.18	6.97	12.81	95.47	98.45	90.95	85.85	90.91	3.06	15.31
FRAG# 2:	38.51	73.20	69.14	3.77	0.96	2.21	2.22	1.47	24.76	24.29
FRAG# 3:	9.31	19.83	18.05	0.77	0.59	6.83	11.93	7.62	72.18	60.40
OP( 1 & 2 )	-0.048	0.006	0.005	0.000	0.000	-0.011	-0.001	-0.001	0.007	0.013
OP( 1 & 3 )	0.011	-0.001	-0.004	0.000	0.004	0.050	0.090	0.027	-0.067	0.036
OP( 2 & 3 )	0.061	0.149	0.139	0.005	0.000	-0.001	-0.005	0.000	0.086	0.084
=====										
Alpha MO:	61	62	63	64	65	66	67	68	69	70
	HOMO	LUMO	LUMO+1	LUMO+2	LUMO+3	LUMO+4	LUMO+5	LUMO+6	LUMO+7	LUMO+8
Energy(eV):	-5.76	-1.85	-1.27	-0.44	-0.40	-0.20	0.03	0.42	0.50	0.51
Symmetry:	na	na	na	na	na	na	na	na	na	na
=====										
FRAG# 1:	18.73	84.56	82.57	17.22	12.56	17.73	62.38	12.06	5.90	10.30
FRAG# 2:	23.37	8.17	11.88	39.58	46.36	49.67	24.92	2.47	67.33	62.66
FRAG# 3:	57.91	7.27	5.55	43.21	41.09	32.59	12.70	85.48	26.77	27.03
OP( 1 & 2 )	0.013	-0.076	-0.142	-0.277	-0.239	-0.551	-0.020	0.931	0.088	0.167
OP( 1 & 3 )	0.024	-0.085	-0.077	-0.421	-0.393	-1.056	-0.238	-2.471	-0.096	-0.340
OP( 2 & 3 )	0.082	0.026	0.001	0.108	0.157	0.087	-0.253	-5.174	-0.383	-0.759

Excitation energies and oscillator strengths:

Excited State 1: Singlet-A 2.9053 eV 426.75 nm f=0.0010 <S\*\*2>=0.000  
 60 -> 62 0.68708  
 This state for optimization and/or second-order correction.  
 Total Energy, E(TD-HF/TD-KS) = -1694.31620642  
 Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Singlet-A 3.0587 eV 405.35 nm f=0.0045 <S\*\*2>=0.000  
 59 -> 62 0.60470  
 59 -> 65 -0.14113  
 60 -> 63 0.13598  
 61 -> 62 0.25997

Excited State 3: Singlet-A 3.1145 eV 398.09 nm f=0.0296 <S\*\*2>=0.000  
 59 -> 62 -0.30536  
 60 -> 63 0.27159  
 61 -> 62 0.53484  
 61 -> 64 -0.11349

Excited State 4: Singlet-A 3.3052 eV 375.12 nm f=0.0001 <S\*\*2>=0.000  
 59 -> 64 -0.22044  
 60 -> 63 0.14604  
 60 -> 64 0.10627  
 61 -> 63 0.58314  
 61 -> 64 0.16741  
 61 -> 65 0.10826

Excited State 5: Singlet-A 3.4452 eV 359.87 nm f=0.0008 <S\*\*2>=0.000  
 59 -> 63 0.42045  
 59 -> 64 0.40944  
 59 -> 69 -0.10884  
 59 -> 73 0.10863  
 60 -> 64 0.11139  
 60 -> 65 -0.16243  
 61 -> 63 0.17437  
 61 -> 65 0.10736

Excited State	6:	Singlet-A	3.4625 eV	358.08 nm	f=0.0010	<S**2>=0.000
	59 -> 63	-0.11737				
	59 -> 65	-0.27126				
	60 -> 63	0.10561				
	60 -> 64	0.36947				
	60 -> 65	-0.23310				
	61 -> 63	-0.22081				
	61 -> 64	0.28834				
	61 -> 65	0.14274				
Excited State	7:	Singlet-A	3.5343 eV	350.80 nm	f=0.0006	<S**2>=0.000
	59 -> 65	0.17474				
	59 -> 66	0.13512				
	60 -> 64	0.25856				
	60 -> 65	0.23351				
	61 -> 64	-0.25968				
	61 -> 65	0.42173				
Excited State	8:	Singlet-A	3.5560 eV	348.67 nm	f=0.0032	<S**2>=0.000
	59 -> 63	0.16564				
	59 -> 64	-0.15708				
	59 -> 65	0.36654				
	59 -> 70	0.10249				
	59 -> 74	0.10652				
	60 -> 64	-0.14267				
	60 -> 65	-0.18440				
	61 -> 62	0.11514				
	61 -> 63	-0.20639				
	61 -> 64	0.30638				
	61 -> 65	0.13922				
	61 -> 72	-0.11738				
Excited State	9:	Singlet-A	3.6396 eV	340.65 nm	f=0.0014	<S**2>=0.000
	59 -> 63	0.49989				
	59 -> 64	-0.25657				
	59 -> 65	-0.17466				
	59 -> 72	0.10731				
	60 -> 65	0.25381				
	60 -> 72	-0.10337				
	61 -> 64	0.10447				
Excited State	10:	Singlet-A	3.8885 eV	318.85 nm	f=0.0029	<S**2>=0.000
	59 -> 64	0.28325				
	60 -> 63	0.12926				
	60 -> 64	-0.23060				
	60 -> 65	0.37417				
	61 -> 64	0.32438				
	61 -> 65	0.17671				

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Kinetic Analyses

Kinetic Analysis of (eta-6-benzophenone)Cr(CO)<sub>3</sub> Transient signals

470 nm excitation

1965 Band Single Exponential Curve Fitting

		Value	Standard Error
1965	y0	-4.19763E-4	4.81883E-5
1965	A1	-0.00206	5.47435E-5
1965	t1	-1.27178E-11	1.07136E-12

Number of Points 86  
Degrees of Freedom 83  
Reduced Chi-Sqr 2.18542E-8  
Residual Sum of Squares 1.8139E-6  
Adj. R-Square 0.94388  
Fit Status Succeeded(100)

2008 Band Single Exponential Curve Fitting

		Value	Standard Error
2008	y0	1.28339E-4	1.39461E-5
2008	A1	0.00132	3.60763E-5
2008	t1	6.77533E-12	3.51052E-13

Number of Points 86  
Degrees of Freedom 83  
Reduced Chi-Sqr 4.94448E-9  
Residual Sum of Squares 4.10392E-7  
Adj. R-Square 0.96038  
Fit Status Succeeded(100)

320 nm Excitation

1843 Single Exponential Curve Fitting

		Value	Standard Error
1843	y0	6.38375E-4	6.15733E-6
1843	A1	-3.37668E-4	7.32654E-6
1843	t1	-5.18538E-11	3.04456E-12

Number of Points 69  
Degrees of Freedom 66  
Reduced Chi-Sqr 2.774E-10  
Residual Sum of Squares 1.83084E-8  
Adj. R-Square 0.96918  
Fit Status Succeeded(100)

Kinetic Analysis of (eta-6-Styrene)Cr(CO)<sub>3</sub> Transient signals

400 nm Excitation

Grow-in of reactive excited state

1966 Single Exponential Curve Fitting

		Value	Standard Error
1966	y0	0.00171	1.00045E-4
1966	A1	-0.00182	1.14507E-4
1966	t1	-2.01035E-12	3.59568E-13

Number of Points 9  
Degrees of Freedom 6  
Reduced Chi-Sqr 6.06619E-9  
Residual Sum of Squares 3.63972E-8



Adj. R-Square 0.96969  
Fit Status Succeeded(100)

Recovery of Parent Absorbances

1983 Band			
		Value	Standard Error
1983	y0	-0.00297	4.27297E-5
1983	A1	-0.00495	1.13001E-4
1983	t1	-2.57462E-11	1.08249E-12

Number of Points 17  
Degrees of Freedom 14  
Reduced Chi-Sqr 6.03311E-9  
Residual Sum of Squares 8.44636E-8  
Adj. R-Square 0.99541  
Fit Status Succeeded(100)

Decay of Reactive Excited State

1966 Band			
		Value	Standard Error
1966	y0	-1.34211E-4	1.67078E-5
1966	A1	0.00209	1.96177E-5
1966	t1	4.98648E-11	1.2656E-12

Number of Points 17  
Degrees of Freedom 14  
Reduced Chi-Sqr 4.19734E-10  
Residual Sum of Squares 5.87627E-9  
Adj. R-Square 0.99861  
Fit Status Succeeded(100)

Kinetic Analysis of (eta-6-Allylbenzene)Cr(CO)3 Transient signals

400 nm Excitation

Grow-in of reactive excited state

1958 Band			
		Value	Standard Error
1958	y0	9.15279E-4	3.33429E-5
1958	A1	-0.00129	7.9541E-5
1958	t1	-1.30047E-12	1.61119E-13

1958  
Number of Points 9  
Degrees of Freedom 6  
Reduced Chi-Sqr 1.60132E-9  
Residual Sum of Squares 9.60791E-9  
Adj. R-Square 0.98122  
Fit Status Succeeded(100)

Decay of Reactive Excited State

1958 Band			
		Value	Standard Error
1958	y0	-1.91262E-5	7.83047E-6
1958	A1	0.00113	1.22143E-5
1958	t1	4.24781E-11	1.09932E-12

Number of Points 16  
Degrees of Freedom 13  
Reduced Chi-Sqr 1.10589E-10  
Residual Sum of Squares 1.43765E-9  
Adj. R-Square 0.99855  
Fit Status Succeeded(100)

Grow-in of CO-loss

1918 Band

		Value	Standard Error
1918	y0	0.00114	1.71716E-5
1918	A1	-0.00131	3.23346E-5
1918	t1	-3.70118E-11	1.97781E-12

Number of Points	16
Degrees of Freedom	13
Reduced Chi-Sqr	6.28767E-10
Residual Sum of Squares	8.17397E-9
Adj. R-Square	0.99359
Fit Status	Succeeded(100)

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( $\eta^6$ -Allylbenzene)Cr(CO)<sub>3</sub> Analytical Data <sup>13</sup>C nmr in C<sub>6</sub>D<sub>12</sub>





