†Electronic Supplementary Information (ESI) for: Dissociative electron attachment and electronic excitation in $Fe(CO)_5$

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Contents

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S1 Geometry of $Fe(CO)_5$

Cartesian coordinates of $Fe(CO)_5$, D_{3h} point group, optimized at BP86/QZ4P level of theory (see section Experimental Methods, Electronically excited states of Fe(CO)5, in the main text):

1.Fe	0.000000	0.000000	0.000000
2.C	0.903371	1.564685	0.000000
3.C	0.903371	-1.564685	0.000000
4.C	-1.806743	0.000000	0.000000
5.C	0.000000	0.000000	1.807515
6.C	0.000000	0.000000	-1.807515
7.O	1.479928	2.563310	0.000000
8.O	1.479928	-2.563310	0.000000
9.O	-2.959856	0.000000	0.000000
10.O	0.000000	0.000000	2.957760
11.O	0.000000	0.000000	-2.957760

S2 Excited states

Tables S1, S2, S3, S4 list the calculated excited states, their energies and oscillator strengths. The excitation energies were calculated at the BP86/QZ4P level of theory (see Figure 10 in the main text). Ground electronic state of $Fe(CO)_5$ is $^1A_1'$, with electronic configuration: ...$(1e'')^4(7e')^4(7a_2'')^2(8e')^4(13a_1')^2(1a_2')^2(2e'')^4$ $(9e')^4(8a_2'')^2(3e'')^4(10e')^4$ $(4e'')^0(14a_1')^0(11e')^0(9a_2'')^0(2a_2')^0(12e')^0$ $(5e'')^0$ $(15a_1')^0(10a_2'')^0(13e')^0(16a_1')^0(17a_1')^0(14e')^0$ $(6e'')^0(11a_2'')^0(18a_1')^0$... Description of electronic states by TD-DFT is given by linear combination of single excitations, as given in Tables S1, S2, S3, S4.

Dipole allowed transitions are to the excited $^1A_2''$ and $^1E'$ states, Tables S1 and S2, respectively. Spin allowed, dipole forbidden transitions are given in Table S3, while singlet-triplet transitions are collected in Table S4.

S2.1 Spin and dipole allowed transitions

Table S1 TDDFT (BP86/QZ4P) $^1A_2''$ transitions, the corresponding oscillator strenghts (f), and description of the dominant one-electron excitations (contributions greater than 10 %) of $Fe(CO)_5$

E (eV)	f	Assignment	%
4.1103	0.22461E-01	10e' → 4e"	95.68
5.3675	0.30392E-03	10e' → 5e"	83.39
		3e" → 11e'	16.54
6.0659	0.12560E-02	3e" → 12e'	98.75
6.5274	0.36667	3e" → 11e'	67.20
		10e' → 5e"	13.51
8.3599	0.30408E-02	3e" → 13e'	99.39
8.5621	0.10066	8a2" → 14a1'	61.93
		9e' → 4e"	27.83
8.9261	0.10169	9e' → 4e"	53.40
		2e" → 11e'	16.16
		8a2" → 14a1'	12.46
9.1243	0.11369E-01	10e' → 6e"	95.69
9.2266	0.75825E-05	8e' → 4e"	97.66
9.3553	0.68589E-01	2e" → 11e'	59.33
		7e' → 4e"	10.45
9.6609	0.25707E-03	13a1' → 9a2"	47.08
		7a2" → 14a1'	36.48
9.7603	0.54551E-03	2e" → 12e'	85.49

Table S1 TDDFT (BP86/QZ4P) $^1A_2''$ transitions of $Fe(CO)_5$

E (eV)	f	Assignment	%
9.7860	0.53044E-03	7e' → 4e"	60.14
		1e" → 11e'	14.01
		9e' → 5e"	12.60
10.076	0.74607E-03	3e" → 14e'	99.23

Table S2 TDDFT (BP86/QZ4P) $^1E'$ transitions, the corresponding oscillator strenghts (f), and description of the dominant one-electron excitations (contributions greater than 10 %) of $Fe(CO)_5$

E (eV)	f	Assignment	%
4.1410	0.14305E-04	10e' → 11e'	98.74
4.2445	0.18436E-03	10e' → 14a1'	93.38
4.5853	0.19820E-02	10e' → 2a2'	66.25
		10e' → 12e'	32.38
5.2567	0.55409E-01	10e' → 12e'	45.08
		3e" → 9a2"	32.44
		10e' → 2a2'	15.71
5.6504	0.12531E-02	3e" → 4e"	77.32
		3e" → 9a2"	18.67
6.0948	0.47277E-01	10e' → 15a1'	49.65
		3e" → 9a2"	21.23
6.2033	0.13858	10e' → 15a1'	49.33
		3e" → 9a2"	17.83
		3e" → 5e"	13.74
6.9906	0.16826	3e" → 5e"	67.03
		10e' → 13e'	10.77
7.0221	0.39796E-01	10e' → 13e'	89.03
7.6597	0.50695E-02	10e' → 16a1'	99.78
8.1833	0.14764E-02	3e" → 10a2"	98.55
8.2574	0.18657E-01	10e' → 17a1'	95.88
8.3509	0.42221E-01	8a2" → 4e"	85.97
8.7396	0.10690E-01	10e' → 14e'	94.74
8.8102	0.17301E-01	9e' → 14a1'	52.17
		9e' → 11e'	40.52
8.9812	0.30071E-01	2e" → 4e"	41.82
		9e' → 11e'	28.42
		9e' → 14a1'	15.95
9.0993	0.43509E-01	2e" → 4e"	46.98
		9e' → 11e'	20.70
9.1620	0.13355E-04	1a2' → 11e'	76.76
		9e' → 2a2'	21.62
9.2187	0.22392E-02	9e' → 2a2'	48.58
		8e' → 14a1'	20.81
		1a2' → 11e'	16.92
9.3043	0.95784E-03	8e' → 14a1'	63.26
		9e' → 2a2'	12.87
9.3959	0.16112E-03	8e' → 11e'	89.77
9.4282	0.12323E-02	2e" → 9a2"	59.52
		13a1' → 11e'	12.93
9.5047	0.33184E-02	9e' → 12e'	55.03

Table S2 TDDFT (BP86/QZ4P) $^1E'$ transitions of $Fe(CO)_5$; f should be multiplied by two due to the degeneracy

E (eV)	f	Assignment	%
		13a1' → 11e'	16.64
9.6211	0.60699E-05	7a2" → 4e"	51.49
		8a2" → 5e"	40.12
9.6866	0.48115E-01	7e' → 14a1'	55.91
9.7055	0.29019E-02	8e' → 2a2'	47.33
		1a2' → 12e'	27.55
		7e' → 14a1'	13.12
9.8111	0.26884E-01	1e" → 4e"	32.29
		7e' → 11e'	18.16
		7a2" → 4e"	10.40
9.8827	0.84912E-02	10e' → 18a1'	61.68
		8e' → 12e'	14.93
		1a2' → 12e'	11.13
9.9054	0.24826E-01	10e' → 18a1'	30.32
		13a1' → 12e'	13.97
		1a2' → 12e'	10.41
		1e" → 4e"	17.78
		8e' → 12e'	11.56
9.9526	0.40831E-01	8a2" → 5e"	27.72
		7e' → 14a1'	17.71
10.028	0.44501E-01	8e' → 12e'	24.66
		7e' → 2a2'	19.66
10.069	0.95595E-02	7e' → 11e'	54.13
		1e" → 4e"	30.68
10.123	0.35522E-01	7e' → 2a2'	51.08
		13a1' → 12e'	11.00
		1e" → 9a2"	10.62

S2.2 Spin allowed, dipole forbidden transitions

Table S3 TDDFT (BP86/QZ4P) spin allowed dipole forbidden, their symmetry label, the corresponding oscillator strenghts (f), and description of the dominant one-electron excitations (contributions greater than 10 %) of $Fe(CO)_5$

E (eV)	f	Symmetry	Assignment	%
3.97882	0.000	A1"	10e' → 4e"	99.86
4.09309	0.1546E-34	A2'	10e' → 11e'	99.79
4.13733	0.000	E"	10e' → 4e"	97.38
4.31740	0.000	E"	10e' → 9a2"	99.74
4.52799	0.9080E-34	A1'	10e' → 11e'	92.14
4.76975	0.2796E-32	A2'	10e' → 12e'	99.58
5.24317	0.7592E-33	A2'	3e" → 4e"	99.98
5.37378	0.000	A1"	10e' → 5e"	98.45
5.37440	0.000	E"	10e' → 5e"	89.68
5.42123	0.000	A1"	3e" → 11e'	98.47
5.42185	0.000	E"	3e" → 14a1'	77.67
			3e" → 11e'	14.17
5.43420	0.2321E-32	A1'	10e' → 12e'	66.27
			3e" → 4e"	30.04
5.52647	0.000	E"	3e" → 11e'	75.83

Table S3 TDDFT (BP86/QZ4P) spin allowed dipole forbidden transitions of $Fe(CO)_5$

E (eV)	f	Symmetry	Assignment	%
			3e" → 14a1'	15.87
5.69542	0.000	E"	3e" → 2a2'	99.71
6.08401	0.000	A1"	3e" → 12e'	99.70
6.36004	0.000	E"	3e" → 12e'	92.82
6.66475	0.9962E-33	A2'	3e" → 5e"	99.97
6.85310	0.000	E"	10e' → 10a2"	99.91
6.95526	0.1722E-34	A1'	10e' → 13e'	87.12
7.03373	0.1868E-34	A2'	10e' → 13e'	99.91
7.13085	0.2123E-33	A1'	3e" → 5e"	74.30
7.45306	0.000	E"	3e" → 15a1'	99.93
7.63541	0.7835E-33	A1'	13a1' → 14a1'	18.42
			3e" → 4e"	33.15
			10e' → 12e'	11.07
			3e" → 5e"	10.61
8.35928	0.000	A1"	3e" → 13e'	99.98
8.36098	0.000	E"	3e" → 13e'	99.47
8.56178	0.000	E"	8a2" → 11e'	94.24
8.62347	0.000	A1"	8a2" → 2a2'	92.79
8.65780	0.000	A1"	9e' → 4e"	93.25
8.70583	0.1571E-35	A1'	10e' → 14e'	85.98
8.74494	0.000	E"	9e' → 4e"	94.42
8.75117	0.7824E-34	A2'	10e' → 14e'	99.57
8.78016	0.1269E-35	A1'	8a2" → 9a2"	66.08
			10e' → 14e'	12.60
			2e" → 4e"	11.90
8.81353	0.3702E-33	A2'	9e' → 11e'	99.70
8.94885	0.000	E"	8a2" → 12e'	92.67
8.97453	0.1356E-32	A2'	2e" → 4e"	99.97
8.98506	0.000	E"	3e" → 16a1'	98.36
9.00755	0.000	E"	2e" → 14a1'	79.33
			9e' → 9a2"	15.14
9.01863	0.2102E-37	A1'	9e' → 11e'	51.41
			2e" → 4e"	39.06
9.02306	0.000	E"	1a2' → 4e"	88.22
9.03057	0.3692E-35	A2'	1a2' → 14a1'	98.46
9.10851	0.000	E"	9e' → 9a2"	36.43
			10e' → 6e"	48.01
9.14287	0.000	A1"	2e" → 11e'	99.64
9.14701	0.000	E"	9e' → 9a2"	27.76
			10e' → 6e"	50.64
9.15846	0.000	A1"	10e' → 6e"	99.26
9.19953	0.000	E"	2e" → 11e'	95.49
9.24456	0.000	A1"	8e' → 4e"	87.74
			1a2' → 9a2"	11.23
9.26854	0.000	E"	8e' → 4e"	65.07
			10e' → 11a2"	26.58
9.27450	0.000	E"	10e' → 11a2"	71.96
			8e' → 4e"	21.59
9.32098	0.000	E"	13a1' → 4e"	87.49

Table S3 TDDFT (BP86/QZ4P) spin allowed dipole forbidden transitions of $Fe(CO)_5$

E (eV)	f	Symmetry	Assignment	%
9.38548	0.3322E-37	A1'	8e' → 11e'	94.85
9.39458	0.1073E-33	A2'	8e' → 11e'	88.31
			9e' → 12e'	11.50
9.40585	0.000	A1"	1a2' → 9a2"	84.53
9.44782	0.000	E"	2e" → 2a2'	86.06
9.47821	0.1555E-34	A1'	9e' → 12e'	36.14
			2e" → 4e"	21.66
9.52448	0.1497E-33	A2'	13a1' → 2a2'	32.04
			9e' → 12e'	59.46
9.54249	0.9112E-37	A1'	1a2' → 2a2'	55.35
			9e' → 12e'	16.03
9.62617	0.000	E"	8e' → 9a2"	76.46
9.65950	0.000	A1"	7e' → 4e"	99.37
9.68546	0.000	E"	3e" → 17a1'	90.12
9.72193	0.4563E-36	A1'	13a1' → 14a1'	29.81
			1a2' → 2a2'	12.09
			1e" → 4e"	12.45
			7e' → 11e'	11.38
9.73461	0.000	E"	7e' → 4e"	78.66
9.80336	0.000	E"	2e" → 12e'	84.01
9.81139	0.000	A1"	2e" → 12e'	89.52
9.82638	0.1086E-33	A2'	7e' → 11e'	99.77
9.85113	0.2226E-34	A2'	1e" → 4e"	99.53
9.86674	0.000	E"	7a2" → 11e'	58.58
			1e" → 14a1'	39.63
9.87010	0.3470E-36	A1'	1e" → 4e"	48.23
			7a2" → 9a2"	13.33
			7e' → 11e'	10.56
9.91135	0.1455E-35	A2'	13a1' → 2a2'	62.14
			9e' → 12e'	23.67
9.97269	0.000	E"	1e" → 14a1'	39.42
			7e' → 9a2"	32.05
			7a2" → 11e'	21.62
10.10506	0.6112E-36	A1'	7a2" → 9a2"	65.89
			2e" → 5e"	12.94
			8e' → 12e'	10.93
10.27079	0.3501E-35	A1'	10e' → 15e'	42.12
			7e' → 12e'	12.83
10.35836	0.1181E-38	A1'	2e" → 5e"	39.45
			10e' → 15e'	25.76
			8e' → 12e'	14.38
10.39938	0.9964E-38	A1'	7e' → 12e'	72.64
			10e' → 15e'	16.74

S2.3 Singlet-triplet transitions

Table S4 TDDFT (BP86/QZ4P) singlet-triplet transitions, their symmetry label, the corresponding oscillator strenghts (f), and description of the dominant one-electron excitations (contributions greater than 10 %) of $Fe(CO)_5$

E (eV)	f	Symmetry	Assignment	%
3.67716	0.000	E'	10e' → 14a1'	99.65
3.72867	0.000	A1'	10e' → 11e'	55.00
			10e' → 12e'	30.92
			3e" → 4e"	13.35
3.74874	0.000	A2"	10e' → 4e"	99.26
3.76176	0.000	E"	10e' → 4e"	99.33
3.77672	0.000	A1"	10e' → 4e"	99.43
3.98357	0.000	E'	10e' → 11e'	93.87
4.07214	0.000	A2'	10e' → 11e'	99.79
4.13400	0.000	A1'	10e' → 12e'	50.13
			10e' → 11e'	43.33
4.16576	0.000	E'	10e' → 2a2'	85.08
			10e' → 12e'	10.56
4.17921	0.000	E"	10e' → 9a2"	99.74
4.43947	0.000	E'	10e' → 12e'	85.19
			10e' → 2a2'	12.72
4.60474	0.000	A2'	10e' → 12e'	99.68
4.69541	0.000	A1'	3e" → 4e"	79.85
			10e' → 12e'	18.42
4.92178	0.000	E'	3e" → 4e"	99.37
4.95119	0.000	E"	3e" → 14a1'	99.64
5.18203	0.000	A2"	3e" → 11e'	59.59
			10e' → 5e"	39.59
5.24168	0.000	A2'	3e" → 4e"	100.0
5.25542	0.000	E"	10e' → 5e"	68.40
			3e" → 11e'	31.09
5.29160	0.000	A1"	10e' → 5e"	99.58
5.33972	0.000	A2"	10e' → 5e"	60.28
			3e" → 11e'	39.53
5.34391	0.000	E"	3e" → 11e'	68.10
			10e' → 5e"	31.18
5.38661	0.000	A1"	3e" → 11e'	98.79
5.51096	0.000	E'	3e" → 9a2"	99.42
5.65626	0.000	E"	3e" → 2a2'	99.35
5.87695	0.000	A1"	3e" → 12e'	98.52
5.88006	0.000	E"	3e" → 12e'	98.80
5.88854	0.000	A2"	3e" → 12e'	99.41
6.10064	0.000	E'	10e' → 15a1'	99.96
6.53885	0.000	A1'	3e" → 5e"	99.47
6.60214	0.000	E'	3e" → 5e"	99.73
6.65961	0.000	A2'	3e" → 5e"	99.99
6.85316	0.000	E"	10e' → 10a2"	99.98
7.01127	0.000	A1'	10e' → 13e'	99.88
7.01616	0.000	E'	10e' → 13e'	99.93
7.02197	0.000	A2'	10e' → 13e'	99.99
7.43546	0.000	E"	3e" → 15a1'	99.94

Table S4 TDDFT (BP86/QZ4P) singlet-triplet transitions of $Fe(CO)_5$

E (eV)	f	Symmetry	Assignment	%
7.65156	0.000	E'	10e' → 16a1'	99.88
7.93391	0.000	E'	8a2" → 4e"	83.29
7.97096	0.000	A2"	8a2" → 14a1'	82.14
8.01477	0.000	A1'	8a2" → 9a2"	52.31
8.07725	0.000	E"	8a2" → 11e'	97.05
8.17355	0.000	E'	3e" → 10a2"	99.18
8.19416	0.000	A1'	9e' → 11e'	38.28
			2e" → 4e"	28.81
			7e' → 11e'	16.58
8.26261	0.000	A2"	9e' → 4e"	51.93
			8a2" → 14a1'	14.82
			2e" → 11e'	14.58
8.34414	0.000	A2"	3e" → 13e'	98.13
8.34827	0.000	E'	10e' → 17a1'	85.85
8.35030	0.000	E"	3e" → 13e'	99.64
8.35684	0.000	A1"	3e" → 13e'	99.90
8.35809	0.000	E'	9e' → 14a1'	17.41
			10e' → 17a1'	13.57
			2e" → 9a2"	11.51
			8a2" → 4e"	10.82
			2e" → 4e"	10.18
8.48589	0.000	E"	9e' → 4e"	88.06
8.50451	0.000	A1"	8a2" → 2a2'	86.97
8.56342	0.000	E'	9e' → 14a1'	62.35
			2e" → 4e"	11.56
			9e' → 11e'	11.48
8.56649	0.000	A1'	8a2" → 9a2"	37.83
			1a2' → 2a2'	15.99
			2e" → 4e"	14.29
8.62190	0.000	A1"	9e' → 4e"	94.42
8.63726	0.000	E'	9e' → 11e'	71.40
			9e' → 14a1'	14.31
8.65179	0.000	A2"	9e' → 4e"	37.81
			2e" → 11e'	32.26
			7e' → 4e"	10.50
8.69675	0.000	A1'	10e' → 14e'	89.50
8.71535	0.000	E'	10e' → 14e'	96.12
8.74389	0.000	A2'	10e' → 14e'	98.06
8.74711	0.000	E"	9e' → 9a2"	41.07
			8a2" → 12e'	18.55
			1a2' → 4e"	15.84
8.78994	0.000	A1'	13a1' → 14a1'	85.35
8.80157	0.000	A2'	9e' → 11e'	98.58
8.81108	0.000	E"	9e' → 9a2"	28.87
			8a2" → 12e'	25.88
			1a2' → 4e"	12.38
8.83194	0.000	E'	9e' → 2a2'	72.12
8.89685	0.000	A1'	1a2' → 2a2'	36.38
			2e" → 4e"	28.29

Table S4 TDDFT (BP86/QZ4P) singlet-triplet transitions of $Fe(CO)_5$

E (eV)	f	Symmetry	Assignment	%
			9e' → 11e'	17.08
			8e' → 12e'	10.20
8.94145	0.000	E'	2e" → 4e"	46.39
			8e' → 2a2'	17.90
8.94911	0.000	E"	8a2" → 12e'	40.51
			1a2' → 4e"	30.06
			2e" → 11e'	16.01
8.94950	0.000	E"	2e" → 14a1'	86.10
8.95070	0.000	A2'	1a2' → 14a1'	87.55
8.97401	0.000	E"	2e" → 11e'	53.71
			1a2' → 4e"	19.67
8.97425	0.000	A2'	2e" → 4e"	99.86
8.97772	0.000	E"	3e" → 16a1'	94.04
8.99430	0.000	A1"	8e' → 4e"	50.09
			1a2' → 9a2"	28.10
9.08442	0.000	E'	2e" → 9a2"	35.05
			8e' → 2a2'	11.01
9.11158	0.000	E"	13a1' → 4e"	87.50
9.11553	0.000	A2"	10e' → 6e"	99.54
9.13439	0.000	E"	10e' → 6e"	88.26
9.13489	0.000	A1'	7e' → 11e'	35.70
			1e" → 4e"	19.95
			9e' → 11e'	18.41
9.13818	0.000	E"	8e' → 4e"	56.66
			1a2' → 4e"	14.60
9.14258	0.000	E'	1a2' → 11e'	64.48
			8e' → 14a1'	26.75
9.14279	0.000	A1"	2e" → 11e'	96.13
9.14668	0.000	A2'	9e' → 12e'	65.78
			13a1' → 2a2'	12.38
			1a2' → 14a1'	11.57
9.15778	0.000	A1"	10e' → 6e"	94.61
9.18554	0.000	E'	8e' → 14a1'	64.38
			1a2' → 11e'	28.61
9.19469	0.000	A2"	8e' → 4e"	94.12
9.24596	0.000	E'	13a1' → 11e'	68.58
			8a2" → 5e"	10.18
9.26948	0.000	A1"	1a2' → 9a2"	58.78
			8e' → 4e"	39.10
9.27251	0.000	E"	10e' → 11a2"	95.78
9.30057	0.000	E"	2e" → 2a2'	47.48
			8e' → 9a2"	14.00
			8e' → 4e"	25.71
9.31790	0.000	A1'	9e' → 12e'	76.99
9.33294	0.000	A2"	13a1' → 9a2"	19.17
			2e" → 11e'	36.79
			7e' → 4e"	26.53
9.33312	0.000	E'	9e' → 12e'	62.77
9.37018	0.000	A2'	8e' → 11e'	89.33

Table S4 TDDFT (BP86/QZ4P) singlet-triplet transitions of $Fe(CO)_5$

E (eV)	f	Symmetry	Assignment	%
			9e' → 12e'	10.14
9.37154	0.000	E'	8e' → 11e'	87.12
9.38292	0.000	A1'	8e' → 11e'	89.32
			9e' → 12e'	10.35
9.42491	0.000	A2"	13a1' → 9a2"	64.78
9.43319	0.000	E'	8a2" → 5e"	25.95
			2e" → 9a2"	17.40
			13a1' → 11e'	15.79
			7a2" → 4e"	12.22
9.46698	0.000	E"	8e' → 9a2"	31.63
			2e" → 2a2'	22.62
			7e' → 4e"	29.91
9.47270	0.000	E'	7e' → 11e'	44.12
			8a2" → 5e"	19.00
			1e" → 4e"	16.88
9.49702	0.000	E"	8e' → 9a2"	33.86
			7e' → 4e"	39.32
9.54262	0.000	A2"	7a2" → 14a1'	85.75
9.56330	0.000	E'	7a2" → 4e"	51.46
			7e' → 14a1'	32.48
9.57784	0.000	A2'	13a1' → 2a2'	83.85
			9e' → 12e'	14.88
9.59796	0.000	A1'	7a2" → 9a2"	38.04
			1a2' → 2a2'	13.03
			7e' → 11e'	17.74
9.60363	0.000	E'	7e' → 14a1'	56.39
			8a2" → 5e"	22.93
			7a2" → 4e"	19.28
9.63833	0.000	A1"	2e" → 12e'	51.57
			7e' → 4e"	36.35
9.65075	0.000	E"	7a2" → 11e'	71.84
			1e" → 14a1'	10.91
9.66293	0.000	A1"	7e' → 4e"	63.35
			2e" → 12e'	32.59
9.69348	0.000	E"	3e" → 17a1'	99.54
9.70348	0.000	E"	2e" → 12e'	79.78
			7a2" → 11e'	12.26
9.70843	0.000	E'	1a2' → 12e'	56.72
			8e' → 2a2'	39.12
9.72155	0.000	A2"	2e" → 12e'	92.34
9.76476	0.000	A1'	8e' → 12e'	67.52
			1a2' → 2a2'	18.07
9.78156	0.000	E"	1e" → 14a1'	81.93
			7a2" → 11e'	11.66
9.80169	0.000	E'	1e" → 4e"	56.65
			7e' → 11e'	24.94
9.82366	0.000	A2'	7e' → 11e'	99.83
9.84326	0.000	E'	13a1' → 12e'	46.08
			8e' → 12e'	26.35

Table S4 TDDFT (BP86/QZ4P) singlet-triplet transitions of $Fe(CO)_5$

E (eV)	f	Symmetry	Assignment	%
9.84939	0.000	A1'	7a2" $\rightarrow$ 9a2"	31.21
			1e" $\rightarrow$ 4e"	50.21
			7e' $\rightarrow$ 11e'	16.88
9.85111	0.000	A2'	1e" $\rightarrow$ 4e"	100.0
9.88891	0.000	E'	10e' $\rightarrow$ 18a1'	95.89