Supporting Information

Ground and excited states of the $[Fe(H_2O)_6]^{2+}$ and $[Fe(H_2O)_6]^{3+}$ clusters: Insight into the electronic structure of the $[Fe(H_2O)_6]^{2+}$ – $[Fe(H_2O)_6]^{3+}$ complex

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Table S1. SS-MCSCF and MR-PT2 absolute energies (a.u.) for the selected electronic states of $Fe^{2+}(H_2O)_6$ and $Fe^{3+}(H_2O)_6$ clusters listed in Table 2 of the manuscript.

State	SS-MCSCF	MR-PT2 [a]	MR-PT2 [b]
		$[Fe(H_2O)_6]^{2+}$	
^5T_g	-1718.496614	-1720.264382	-1720.269969
^5E_g	-1718.479681	-1720.233696	-1720.239887
$^3B_{3g}$	-1718.415558	-1720.185548	
^1A_g	-1718.399287	-1720.173256	
^7A_g	-1718.309056	-1720.074916	
	-1718.305390	-1720.053292	
^5A_g	-1718.288374	n/a [c]	
		$[Fe(H_2O)_6]^{3+}$	
^6A_g	-1717.937523	-1719.662969	-1719.668084
$^4B_{1g}$	-1717.815381	-1719.566828	
$^2B_{2g}$	-1717.781709	-1719.546553	
^6A_u	-1717.708841	-1719.502504	
$1\ ^4A_u$	-1717.706875	n/a [c]	
^2A_u	-1717.619828	-1719.424375	
$2\ ^4A_u$	-1717.618156	n/a [c]	
$^8B_{2g}$	-1717.532120	n/a [c]	

[a] MR-PT2//SS-MCSCF.

[b] MR-PT2//MR-PT2.

[c] No convergence was achieved probably due to the existing nearly degenerate electronic states (intruder states).

Table S2. Potential energy curves for various electronic states of the $[Fe(H_2O)_6]^{2+}$ cluster. Energies are reported in kcal/mol and *R*(Fe-O) distances in Å.

***R*(Fe-O)**	**1** ^5A_g	**2** ^5A_g	**3** ^5A_g	**4** ^5A_g	**5** ^5A_g	**6** ^5A_g	**7** ^5A_g
10.00	33.2	59.5	82.3	82.3	101.7	101.7	101.7
9.00	34.4	60.6	78.4	78.4	102.9	102.9	102.9
8.00	35.5	61.7	72.9	72.9	104.0	104.0	104.0
7.00	36.3	62.5	64.8	64.8	104.8	104.8	104.9
6.00	36.1	52.0	52.0	62.3	104.6	104.6	104.7
5.00	29.8	29.9	33.4	59.6	101.8	102.0	102.0
4.50	12.3	12.4	30.2	56.4	98.6	98.8	98.9
4.00	-12.8	-12.6	25.1	51.3	93.5	93.8	93.9
3.70	-33.2	-33.0	21.0	47.1	89.3	89.7	89.9
3.35	-64.3	-64.0	15.6	41.7	83.7	84.2	84.7
3.00	-105.0	-104.6	11.7	37.0	79.2	79.8	81.0
2.80	-134.4	-133.8	12.3	35.9	62.3	79.1	79.9
2.70	-149.0	-148.4	14.1	35.3	55.4	80.0	80.9
2.60	-163.8	-163.3	17.2	33.9	51.8	81.7	82.9
2.50	-178.7	-178.2	21.5	30.9	50.8	84.4	85.6
2.40	-191.6	-191.2	25.3	26.1	50.5	86.3	87.8
2.30	-198.6	-198.6	16.1	26.7	47.1	84.9	86.7
2.20	-200.7	-200.5	-25.5	30.0	45.3	64.4	64.4
2.10	-186.5	-186.2	-52.1	29.5	40.7	40.9	55.5
2.00	-153.0	-152.2	-65.7	23.8	27.9	28.0	48.3
1.90	-96.0	-94.8	-46.9	42.7	45.8	46.0	66.9
1.80	0.0	1.2	10.9	98.4	101.1	101.6	122.3
1.70	125.9	156.6	159.1	211.3	213.7	214.5	234.5
1.60	330.0	407.3	408.8	411.1	413.2	414.2	432.8
1.50	657.9	733.0	734.9	736.0	753.5	755.0	792.2
1.35	1910.6	1914.7	2179.1	2264.9	2270.4	2273.5	2274.8
1.20	3223.9	3244.6	3264.1	3268.0	3293.9	3296.2	3309.3
1.00	7955.6	7979.6	8012.4	8077.2	8080.0	8109.6	8110.2

R(Fe-O)	$1\,^5B_{3u}$	$2\,^5B_{3u}$	$3\,^5B_{3u}$	$4\,^5B_{3u}$	$5\,^5B_{3u}$	$6\,^5B_{3u}$
10.00	33.2	33.2	59.4	59.5	101.7	101.7
9.00	34.4	34.4	60.6	60.7	102.9	102.9
8.00	35.5	35.6	61.7	61.8	104.0	104.0
7.00	36.3	36.4	62.5	62.7	104.8	104.9
6.00	36.0	36.3	62.2	62.5	104.6	104.7
5.00	33.3	33.7	59.5	60.0	101.9	102.0
4.50	30.1	30.7	56.3	57.0	98.8	98.9
4.00	25.0	25.9	51.3	52.3	93.8	94.0
3.70	21.0	22.1	47.3	48.5	89.7	90.0
3.35	15.9	17.5	42.3	43.9	84.5	84.8
3.00	12.8	15.1	39.1	41.2	81.0	81.3
2.80	14.6	17.7	40.4	42.8	82.3	82.7
2.70	17.5	20.9	42.3	44.8	84.5	84.8
2.60	22.1	26.0	45.0	47.7	88.1	88.3
2.50	28.4	33.0	47.5	50.8	93.0	93.1
2.40	35.2	40.7	47.6	52.0	97.7	97.9
2.30	40.3	46.6	46.9	52.4	100.1	100.9
2.20	51.4	56.0	59.1	63.1	109.3	111.3
2.10	70.5	74.1	79.7	82.9	124.6	128.0
2.00	107.6	110.7	117.5	120.8	154.3	159.4
1.90	164.1	167.3	174.9	178.8	200.1	206.5
1.80	259.1	262.5	270.8	275.6	279.8	287.2
1.70	414.3	414.9	418.8	422.4	427.3	433.4
1.60	635.2	643.5	657.6	664.3	671.2	678.0
1.50	987.1	1006.3	1012.1	1042.5	1045.1	1050.4
1.35	2370.6	2415.1	2426.5	2429.9	2448.4	2452.5
1.20	3370.3	3387.2	3432.9	3460.1	3482.9	3513.8
1.00	8013.1	8019.6	8059.1	8065.0	8078.9	8105.5

R(Fe-O)	$1\,^5B_{2u}$	$2\,^5B_{2u}$	$3\,^5B_{2u}$	$4\,^5B_{2u}$	$5\,^5B_{2u}$
10.00	33.2	59.5	101.7	101.7	101.7
9.00	34.4	60.7	102.9	102.9	102.9
8.00	35.6	61.8	104.0	104.0	104.0
7.00	36.4	62.7	104.8	104.8	104.9
6.00	36.3	62.5	104.6	104.7	104.7
5.00	33.7	60.0	101.9	102.0	102.1
4.50	30.6	56.9	98.8	98.9	98.9
4.00	25.7	52.0	93.7	93.8	93.9
3.70	21.8	48.1	89.7	89.8	89.9
3.35	16.7	43.0	84.2	84.4	84.6
3.00	13.3	39.1	79.6	80.2	81.0
2.80	14.6	39.2	79.4	80.6	82.1
2.70	16.7	40.2	80.0	82.0	83.8
2.60	20.4	41.7	81.4	84.6	86.8
2.50	25.5	42.9	84.1	88.1	90.7
2.40	30.7	41.7	87.1	91.0	94.1
2.30	33.0	38.7	86.8	90.8	95.0
2.20	41.1	45.1	91.9	96.3	102.6
2.10	55.3	58.6	101.6	106.4	115.9
2.00	84.4	87.7	123.5	129.1	144.3
1.90	130.5	134.5	159.2	165.5	189.2
1.80	211.1	216.2	225.4	232.1	268.0
1.70	341.4	347.3	348.3	354.1	401.8
1.60	536.8	543.6	570.6	580.1	620.8
1.50	871.5	880.9	910.4	940.3	950.9
1.35	2219.8	2252.8	2430.4	2489.5	2662.4
1.20	3155.7	3176.8	3227.1	3300.3	3307.6
1.00	7720.3	7746.0	7786.2	7935.0	7939.3

R(Fe-O)	$1\,^5B_{1g}$	$2\,^5B_{1g}$	$3\,^5B_{1g}$	$4\,^5B_{1g}$	$5\,^5B_{1g}$	$6\,^5B_{1g}$
10.00	33.2	59.5	82.3	101.7	101.7	101.7
9.00	34.4	60.6	78.4	102.9	102.9	102.9
8.00	35.5	61.7	72.9	104.0	104.0	104.0
7.00	36.3	62.5	64.8	104.8	104.8	104.9
6.00	36.1	52.0	62.3	104.6	104.6	104.7
5.00	29.8	33.4	59.6	101.8	102.0	102.0
4.50	12.3	30.2	56.4	98.6	98.8	98.9
4.00	-12.8	25.1	51.3	93.5	93.8	93.9
3.70	-33.3	21.0	47.2	89.3	89.7	89.9
3.35	-64.8	15.6	41.8	83.7	84.2	84.7
3.00	-106.4	11.8	37.4	79.2	79.9	81.0
2.80	-137.1	12.5	37.3	79.0	80.2	82.1
2.70	-152.7	14.4	38.1	79.8	81.3	83.8
2.60	-169.0	17.6	39.4	81.3	83.4	86.5
2.50	-185.7	22.0	40.4	83.2	86.4	90.4
2.40	-201.3	26.0	38.9	83.9	89.2	93.9
2.30	-212.1	27.1	35.7	80.3	88.5	94.9
2.20	-218.4	30.8	41.6	56.5	66.9	86.4
2.10	-210.2	27.1	31.0	46.3	54.2	66.2
2.00	-185.2	8.2	20.1	38.9	58.3	80.6
1.90	-139.2	16.5	32.7	55.0	81.9	109.4
1.80	-58.0	58.4	77.3	108.5	142.0	175.1
1.70	79.0	151.7	171.9	219.8	257.1	304.4
1.60	303.4	323.8	343.6	418.6	456.8	529.3
1.50	605.5	625.4	685.6	742.4	779.0	889.1
1.35	2072.2	2121.3	2140.4	2285.0	2287.2	2312.0
1.20	3040.1	3050.2	3095.5	3244.1	3249.1	3302.9
1.00	7834.3	7856.3	7889.4	7941.3	7968.4	7976.7

R(Fe-O)	$1\,^5B_{1u}$	$2\,^5B_{1u}$	$3\,^5B_{1u}$	$4\,^5B_{1u}$	$5\,^5B_{1u}$
10.00	33.2	59.5	101.7	101.7	101.7
9.00	34.4	60.6	102.9	102.9	102.9
8.00	35.5	61.7	104.0	104.0	104.0
7.00	36.3	62.5	104.8	104.8	104.9
6.00	36.1	62.3	104.6	104.6	104.7
5.00	33.4	59.6	101.8	102.0	102.1
4.50	30.2	56.4	98.7	98.9	98.9
4.00	25.1	51.3	93.5	93.8	93.9
3.70	21.0	47.2	89.4	89.7	89.9
3.35	15.7	41.8	83.8	84.3	84.8
3.00	11.9	37.4	79.3	80.0	81.2
2.80	12.7	37.2	79.3	80.3	82.3
2.70	14.7	37.9	80.3	81.6	84.0
2.60	18.1	39.2	82.2	84.0	86.9
2.50	22.8	40.1	84.9	87.5	90.8
2.40	27.3	38.4	86.9	90.8	94.5
2.30	28.9	35.0	85.5	91.5	95.6
2.20	36.2	40.7	89.6	98.6	103.4
2.10	50.5	54.1	98.0	110.9	117.7
2.00	79.3	82.5	119.0	136.1	146.5
1.90	125.1	128.4	154.0	175.2	191.7
1.80	205.7	209.2	219.1	244.5	271.2
1.70	333.9	342.1	346.1	362.9	405.8
1.60	527.7	559.9	566.0	571.2	626.8
1.50	860.7	893.6	927.5	937.9	946.5
1.35	2236.5	2250.6	2425.3	2491.8	2646.9
1.20	3139.8	3157.0	3206.3	3320.3	3332.4
1.00	7708.7	7726.3	7759.0	7868.7	7890.2

R(Fe-O)	$1\ ^5B_{2g}$	$2\ ^5B_{2g}$	$3\ ^5B_{2g}$	$4\ ^5B_{2g}$	$5\ ^5B_{2g}$	$6\ ^5B_{2g}$	$7\ ^5B_{2g}$
10.00	33.2	33.2	59.4	59.5	82.3	101.7	101.7
9.00	34.4	34.4	60.6	60.7	78.4	102.9	102.9
8.00	35.5	35.6	61.7	61.8	72.9	104.0	104.0
7.00	36.3	36.4	62.5	62.7	64.8	104.8	104.8
6.00	36.0	36.3	51.9	62.2	62.5	104.6	104.7
5.00	29.8	33.3	33.7	59.5	60.0	101.9	102.0
4.50	12.2	30.1	30.7	56.3	57.0	98.8	98.9
4.00	-12.9	25.0	25.9	51.3	52.2	93.7	93.9
3.70	-33.5	20.9	22.1	47.3	48.5	89.7	89.9
3.35	-65.0	15.8	17.4	42.3	43.8	84.4	84.7
3.00	-106.7	12.5	14.9	39.0	41.1	80.9	81.2
2.80	-137.4	14.2	17.3	40.3	42.7	82.2	82.5
2.70	-153.0	16.8	20.3	42.2	44.8	84.2	84.5
2.60	-169.3	21.1	25.1	45.0	47.7	87.4	88.1
2.50	-186.1	27.0	31.6	47.6	50.9	91.3	93.0
2.40	-201.7	33.1	38.7	47.8	52.3	94.7	97.8
2.30	-212.4	37.2	43.7	47.2	52.8	94.4	100.7
2.20	-219.0	43.3	50.8	56.6	63.5	65.3	69.0
2.10	-210.2	31.1	38.2	50.9	58.8	73.4	74.8
2.00	-184.8	11.0	23.6	45.5	52.8	86.1	89.7
1.90	-138.6	19.4	36.9	60.6	79.5	110.4	116.7
1.80	-56.8	61.5	83.0	113.5	143.0	171.1	185.0
1.70	80.8	155.0	179.1	224.6	260.6	296.8	315.1
1.60	306.1	326.6	352.4	423.3	461.2	520.3	539.6
1.50	606.8	632.0	692.1	745.2	782.5	883.3	902.4
1.35	2081.8	2122.2	2128.1	2285.4	2337.3	2393.7	2450.7
1.20	3040.6	3049.8	3096.0	3329.2	3352.7	3455.8	3463.5
1.00	7832.9	7845.9	7883.1	7891.5	8069.5	8148.2	8176.3

R(Fe-O)	$1\ ^5B_{3g}$	$2\ ^5B_{3g}$	$3\ ^5B_{3g}$	$4\ ^5B_{3g}$	$5\ ^5B_{3g}$	$6\ ^5B_{3g}$
10.00	33.2	59.5	82.3	101.7	101.7	101.7
9.00	34.4	60.7	78.4	102.9	102.9	102.9
8.00	35.6	61.8	72.9	104.0	104.0	104.0
7.00	36.4	62.7	64.8	104.8	104.8	104.9
6.00	36.3	51.9	62.5	104.6	104.7	104.7
5.00	29.8	33.7	59.9	101.9	102.0	102.0
4.50	12.2	30.6	56.9	98.8	98.9	98.9
4.00	-12.9	25.7	52.0	93.7	93.8	93.9
3.70	-33.5	21.7	48.1	89.6	89.7	89.8
3.35	-64.9	16.6	43.0	84.1	84.3	84.6
3.00	-106.7	13.1	39.0	79.4	80.0	80.9
2.80	-137.4	14.2	39.2	79.0	80.4	81.9
2.70	-153.0	16.2	40.1	79.4	81.7	83.7
2.60	-169.2	19.5	41.7	80.4	83.9	86.6
2.50	-186.0	24.2	43.0	82.4	87.0	90.5
2.40	-201.6	28.7	41.9	84.2	89.0	93.8
2.30	-212.3	30.2	39.0	81.5	87.2	94.8
2.20	-218.8	34.1	45.5	57.2	67.1	86.4
2.10	-210.7	27.5	32.2	48.2	58.8	67.0
2.00	-185.6	8.5	20.8	39.7	58.8	82.8
1.90	-139.4	16.8	33.8	55.6	82.6	110.2
1.80	-58.0	58.6	78.8	108.9	143.0	175.4
1.70	79.1	151.9	173.9	220.1	258.5	304.4
1.60	303.5	323.7	346.2	418.8	458.5	529.3
1.50	605.2	627.7	685.5	742.7	780.3	889.3
1.35	2104.8	2113.6	2135.9	2259.4	2286.2	2324.3
1.20	3035.7	3040.8	3087.4	3239.2	3252.5	3304.4
1.00	7825.9	7836.5	7871.3	7879.5	7976.4	7996.4

R(Fe-O)	$1\ ^5A_u$	$2\ ^5A_u$	$3\ ^5A_u$	$4\ ^5A_u$	$5\ ^5A_u$
10.00	33.2	59.5	101.7	101.7	101.7
9.00	34.4	60.6	102.9	102.9	102.9
8.00	35.5	61.7	104.0	104.0	104.0
7.00	36.3	62.5	104.8	104.8	104.9
6.00	36.1	62.3	104.6	104.6	104.7
5.00	33.4	59.6	101.8	102.0	102.1
4.50	30.2	56.4	98.7	98.9	98.9
4.00	25.1	51.3	93.5	93.8	93.9
3.70	21.1	47.2	89.4	89.8	89.9
3.35	15.8	41.8	83.8	84.3	84.8
3.00	12.0	37.5	79.4	80.1	81.2
2.80	12.9	37.3	79.4	80.4	82.3
2.70	15.0	38.1	80.4	81.7	84.0
2.60	18.4	39.4	82.4	84.0	86.8
2.50	23.3	40.3	85.2	87.5	90.8
2.40	27.9	38.7	87.0	90.9	94.5
2.30	29.8	35.4	85.6	91.7	95.6
2.20	37.2	41.2	89.6	98.7	103.6
2.10	50.8	54.1	98.4	111.0	117.5
2.00	79.5	82.9	119.7	136.1	146.2
1.90	125.3	129.3	154.8	175.1	191.3
1.80	205.7	210.8	220.3	244.2	270.5
1.70	335.7	341.7	348.7	362.4	404.5
1.60	530.5	559.1	565.1	574.7	624.7
1.50	866.8	893.4	913.9	936.0	940.4
1.35	2241.2	2275.3	2437.6	2485.8	2621.6
1.20	3144.0	3154.3	3204.2	3316.4	3328.8
1.00	7713.5	7728.5	7759.9	7944.7	7958.3

R(Fe-O)	$1\,^7A_g$	$1\,^7B_{3u}$	$2\,^7B_{3u}$	$1\,^7B_{2u}$	$1\,^7B_{1g}$	$1\,^7B_{1u}$	$1\,^7B_{2g}$	$2\,^7B_{2g}$	$1\,^7B_{3g}$	$1\,^7A_u$
10.00	33.2	33.2	33.3	33.3	33.2	33.2	33.2	33.3	33.3	33.2
9.00	34.4	34.4	34.5	34.5	34.4	34.4	34.4	34.5	34.5	34.4
8.00	35.5	35.5	35.6	35.6	35.5	35.5	35.5	35.6	35.6	35.5
7.00	36.3	36.3	36.4	36.4	36.3	36.3	36.3	36.4	36.4	36.3
6.00	36.1	36.0	36.3	36.3	36.1	36.1	36.0	36.3	36.3	36.1
5.00	33.4	33.3	33.8	33.7	33.4	33.4	33.3	33.7	33.7	33.4
4.50	30.2	30.1	30.7	30.6	30.2	30.2	30.1	30.7	30.6	30.2
4.00	24.9	24.9	25.9	25.7	25.0	25.1	24.9	25.8	25.7	25.1
3.70	20.8	20.8	22.0	21.7	20.9	20.9	20.8	22.0	21.6	20.9
3.35	15.4	15.4	17.1	16.4	15.3	15.4	15.4	17.1	16.4	15.4
3.00	-18.2	11.8	14.3	12.6	11.1	11.1	11.7	14.2	12.6	11.2
2.80	-40.0	13.0	16.1	13.3	11.4	11.4	12.9	16.0	13.2	11.5
2.70	-50.1	15.4	18.8	15.1	13.1	13.1	15.4	18.8	15.1	13.1
2.60	-59.0	20.2	24.1	19.0	17.0	17.4	20.4	24.3	19.2	16.8
2.50	-65.6	26.1	30.5	23.7	21.5	22.0	26.5	30.8	24.0	21.2
2.40	-69.0	32.6	37.5	28.3	26.0	26.3	33.1	38.0	28.8	25.6
2.30	-68.4	37.6	43.1	30.4	28.1	28.0	38.3	43.9	31.1	27.4
2.20	-66.2	44.1	50.2	32.8	30.6	30.3	45.1	51.3	34.0	29.5
2.10	-68.7	58.4	65.1	41.6	39.5	38.9	59.8	66.6	43.2	38.0
2.00	-65.7	88.1	95.4	63.7	61.7	60.8	89.9	97.4	65.7	59.7
1.90	-42.1	143.2	151.0	108.3	106.6	105.4	145.5	153.5	110.9	104.1
1.80	17.5	238.1	246.4	188.9	187.5	186.1	241.0	249.5	192.2	184.4
1.70	84.9	394.2	402.9	325.6	324.5	323.1	397.5	406.3	329.4	320.9
1.60	292.3	642.5	651.4	548.4	547.6	546.7	646.2	654.9	552.6	543.8

R(Fe-O)	$1\,^3A_g$	$2\,^3A_g$	$3\,^3A_g$	$4\,^3A_g$	$1\,^1B_{3u}$	$2\,^1B_{3u}$	$3\,^1B_{3u}$	$4\,^1B_{3u}$	$1\,^1B_{2u}$	$2\,^1B_{2u}$	$3\,^1B_{2u}$	$4\,^1B_{2u}$
10.00	57.5	99.7	99.8	99.8	57.5	57.6	99.8	99.8	57.6	99.8	99.8	99.8
9.00	58.7	100.9	101.0	101.0	58.7	58.8	100.9	101.0	58.8	100.9	101.0	101.0
8.00	59.8	102.0	102.1	102.1	59.8	59.9	102.1	102.1	59.9	102.1	102.1	102.1
7.00	60.6	102.8	102.9	102.9	60.5	60.7	102.9	102.9	60.7	102.9	102.9	102.9
6.00	60.4	102.6	102.7	102.7	60.3	60.6	102.7	102.7	60.6	102.7	102.7	102.7
5.00	60.6	80.2	80.2	89.7	60.2	60.7	104.0	104.2	60.6	104.0	104.1	104.1
4.50	57.4	62.5	62.5	72.0	57.1	57.7	101.0	101.1	57.6	101.0	101.0	101.1
4.00	31.4	31.5	40.9	48.2	56.4	57.3	100.1	100.3	57.0	100.0	100.1	100.2
3.70	10.4	10.4	19.9	27.2	52.6	53.7	96.4	96.6	53.2	96.3	96.4	96.5
3.35	-21.6	-21.5	-12.1	-4.9	47.8	49.1	91.7	92.1	48.1	91.3	91.5	91.9
3.00	-62.9	-62.9	-53.5	-46.6	44.4	46.1	88.9	89.2	43.8	87.4	87.9	88.9
2.80	-90.6	-90.5	-81.2	-74.6	44.9	46.7	90.4	90.7	43.0	87.1	88.4	90.0
2.70	-105.1	-105.0	-95.6	-89.3	46.2	48.1	92.8	92.9	43.3	87.9	90.0	92.0
2.60	-119.5	-119.5	-110.1	-104.1	48.1	50.1	96.5	96.6	43.8	89.4	92.6	95.1
2.50	-133.5	-133.4	-123.9	-118.2	49.5	51.9	101.1	101.3	43.8	91.6	95.9	98.8
2.40	-145.5	-145.4	-135.5	-130.3	49.0	52.5	104.9	105.5	41.7	93.2	97.9	100.5
2.30	-153.7	-153.6	-142.9	-138.2	48.6	53.3	105.6	106.8	39.2	91.6	96.1	97.2
2.20	-156.0	-155.9	-143.8	-139.1	52.8	58.7	104.8	107.7	39.9	89.5	94.7	94.7
2.10	-149.5	-149.3	-134.8	-129.6	66.2	73.2	102.7	116.7	48.4	93.0	98.0	99.1
2.00	-128.7	-128.3	-110.1	-103.2	95.8	103.9	110.1	139.1	70.9	108.0	112.9	115.1
1.90	-85.2	-84.4	-61.1	-50.8	134.4	151.3	160.7	183.9	116.6	142.8	147.5	150.7
1.80	112.0	139.7	144.3	158.8	-6.1	-5.0	24.9	41.5	186.6	247.3	257.9	264.3
1.70	-66.1	-49.5	-17.3	-12.1	194.0	206.1	210.6	228.6	128.5	129.2	166.4	194.7
1.60	48.7	67.1	117.0	121.3	48.9	67.7	116.6	120.8	322.8	326.9	333.2	347.7
1.50	515.4	526.1	540.1	546.2	245.4	263.4	305.7	338.2	245.5	264.6	318.3	338.3
1.35	534.6	578.3	585.2	640.1	832.3	844.5	849.1	856.2	526.5	566.3	596.2	628.7
1.20	1577.7	1617.7	1624.8	1639.5	1280.9	1336.8	1445.1	1449.0	1569.3	1610.5	1627.1	1630.4
1.00	3027.5	3081.7	3095.6	3382.8	3112.6	3153.9	3165.7	3170.2	2873.0	2925.0	2931.1	3023.5

R(Fe-O)	$1\,^3B_{1g}$	$2\,^3B_{1g}$	$3\,^3B_{1g}$	$4\,^3B_{1g}$	$1\,^3B_{1u}$	$2\,^3B_{1u}$	$3\,^3B_{1u}$	$4\,^3B_{1u}$	$1\,^3B_{2g}$	$2\,^3B_{2g}$	$3\,^3B_{2g}$	$4\,^3B_{2g}$
10.00	57.5	99.7	99.8	99.8	57.5	99.7	99.8	99.8	57.5	57.6	99.8	99.8
9.00	58.7	100.9	101.0	101.0	58.7	100.9	101.0	101.0	58.7	58.8	100.9	101.0
8.00	59.8	102.0	102.1	102.1	59.8	102.0	102.1	102.1	59.8	59.9	102.1	102.1
7.00	60.6	102.8	102.9	102.9	60.6	102.8	102.9	102.9	60.5	60.7	102.9	102.9
6.00	60.4	102.6	102.7	102.7	60.4	102.6	102.7	102.7	60.3	60.6	102.7	102.7
5.00	60.6	80.2	80.2	80.2	60.2	103.9	104.1	104.1	60.6	61.0	80.2	80.2
4.50	57.4	62.4	62.5	62.5	57.1	100.8	101.0	101.1	57.4	58.0	62.4	62.5
4.00	31.3	31.3	31.4	38.7	56.4	99.8	100.1	100.3	31.3	31.3	31.5	38.6
3.70	10.1	10.2	10.4	17.5	52.4	96.0	96.4	96.6	10.1	10.2	10.4	17.5
3.35	-22.2	-22.0	-21.5	-14.6	47.1	91.0	91.5	92.0	-22.3	-22.0	-21.5	-14.7
3.00	-64.7	-64.2	-62.9	-56.7	42.4	87.2	87.8	89.1	-64.7	-64.2	-62.8	-56.7
2.80	-93.7	-92.7	-90.8	-85.1	41.2	87.2	88.2	90.2	-93.7	-92.7	-90.7	-85.1
2.70	-109.3	-108.0	-105.6	-100.0	41.4	88.4	89.7	92.1	-109.3	-108.0	-105.5	-100.1
2.60	-125.3	-123.4	-120.7	-115.0	41.7	90.3	92.3	95.0	-125.4	-123.5	-120.6	-115.0
2.50	-141.4	-138.8	-135.6	-129.4	41.3	92.8	95.4	98.7	-141.5	-138.8	-135.5	-129.4
2.40	-156.8	-152.8	-149.1	-141.8	38.6	93.9	97.5	99.2	-156.8	-152.8	-149.0	-141.8
2.30	-169.2	-163.5	-158.9	-150.4	35.6	91.1	95.6	97.0	-169.1	-163.6	-158.9	-150.5
2.20	-177.1	-169.2	-162.9	-154.7	35.6	88.4	93.1	96.9	-176.9	-169.3	-163.1	-154.8
2.10	-177.2	-166.8	-157.9	-150.5	43.3	91.3	96.1	103.1	-176.9	-167.1	-158.1	-150.6
2.00	-164.6	-151.5	-138.3	-131.8	65.2	105.8	110.7	121.3	-164.3	-152.0	-138.4	-131.8
1.90	-131.7	-115.8	-95.5	-90.0	110.1	140.0	145.3	159.6	-131.4	-116.8	-95.7	-89.8
1.80	199.0	209.6	214.1	218.1	-66.8	-48.1	-16.9	-12.3	191.5	206.0	212.3	229.5
1.70	283.5	400.0	404.5	405.1	327.3	331.4	334.5	338.9	48.2	68.0	117.4	121.3
1.60	351.6	353.4	389.6	396.3	448.8	623.5	628.5	631.7	522.6	525.7	529.4	533.6
1.50	517.2	520.9	540.0	545.3	670.0	681.0	689.8	706.5	740.4	977.2	982.3	984.5
1.35	531.7	571.9	597.7	628.7	837.8	841.8	855.9	864.8	1481.2	1494.1	1519.2	1526.6
1.20	1278.3	1334.4	1456.0	1459.2	1283.1	1344.2	1442.7	1455.8	1566.2	1605.3	1611.4	1628.0
1.00	3099.3	3141.9	3153.2	3158.1	2872.1	2924.3	2928.9	3027.3	2878.7	2929.5	2940.3	3015.9

R(Fe-O)	$1\,^3B_{3g}$	$2\,^3B_{3g}$	$3\,^3B_{3g}$	$4\,^3B_{3g}$	$1\,^3A_u$	$2\,^3A_u$	$3\,^3A_u$	$4\,^3A_u$
10.00	57.6	99.8	99.8	99.8	57.5	99.7	99.8	99.8
9.00	58.8	100.9	101.0	101.0	58.7	100.9	101.0	101.0
8.00	59.9	102.1	102.1	102.1	59.8	102.0	102.1	102.1
7.00	60.7	102.9	102.9	102.9	60.6	102.8	102.9	102.9
6.00	60.6	102.7	102.7	102.7	60.4	102.6	102.7	102.7
5.00	60.9	80.2	80.2	80.2	60.2	103.9	104.1	104.1
4.50	57.9	62.4	62.5	62.5	57.1	100.8	101.0	101.1
4.00	31.3	31.3	31.5	38.6	56.4	99.8	100.1	100.3
3.70	10.1	10.2	10.4	17.5	52.5	96.0	96.4	96.6
3.35	-22.3	-22.1	-21.5	-14.7	47.1	91.0	91.5	92.0
3.00	-64.7	-64.2	-62.8	-56.7	42.4	87.2	87.8	89.1
2.80	-93.7	-92.8	-90.7	-85.2	41.4	87.3	88.2	90.2
2.70	-109.3	-108.0	-105.5	-100.1	41.6	88.4	89.7	92.1
2.60	-125.3	-123.5	-120.6	-115.1	42.0	90.4	92.2	95.0
2.50	-141.4	-138.8	-135.6	-129.4	41.7	92.8	95.4	98.7
2.40	-156.7	-152.9	-149.1	-141.9	39.1	93.7	97.5	99.3
2.30	-169.0	-163.6	-159.0	-150.6	36.2	90.8	95.6	97.0
2.20	-176.9	-169.4	-163.2	-154.9	36.5	88.0	92.9	96.9
2.10	-176.8	-167.0	-158.2	-150.7	44.5	90.9	95.8	102.9
2.00	-164.2	-152.0	-138.6	-131.9	66.7	105.4	110.1	120.9
1.90	-131.2	-116.6	-95.9	-90.0				
1.80	-66.3	-49.8	-17.0	-11.8				
1.70	321.9	329.9	329.9	347.7				
1.60	244.1	266.5	320.8	339.7				
1.50	845.1	849.2	850.0	852.9				
1.35	1564.4	1627.5	1791.7	1815.3				
1.20	3077.7	3087.2	3094.1	3099.6				
1.00	3096.3	3134.3	3141.8	3145.6				

R(Fe-O)	$1\,^1A_g$	$2\,^1A_g$	$3\,^1A_g$	$4\,^1A_g$	$5\,^1A_g$	$6\,^1A_g$	$1\,^1B_{3u}$	$2\,^1B_{3u}$	$3\,^1B_{3u}$
6.00	111.2	111.2	111.2	118.4	120.6	120.6	111.2	111.2	120.6
5.00	108.5	108.5	108.5	115.7	117.9	118.0	108.5	108.5	117.9
4.50	83.4	83.6	83.6	83.6	88.5	88.6	111.4	111.6	120.9
4.00	56.1	56.4	56.4	56.5	61.2	61.3	108.1	108.2	117.5
3.70	34.8	35.3	35.4	35.4	39.9	40.1	104.4	104.4	113.7
3.35	2.3	3.2	3.4	3.5	7.5	7.9	99.5	99.6	108.8
3.00	-40.9	-38.3	-38.0	-37.9	-35.0	-34.0	95.9	96.0	104.9
2.80	-71.0	-66.1	-65.9	-65.7	-63.6	-62.0	96.0	96.2	104.9
2.70	-87.6	-80.7	-80.6	-80.5	-78.7	-76.5	97.1	97.3	105.9
2.60	-104.9	-95.7	-95.6	-95.1	-93.9	-90.8	98.7	99.1	107.7
2.50	-122.7	-110.4	-110.3	-108.9	-108.5	-104.0	100.1	100.7	109.5
2.40	-139.9	-123.5	-123.3	-121.4	-120.4	-114.6	100.2	101.1	110.2
2.30	-155.2	-133.2	-133.0	-130.7	-128.1	-121.0	99.5	100.8	110.4
2.20	-167.2	-137.4	-137.0	-134.5	-129.4	-120.5	101.2	103.5	104.5
2.10	-173.1	-132.4	-131.9	-129.2	-120.7	-109.4	101.5	110.4	113.7
2.00	-168.0	-113.0	-112.3	-109.4	-97.1	-82.7	108.7	132.9	137.4
1.90	-145.5	-70.6	-69.7	-66.8	-50.4	-31.9	132.7	178.0	183.4
1.80	-94.9	7.4	8.6	11.6	31.4	54.8	184.5	258.9	265.3
1.70	0.5	141.3	143.2	146.1	168.0	195.4	279.5	396.9	403.8
1.60	168.8	358.6	361.2	364.1	385.8	389.5	446.4	621.2	628.0
1.50	473.2	654.4	680.6	684.0	708.1	710.8	737.6	970.2	980.0
1.35	1357.4	1458.0	1488.6	1510.0	1512.0	1523.5	1556.3	1622.8	1627.9

R(Fe-O)	$1\,^1B_{2u}$	$2\,^1B_{2u}$	$3\,^1B_{2u}$	$4\,^1B_{2u}$	$5\,^1B_{2u}$	$6\,^1B_{2u}$	$1\,^1B_{1g}$	$2\,^1B_{1g}$	$3\,^1B_{1g}$	$4\,^1B_{1g}$	$5\,^1B_{1g}$	$6\,^1B_{1g}$
6.00	111.2	111.2	111.2	118.4	120.6	120.6	111.2	111.2	111.2	118.4	120.6	120.6
5.00	108.5	108.5	108.5	115.7	117.9	117.9	108.5	108.5	108.5	115.7	117.9	118.0
4.50	111.2	111.4	111.6	118.6	120.8	120.9	83.4	83.5	83.6	88.6	88.7	111.5
4.00	107.9	108.0	108.2	115.2	117.4	117.5	56.1	56.2	56.4	61.2	61.5	86.7
3.70	104.0	104.1	104.5	111.4	113.6	113.7	34.9	35.0	35.3	40.0	40.5	65.4
3.35	98.8	99.0	99.6	106.2	108.5	108.7	2.5	2.7	3.3	7.8	8.6	33.0
3.00	94.2	94.7	96.0	101.7	104.4	105.3	-40.3	-39.7	-38.1	-34.4	-32.5	-9.4
2.80	93.2	94.0	96.0	100.9	104.1	105.8	-69.8	-68.4	-65.7	-62.7	-59.6	-38.2
2.70	93.4	94.4	96.8	101.6	105.0	107.1	-85.7	-83.7	-80.2	-77.6	-73.7	-53.6
2.60	93.8	95.1	98.0	103.0	106.4	108.9	-102.1	-99.3	-94.6	-92.5	-87.5	-69.1
2.50	93.6	95.3	98.7	104.4	107.6	110.7	-118.6	-114.5	-108.3	-106.6	-100.3	-84.2
2.40	91.2	93.6	97.7	104.4	107.0	111.7	-134.0	-128.1	-120.0	-118.7	-110.7	-97.5
2.30	87.0	90.4	95.5	103.2	105.0	111.8	-146.7	-138.3	-127.9	-126.9	-116.8	-107.2
2.20	84.1	88.6	95.7	104.6	105.3	114.8	-155.0	-143.2	-130.1	-129.0	-116.7	-110.7
2.10	87.0	92.9	103.3	112.6	113.8	119.4	-155.6	-139.3	-123.9	-121.5	-107.4	-103.4
2.00	101.9	109.0	124.8	133.7	134.0	136.6	-143.6	-121.7	-104.8	-99.1	-84.8	-79.0
1.90	136.7	144.9	167.7	169.1	178.3	182.3	-111.4	-83.0	-64.6	-53.6	-40.4	-28.6
1.80	203.5	212.5	233.3	249.4	258.6	259.9	-47.5	-12.6	10.5	27.6	38.5	60.7
1.70	320.8	330.1	348.5	376.2	385.3	395.1	67.1	106.9	142.6	164.2	172.1	187.8
1.60	517.1	526.2	541.9	569.0	606.8	617.2	259.6	301.3	318.2	359.0	382.8	387.8
1.50	840.1	845.9	854.9	861.5	887.9	959.7	527.9	585.8	631.6	655.7	665.1	691.2
1.35	1578.8	1617.7	1627.5	1638.7	1640.8	1678.1	1276.0	1331.7	1337.1	1463.9	1477.7	1486.2

R(Fe-O)	$1\,^1B_{1u}$	$2\,^1B_{1u}$	$3\,^1B_{1u}$	$4\,^1B_{1u}$	$5\,^1B_{1u}$	$6\,^1B_{1u}$	$1\,^1B_{2g}$	$2\,^1B_{2g}$	$3\,^1B_{2g}$
6.00	111.2	111.2	111.2	118.4	120.6	120.6	111.2	111.2	120.6
5.00	108.5	108.5	108.5	115.8	117.9	118.0	108.5	108.5	117.9
4.50	111.4	111.4	111.5	118.8	120.8	121.0	83.5	83.5	83.6
4.00	107.9	108.0	108.2	115.3	117.4	117.6	56.2	56.2	56.4
3.70	104.0	104.1	104.5	111.5	113.6	113.8	34.9	35.0	35.4
3.35	98.7	98.9	99.6	106.4	108.7	108.9	2.4	2.7	3.5
3.00	94.0	94.6	96.0	102.0	104.8	105.2	-40.3	-39.7	-37.9
2.80	92.7	93.9	95.9	101.3	104.7	105.5	-69.7	-68.5	-65.6
2.70	92.7	94.3	96.6	101.9	105.7	106.7	-85.7	-83.8	-80.0
2.60	92.9	95.2	97.6	103.3	107.1	108.6	-102.1	-99.4	-94.5
2.50	92.5	95.6	98.2	104.7	108.2	110.3	-118.5	-114.6	-108.2
2.40	90.0	94.3	97.2	104.8	107.5	110.7	-133.9	-128.1	-119.9
2.30	85.8	91.7	95.2	103.6	105.8	110.7	-146.6	-138.4	-128.0
2.20	82.8	91.1	95.6	103.9	106.8	114.5	-154.8	-143.2	-130.4
2.10	85.7	97.0	103.4	110.9	115.6	117.7	-155.5	-139.3	-124.4
2.00	100.7	115.4	125.1	131.3	131.6	138.1	-143.5	-121.7	-105.6
1.90	135.8	154.0	164.9	169.5	174.6	183.3	-111.3	-83.4	-65.6
1.80	203.2	224.9	230.0	250.1	253.9	264.4	-47.3	-13.9	9.9
1.70	321.1	344.2	345.8	386.6	387.8	390.5	67.5	103.9	142.3
1.60	518.5	537.0	544.7	583.4	609.4	611.8	260.3	295.9	304.2
1.50	845.9	858.0	866.1	872.0	901.3	961.3	519.5	592.5	619.5
1.35	1585.1	1607.9	1619.5	1643.0	1647.2	1668.8	1273.3	1329.2	1333.1

R(Fe-O)	$1\,^1B_{3g}$	$2\,^1B_{3g}$	$3\,^1B_{3g}$	$4\,^1B_{3g}$	$5\,^1B_{3g}$	$6\,^1B_{3g}$	$1\,^1A_u$	$2\,^1A_u$	$3\,^1A_u$	$4\,^1A_u$	$5\,^1A_u$	$6\,^1A_u$
6.00	111.2	111.2	111.2	118.4	120.6	120.6	111.2	111.2	111.2	118.4	120.6	120.6
5.00	108.5	108.5	108.5	115.7	117.9	117.9	108.5	108.5	108.5	115.8	117.9	118.0
4.50	83.5	83.5	83.6	88.6	88.7	111.5	111.2	111.4	111.5	118.7	120.9	121.0
4.00	56.2	56.2	56.4	61.3	61.5	86.6	107.9	108.0	108.2	115.4	117.4	117.6
3.70	34.9	35.0	35.4	40.1	40.5	65.4	104.0	104.1	104.4	111.5	113.6	113.8
3.35	2.4	2.7	3.4	7.7	8.6	33.1	98.7	99.0	99.6	106.4	108.7	108.9
3.00	-40.3	-39.7	-38.0	-34.4	-32.5	-9.4	94.0	94.6	96.0	102.0	104.8	105.2
2.80	-69.7	-68.5	-65.6	-62.7	-59.6	-38.1	92.7	93.9	95.9	101.3	104.7	105.5
2.70	-85.6	-83.8	-80.1	-77.6	-73.7	-53.5	92.6	94.3	96.6	101.9	105.6	106.8
2.60	-102.1	-99.4	-94.5	-92.4	-87.5	-69.0	92.7	95.1	97.6	103.3	107.0	108.7
2.50	-118.5	-114.6	-108.3	-106.6	-100.3	-84.1	92.2	95.6	98.3	104.6	108.1	110.5
2.40	-133.8	-128.2	-120.0	-118.7	-110.6	-97.5	89.6	94.3	97.4	104.7	107.5	110.9
2.30	-146.5	-138.4	-128.0	-127.0	-116.8	-107.3	85.2	91.7	95.4	103.5	105.9	110.8
2.20	-154.7	-143.3	-130.5	-129.1	-116.7	-110.9	82.0	91.0	96.0	103.9	107.1	114.3
2.10	-155.3	-139.4	-124.5	-121.4	-107.5	-103.6	84.6	96.7	104.0	110.9	116.0	117.7
2.00	-143.3	-121.8	-105.7	-99.0	-85.1	-79.1	99.2	114.7	125.9	131.4	131.6	138.7
1.90	-111.0	-83.4	-65.6	-53.3	-40.7	-28.6	133.7	152.7	165.0	170.6	174.8	184.2
1.80	-46.9	-13.5	9.7	28.0	38.0	60.8	200.3	222.7	230.2	251.3	254.5	265.4
1.70	68.0	104.6	141.8	164.6	171.7	185.6	317.2	342.0	344.7	387.0	388.3	390.9
1.60	260.9	298.3	315.6	358.4	383.0	387.0	513.2	537.1	540.0	582.0	610.6	613.5
1.50	525.9	589.1	628.3	656.2	666.6	693.1	835.7	852.1	859.2	864.8	900.6	963.1
1.35	1280.1	1335.3	1342.8	1460.0	1476.0	1480.2	1562.6	1610.4	1611.8	1622.3	1623.0	1665.5

Table S3. Potential energy curves of the electronic states of the $[Fe(H_2O)_6]^{3+}$ cluster. Energies are reported in kcal/mol and *R*(Fe-O) distances in Å.

***R*(Fe-O)**	**1** ^6A_g	**2** ^6A_g	**3** ^6A_g	**4** ^6A_g	**5** ^6A_g	**6** ^6A_g	**7** ^6A_g	**8** ^6A_g	**9** ^6A_g	**10** ^6A_g	**11** ^6A_g
10.00	83.0	83.1	101.7	143.6	298.3	298.3	314.2	323.4	367.4	368.9	480.9
9.00	88.9	89.1	107.6	146.2	300.9	301.0	316.9	326.0	370.0	371.6	474.8
8.00	95.9	96.1	114.6	148.8	303.5	303.6	319.5	328.6	372.6	374.2	466.2
7.00	103.9	104.3	122.7	150.9	305.6	305.7	321.5	330.7	374.7	376.2	453.5
6.00	113.0	113.6	131.9	151.1	305.8	305.9	321.8	330.9	374.9	376.5	433.0
5.00	122.7	123.8	141.9	146.2	301.1	301.1	317.0	326.1	370.2	371.7	397.2
4.50	127.4	129.0	139.4	146.8	294.4	294.4	310.3	319.4	363.5	365.0	367.7
4.00	126.5	131.6	134.2	151.6	281.9	282.0	297.9	307.0	323.6	351.0	352.5
3.70	114.2	134.0	137.5	154.6	270.3	270.4	286.1	286.2	295.4	339.4	340.9
3.35	93.4	137.0	142.2	159.7	227.5	251.5	251.6	267.4	276.6	320.6	322.1
3.00	63.9	142.5	148.6	150.6	170.7	227.4	227.6	243.5	252.5	296.6	297.9
2.80	43.0	93.6	149.6	159.8	184.0	213.0	213.3	229.3	238.1	282.3	283.5
2.70	31.4	64.2	155.2	166.6	194.0	206.6	207.0	223.4	231.8	276.2	277.2
2.60	17.2	34.6	164.1	175.9	200.4	201.4	207.8	218.3	226.0	270.7	271.5
2.50	-7.8	17.3	174.4	187.2	197.5	199.0	216.5	223.3	225.2	268.7	269.0
2.40	-39.2	8.3	187.1	195.8	199.3	204.2	219.7	224.3	246.2	270.1	271.0
2.30	-71.4	5.5	198.5	201.7	206.6	219.3	227.4	232.2	269.7	276.3	279.2
2.20	-101.6	12.2	205.5	211.5	217.6	233.6	237.7	247.6	287.1	291.7	294.3
2.10	-121.8	32.8	207.7	217.8	229.4	243.3	249.4	264.0	297.5	309.0	314.6
2.00	-123.3	64.9	209.9	223.6	252.5	255.2	277.2	288.9	312.8	331.6	340.8
1.90	-100.1	118.0	226.1	242.0	280.8	300.2	325.8	334.8	356.9	379.9	383.8
1.80	-58.5	254.6	266.0	274.7	337.0	350.5	364.1	374.9	406.0	432.3	463.2
1.70	63.6	339.5	351.4	410.6	433.7	442.6	461.8	500.8	541.7	572.8	594.6
1.60	276.1	496.4	506.7	604.2	615.6	640.0	670.8	712.3	776.8	809.0	816.4
1.50	627.8	776.7	782.4	907.2	917.3	995.9	1017.6	1058.2	1159.1	1175.8	1191.8
1.35	1575.9	1596.2	1598.4	1758.9	1765.5	1902.7	1954.4	1989.8	2148.5	2164.7	2192.1

R(Fe-O)	1 $^6B_{3u}$	2 $^6B_{3u}$	3 $^6B_{3u}$	4 $^6B_{3u}$	5 $^6B_{3u}$	6 $^6B_{3u}$	7 $^6B_{3u}$	8 $^6B_{3u}$	9 $^6B_{3u}$	10 $^6B_{3u}$	11 $^6B_{3u}$	12 $^6B_{3u}$
100.00	3.3	32.0	71.3	71.3	71.3	78.3	80.4	80.4	87.9	87.9	91.0	91.0
50.00	11.2	39.9	79.2	79.2	79.2	86.2	88.3	88.3	95.8	95.8	98.8	98.8
20.00	33.1	61.9	101.1	101.1	101.1	108.2	110.3	110.3	117.7	117.7	120.8	120.8
10.00	64.2	93.0	132.2	132.3	132.3	139.3	141.3	141.4	148.8	148.9	151.9	152.0
9.00	70.2	99.0	138.2	138.3	138.3	145.3	147.3	147.4	154.8	154.8	157.9	158.1
8.00	77.2	105.9	145.2	145.3	145.3	152.3	154.3	154.4	161.8	161.8	164.9	165.2
7.00	85.4	114.1	153.3	153.4	153.5	160.4	162.4	162.6	169.9	170.0	173.0	173.5
6.00	94.6	123.2	162.6	162.7	162.7	169.7	171.6	171.9	179.1	179.2	182.3	183.2
5.00	104.3	132.8	172.2	172.5	172.5	179.4	181.2	181.7	188.6	188.9	192.4	193.8
4.50	108.8	137.2	176.7	177.0	177.1	183.9	185.6	186.3	192.9	193.3	197.3	199.2
4.00	112.6	140.7	180.4	180.7	180.9	187.6	189.1	190.2	193.0	194.2	196.2	196.9
3.70	114.4	142.3	181.2	182.2	182.4	182.7	182.8	189.4	190.6	192.1	197.6	198.6
3.35	116.7	144.1	161.2	163.5	184.0	184.3	185.0	191.3	192.0	194.3	199.0	200.5
3.00	121.2	132.8	136.0	147.6	186.6	188.4	189.0	193.8	195.5	198.5	202.4	204.4
2.80	112.8	116.6	127.2	152.1	189.5	193.1	193.7	198.0	200.8	204.0	207.7	210.1
2.70	102.0	106.3	131.9	155.6	191.6	195.8	198.0	202.2	205.1	208.6	212.3	215.0
2.60	88.1	92.7	138.9	160.2	195.6	200.6	203.9	208.6	211.4	215.4	219.0	222.2
2.50	77.9	82.9	147.5	165.6	199.8	206.2	211.1	216.2	219.0	223.9	227.0	230.7
2.40	68.4	73.8	157.1	171.2	208.1	216.1	218.6	224.6	227.9	234.3	236.4	240.8
2.30	62.9	68.5	165.3	176.3	219.6	225.0	228.6	232.9	237.3	245.3	246.2	251.5
2.20	65.5	71.2	172.9	183.1	228.7	233.4	238.5	244.0	248.7	257.9	258.5	264.6
2.10	78.0	83.8	185.7	195.4	239.2	247.7	251.9	259.3	265.6	276.5	278.6	291.4
2.00	105.1	111.4	210.2	218.6	260.7	273.0	277.0	284.8	293.9	306.2	310.2	315.2
1.90	162.5	169.3	251.3	260.6	307.7	309.3	320.1	323.3	326.7	332.3	343.9	356.1
1.80	266.3	275.2	310.4	320.8	376.6	387.7	390.1	394.6	404.0	408.5	414.4	436.9
1.70	420.5	440.2	440.9	442.2	506.1	506.7	509.1	520.5	526.2	535.1	557.1	568.2
1.60	633.8	651.0	697.5	701.4	712.3	715.6	718.3	729.0	733.9	741.7	777.7	782.4
1.50	980.0	998.8	1051.1	1054.4	1059.6	1068.3	1074.1	1078.6	1104.7	1110.2	1120.0	1123.0
1.35	1941.6	1952.9	1960.8	1973.5	1980.6	1986.7	1988.0	1996.2	1998.0	2006.4	2021.2	2026.0

R(Fe-O)	13 $^6B_{3u}$	14 $^6B_{3u}$	15 $^6B_{3u}$	16 $^6B_{3u}$	1 $^6B_{2u}$	2 $^6B_{2u}$	3 $^6B_{2u}$	4 $^6B_{2u}$	5 $^6B_{2u}$	6 $^6B_{2u}$	7 $^6B_{2u}$
100.00	111.1	140.3	169.7	169.7	3.3	32.0	71.3	71.3	71.3	78.3	80.4
50.00	119.0	148.2	175.7	175.7	11.2	39.9	79.2	79.2	79.2	86.2	88.3
20.00	141.0	170.1	191.4	191.4	33.1	61.9	101.1	101.1	101.1	108.2	110.3
10.00	172.1	201.2	209.4	209.5	64.2	93.0	132.2	132.3	132.3	139.3	141.3
9.00	178.1	207.2	212.1	212.2	70.2	99.0	138.2	138.3	138.3	145.3	147.3
8.00	185.1	214.1	214.6	214.7	77.2	105.9	145.2	145.3	145.3	152.3	154.3
7.00	193.3	216.5	216.8	222.3	85.4	114.1	153.3	153.4	153.5	160.4	162.4
6.00	202.5	216.7	217.0	231.5	94.6	123.2	162.6	162.7	162.7	169.7	171.6
5.00	211.9	212.3	212.5	241.3	104.3	132.8	172.2	172.5	172.5	179.4	181.2
4.50	205.3	206.1	216.9	245.8	108.8	137.2	176.7	177.0	177.1	183.9	185.6
4.00	201.6	204.2	220.6	249.5	112.6	140.8	180.4	180.7	180.9	187.6	189.1
3.70	203.7	206.9	222.5	250.8	114.5	142.4	182.2	182.3	182.5	182.7	189.4
3.35	205.8	209.9	224.5	251.3	116.8	144.3	162.8	184.1	184.3	184.9	191.3
3.00	209.3	214.3	228.5	251.2	121.5	134.3	147.9	186.7	188.4	189.0	193.9
2.80	214.6	219.6	233.5	252.6	113.6	127.6	152.7	189.7	193.0	193.7	198.1
2.70	219.2	224.0	237.4	254.7	102.3	132.5	156.5	191.8	195.7	197.9	202.3
2.60	226.3	231.0	243.4	260.1	87.5	139.7	161.4	195.8	200.6	203.7	208.8
2.50	235.0	239.3	250.2	265.9	75.8	148.7	167.1	199.9	206.2	210.6	216.6
2.40	245.2	250.3	260.0	276.2	64.3	158.7	173.4	208.2	216.4	217.7	225.5
2.30	256.8	263.0	271.1	291.1	55.7	167.5	179.4	219.3	223.8	229.8	234.5
2.20	274.1	278.9	283.2	312.1	54.0	176.2	187.5	226.2	233.7	241.3	246.0
2.10	299.0	301.9	312.8	326.3	60.4	190.6	201.9	234.6	248.4	256.8	262.1
2.00	320.3	332.6	340.4	354.8	79.5	218.6	230.0	252.1	272.8	285.7	289.8
1.90	381.6	394.1	395.5	401.7	127.3	275.0	287.9	288.7	315.6	341.9	346.2
1.80	448.7	454.8	478.4	480.0	217.5	341.8	364.8	375.4	388.5	423.4	429.9
1.70	574.3	583.8	622.9	625.3	363.4	440.8	474.1	501.0	538.0	549.1	558.2
1.60	795.9	815.9	840.4	858.2	598.4	617.9	654.6	714.3	758.3	766.6	775.9
1.50	1134.2	1154.2	1178.9	1190.3	919.7	950.1	978.6	1060.2	1097.8	1106.1	1138.6
1.35	2050.8	2060.1	2134.4	2148.4	1772.4	1799.9	1887.8	1985.5	1999.9	2017.2	2041.3

R(Fe-O)	$8\ ^6B_{2u}$	$9\ ^6B_{2u}$	$10\ ^6B_{2u}$	$11\ ^6B_{2u}$	$12\ ^6B_{2u}$	$13\ ^6B_{2u}$	$14\ ^6B_{2u}$	$15\ ^6B_{2u}$	$1\ ^6B_{1g}$	$2\ ^6B_{1g}$
100.00	80.4	87.9	87.9	91.0	91.0	111.1	140.3	169.7	3.3	169.7
50.00	88.3	95.8	95.8	98.8	98.8	119.0	148.2	175.7	11.2	175.7
20.00	110.3	117.7	117.7	120.8	120.8	141.0	170.1	191.4	33.2	191.4
10.00	141.4	148.8	148.9	151.9	152.0	172.1	201.2	209.5	64.3	209.5
9.00	147.4	154.8	154.8	157.9	158.1	178.1	207.2	212.2	70.3	212.1
8.00	154.4	161.8	161.8	164.9	165.2	185.1	214.1	214.7	77.4	214.6
7.00	162.6	169.9	170.0	173.0	173.5	193.3	216.8	222.3	85.6	216.6
6.00	171.9	179.1	179.2	182.3	183.2	202.5	217.0	231.5	95.0	216.8
5.00	181.7	188.6	188.8	192.4	193.8	212.3	212.4	241.3	104.9	212.0
4.50	186.3	192.9	193.3	197.3	199.2	206.0	216.9	245.9	109.7	205.4
4.00	190.2	194.0	196.2	196.9	201.6	204.2	220.6	249.5	113.8	193.2
3.70	190.6	192.1	197.6	198.6	203.7	206.9	222.4	250.9	116.0	181.4
3.35	191.9	194.2	199.0	200.4	205.8	209.9	224.5	251.5	118.7	161.4
3.00	195.5	198.4	202.4	204.3	209.5	214.3	228.4	251.6	124.1	132.5
2.80	200.9	203.8	207.8	210.1	214.8	219.6	233.4	253.2	111.7	130.8
2.70	205.3	208.2	212.4	215.0	219.4	224.0	237.3	255.4	100.3	136.1
2.60	211.8	215.0	219.2	222.4	226.4	231.0	243.2	260.9	85.3	143.6
2.50	219.5	223.3	227.4	231.0	235.0	239.2	250.1	266.8	73.8	153.0
2.40	228.7	233.5	237.1	241.2	245.3	250.1	259.8	277.2	62.2	163.9
2.30	238.3	244.1	247.2	251.6	257.0	262.6	270.9	292.3	53.7	174.6
2.20	250.2	256.1	259.8	264.3	274.1	278.3	283.2	313.4	52.2	185.3
2.10	268.6	274.2	280.0	291.8	298.5	300.8	313.5	347.9	59.3	201.1
2.00	299.7	306.2	314.7	330.9	342.1	354.8	381.4	385.6	79.4	230.3
1.90	359.0	362.8	371.0	379.5	390.2	395.1	410.5	415.3	128.0	288.7
1.80	441.3	445.1	453.0	460.5	468.1	477.5	485.9	507.4	217.6	379.0
1.70	574.2	584.3	596.0	600.6	611.6	620.9	626.0	649.4	363.5	475.4
1.60	798.3	807.2	829.9	833.7	844.2	852.8	858.8	872.6	598.3	651.9
1.50	1150.0	1177.5	1181.2	1202.6	1206.9	1210.2	1220.2	1227.1	946.4	968.9
1.35	2050.6	2078.9	2100.4	2120.0	2126.8	2136.5	2145.7	2184.4	1796.0	1818.3

R(Fe-O)	$1\ ^6B_{1u}$	$2\ ^6B_{1u}$	$3\ ^6B_{1u}$	$4\ ^6B_{1u}$	$5\ ^6B_{1u}$	$6\ ^6B_{1u}$	$7\ ^6B_{1u}$	$8\ ^6B_{1u}$	$9\ ^6B_{1u}$	$10\ ^6B_{1u}$
100.00	3.3	3.3	32.0	32.0	71.3	71.3	80.4	87.9	87.9	87.9
50.00	11.2	11.2	39.9	39.9	79.2	79.2	88.3	95.8	95.8	95.8
20.00	33.1	33.2	61.9	61.9	101.1	101.1	110.3	117.7	117.7	117.7
10.00	64.2	64.3	92.9	93.1	132.3	132.3	141.4	148.8	148.9	148.9
9.00	70.2	70.3	98.9	99.1	138.2	138.3	147.4	154.8	154.8	154.9
8.00	77.2	77.4	105.9	106.1	145.2	145.3	154.4	161.8	161.8	161.9
7.00	85.3	85.6	114.0	114.4	153.4	153.5	162.6	169.9	170.0	170.1
6.00	94.5	95.0	123.1	123.7	162.6	162.7	171.8	179.1	179.3	179.3
5.00	104.1	105.0	132.7	133.6	172.4	172.5	181.6	188.6	189.0	189.2
4.50	108.5	109.8	137.0	138.3	176.9	177.1	186.2	192.9	193.6	193.8
4.00	112.2	114.0	140.7	142.3	180.7	180.9	190.1	193.2	196.2	197.4
3.70	114.0	116.3	142.5	144.4	181.4	182.6	182.8	192.0	197.6	199.3
3.35	116.2	119.5	144.9	147.2	161.3	184.9	185.0	194.5	199.0	201.6
3.00	121.0	126.0	132.3	150.0	152.6	189.5	189.6	199.3	201.9	206.3
2.80	111.4	127.7	134.0	156.6	159.1	195.4	195.9	205.4	206.6	212.5
2.70	99.9	133.1	140.2	161.6	164.0	200.2	201.0	209.9	211.1	217.4
2.60	84.9	141.0	149.1	168.1	170.6	207.2	208.2	216.6	218.0	224.4
2.50	73.2	151.3	160.2	175.7	178.5	215.7	217.1	224.4	226.7	233.0
2.40	61.5	163.2	173.2	183.3	187.8	225.9	227.4	235.2	236.8	242.7
2.30	52.7	175.1	186.0	190.2	197.9	235.3	237.8	246.0	249.9	252.1
2.20	50.9	187.8	199.9	200.6	211.3	244.6	249.5	257.3	262.8	266.0
2.10	57.4	207.5	220.0	221.2	232.6	258.7	267.4	275.5	280.8	288.1
2.00	76.1	242.6	255.5	258.8	270.5	284.3	298.5	308.9	315.3	325.6
1.90	122.9	307.8	323.8	325.5	331.2	340.7	349.6	357.7	370.0	373.1
1.80	212.9	374.0	386.5	403.1	412.4	433.9	438.6	438.9	458.2	472.8
1.70	359.3	468.8	485.9	518.2	551.0	570.5	591.8	608.2	627.2	629.3
1.60	595.4	644.6	663.0	722.6	759.6	809.1	834.2	864.8	868.3	873.3
1.50	942.7	958.1	977.8	1062.6	1099.4	1191.7	1214.2	1222.1	1238.2	1248.9
1.35	1800.4	1811.4	1893.1	1999.7	2031.1	2177.0	2184.6	2200.5	2214.0	2224.2

R(Fe-O)	11 $^6B_{1u}$	12 $^6B_{1u}$	13 $^6B_{1u}$	14 $^6B_{1u}$	15 $^6B_{1u}$	1 $^6B_{2g}$	2 $^6B_{2g}$	3 $^6B_{2g}$	1 $^6B_{3g}$	2 $^6B_{3g}$
100.00	91.0	111.1	111.1	135.5	169.7	3.3	169.7	169.7	3.3	169.7
50.00	98.8	119.0	119.0	143.4	175.7	11.2	175.7	175.7	11.2	175.7
20.00	120.8	141.0	141.0	165.4	191.4	33.1	191.4	191.4	33.1	191.4
10.00	151.9	172.1	172.1	196.5	209.5	64.2	209.4	209.5	64.2	209.5
9.00	157.9	178.1	178.1	202.5	212.1	70.2	212.1	212.2	70.2	212.2
8.00	165.0	185.1	185.1	209.5	214.6	77.2	214.6	214.7	77.2	214.7
7.00	173.2	193.3	193.3	216.6	217.7	85.4	216.5	216.8	85.4	216.8
6.00	182.7	202.5	202.6	216.8	226.9	94.6	216.7	217.0	94.6	217.0
5.00	193.1	212.0	212.3	212.4	236.7	104.3	211.9	212.5	104.3	212.4
4.50	198.3	205.4	216.9	217.0	241.3	108.8	205.3	206.1	108.8	206.0
4.00	197.8	203.2	220.9	221.0	245.4	112.6	193.0	194.2	112.6	194.0
3.70	199.8	205.9	222.9	223.0	247.8	114.4	181.2	182.8	114.4	182.5
3.35	202.4	209.0	225.5	225.5	252.0	116.6	161.3	163.5	116.7	162.8
3.00	207.6	214.1	230.6	230.8	262.6	121.0	133.0	136.2	121.3	134.4
2.80	214.3	220.3	237.1	237.6	276.6	113.0	116.9	126.9	114.0	127.3
2.70	219.6	225.4	242.3	243.0	287.8	102.4	106.7	131.6	102.7	132.2
2.60	227.1	233.3	249.6	250.7	304.7	88.6	93.3	138.4	88.0	139.3
2.50	236.3	242.4	258.6	260.2	321.2	78.6	83.6	147.1	76.6	148.4
2.40	246.9	254.4	269.0	271.5	330.1	69.3	74.7	156.9	65.2	158.8
2.30	257.8	269.7	279.5	283.9	338.5	64.0	69.7	166.3	56.9	168.9
2.20	270.4	289.0	291.7	302.3	347.5	67.0	72.8	175.3	55.6	179.0
2.10	290.5	311.2	312.8	342.5	362.5	80.2	86.2	188.7	62.8	194.1
2.00	327.1	346.9	351.0	378.8	393.2	108.9	115.3	213.1	83.5	222.4
1.90	382.8	394.0	396.5	411.8	414.7	168.2	174.9	254.6	132.8	279.8
1.80	485.8	494.4	501.4	506.8	508.4	272.3	280.6	309.9	223.1	373.4
1.70	633.7	646.6	658.8	663.4	667.3	422.6	435.7	446.6	369.2	470.9
1.60	875.7	894.8	900.4	915.2	925.2	622.0	657.4	704.2	604.6	646.0
1.50	1281.9	1287.2	1296.5	1302.6	1308.4	951.2	1002.3	1062.3	944.9	968.8
1.35	2228.3	2269.5	2275.8	2279.9	2284.9	1891.3	1972.2	2009.5	1794.7	1818.0

R(Fe-O)	$1\ ^6A_u$	$2\ ^6A_u$	$3\ ^6A_u$	$4\ ^6A_u$	$5\ ^6A_u$	$6\ ^6A_u$	$7\ ^6A_u$	$8\ ^6A_u$	$9\ ^6A_u$	$10\ ^6A_u$
100.00	3.3	32.0	71.3	71.3	71.3	78.3	80.4	80.4	87.9	87.9
50.00	11.2	39.9	79.2	79.2	79.2	86.2	88.3	88.3	95.8	95.8
20.00	33.2	61.9	101.1	101.1	101.1	108.2	110.3	110.3	117.7	117.7
10.00	64.3	93.1	132.3	132.3	132.3	139.3	141.4	141.4	148.8	148.9
9.00	70.3	99.1	138.2	138.3	138.3	145.3	147.4	147.4	154.8	154.9
8.00	77.4	106.1	145.2	145.3	145.3	152.3	154.4	154.4	161.8	161.9
7.00	85.6	114.4	153.4	153.5	153.5	160.5	162.5	162.6	169.9	170.1
6.00	95.0	123.7	162.6	162.7	162.8	169.7	171.8	171.9	179.1	179.3
5.00	104.9	133.6	172.4	172.5	172.5	179.4	181.6	181.8	188.6	189.2
4.50	109.7	138.2	176.9	177.0	177.0	183.9	186.2	186.4	192.8	193.8
4.00	113.8	142.1	180.7	180.8	180.8	187.6	190.0	190.2	193.2	196.1
3.70	116.0	144.1	181.4	182.3	182.5	182.6	189.4	191.9	192.0	197.3
3.35	118.8	146.4	161.3	183.7	184.5	184.9	191.4	194.0	194.3	198.3
3.00	124.3	132.3	150.6	185.2	188.2	189.5	195.6	198.2	198.9	200.1
2.80	111.4	131.1	155.8	186.6	193.1	195.4	201.3	203.3	204.4	205.0
2.70	99.8	136.4	159.7	187.9	196.9	200.1	205.9	206.5	209.5	209.9
2.60	84.8	143.9	164.8	191.0	202.7	206.7	211.8	212.7	216.9	217.1
2.50	73.0	153.3	170.9	194.2	209.4	214.6	218.0	220.5	225.5	225.9
2.40	61.3	163.8	177.9	201.8	218.4	223.3	226.0	229.6	234.5	236.0
2.30	52.4	173.1	184.9	213.1	226.7	231.5	235.8	239.2	243.1	247.0
2.20	50.6	182.4	193.7	224.2	232.8	240.3	248.0	250.5	255.2	259.6
2.10	56.8	197.5	208.9	237.0	242.1	255.0	265.5	266.5	278.0	283.6
2.00	75.5	226.4	238.0	257.5	260.7	283.5	295.4	296.8	310.7	323.3
1.90	122.4	283.5	294.8	297.6	299.9	341.7	350.7	357.1	368.2	376.8
1.80	212.0	346.9	359.3	375.8	398.9	428.6	433.5	439.4	443.4	445.5
1.70	357.6	446.3	461.9	506.9	549.1	553.6	559.7	569.3	580.4	590.6
1.60	591.5	624.8	641.4	719.4	762.2	768.2	778.6	788.3	815.4	824.9
1.50	922.9	941.9	970.6	1064.3	1103.4	1105.6	1116.8	1162.8	1172.1	1191.5
1.35	1774.7	1791.9	1881.5	1989.5	1998.9	2004.3	2041.2	2052.6	2084.9	2112.3

R(Fe-O)	11 ^6A_u	12 ^6A_u	13 ^6A_u	14 ^6A_u	15 ^6A_u
100.00	91.0	91.0	111.1	140.3	169.7
50.00	98.8	98.8	119.0	148.2	175.7
20.00	120.8	120.8	141.0	170.1	191.4
10.00	151.9	151.9	172.1	201.4	209.5
9.00	157.8	157.9	178.1	207.4	212.1
8.00	164.8	165.0	185.1	214.5	214.6
7.00	172.9	173.2	193.3	216.6	222.9
6.00	182.2	182.7	202.5	216.8	232.4
5.00	192.1	193.0	212.0	212.3	242.7
4.50	196.8	198.2	205.4	216.9	247.7
4.00	197.8	200.8	202.9	220.8	252.0
3.70	199.8	202.6	205.4	222.7	253.8
3.35	202.3	204.0	208.1	225.1	255.0
3.00	206.2	207.6	212.2	229.9	255.7
2.80	210.0	214.3	217.6	235.9	257.3
2.70	213.6	219.6	221.9	240.7	259.3
2.60	219.7	227.1	228.7	247.6	264.4
2.50	227.5	236.2	236.7	255.8	269.8
2.40	238.9	246.1	247.6	265.2	281.8
2.30	251.2	257.4	259.4	274.4	300.7
2.20	265.4	273.7	274.1	285.9	325.0
2.10	286.7	296.2	298.3	314.9	361.2
2.00	328.5	340.4	345.7	383.5	389.6
1.90	384.0	386.2	398.3	407.9	416.9
1.80	460.6	468.4	485.3	493.2	510.8
1.70	600.6	614.1	629.7	635.4	654.6
1.60	832.5	849.5	862.2	867.3	870.5
1.50	1201.5	1207.8	1220.9	1228.3	1238.9
1.35	2119.8	2129.0	2144.0	2155.2	2207.4

R(Fe-O)	$1\,^8B_{3u}$	$2\,^8B_{3u}$	$1\,^8B_{2u}$	$1\,^8B_{1u}$	$2\,^8B_{1u}$	$3\,^8B_{1u}$	$1\,^8B_{2g}$	$1\,^8A_u$
10.00	28.0	243.4	28.0	28.0	28.1	96.3	243.4	28.1
9.00	34.0	246.0	34.0	33.9	34.1	102.3	246.0	34.1
8.00	41.0	248.6	41.0	40.9	41.2	109.3	248.6	41.2
7.00	49.1	250.6	49.1	49.0	49.4	117.5	250.6	49.4
6.00	58.3	250.8	58.3	58.2	58.8	126.8	250.8	58.8
5.00	68.1	246.2	68.1	67.8	68.8	136.5	246.2	68.8
4.50	72.6	239.8	72.6	72.2	73.6	141.2	239.8	73.5
4.00	76.4	227.9	76.4	75.8	78.0	145.3	227.9	77.7
3.70	78.2	216.9	78.2	77.5	80.3	147.8	216.9	80.0
3.35	80.4	199.2	80.5	79.6	83.5	152.2	199.1	82.8
3.00	84.7	176.7	85.0	84.1	90.0	162.6	176.6	88.2
2.80	90.3	163.8	91.0	90.6	97.9	175.8	163.4	94.9
2.70	94.8	158.5	95.9	96.0	104.1	186.0	157.9	100.1
2.60	100.9	155.1	102.5	103.5	112.5	199.5	153.9	107.2
2.50	108.6	154.8	111.4	113.6	123.6	217.2	152.6	116.6
2.40	117.8	159.5	122.5	126.5	137.6	239.9	155.6	128.2
2.30	126.8	170.6	133.9	140.7	153.0	268.0	164.5	140.3
2.20	133.6	184.1	143.6	154.4	167.9	300.6	175.4	150.6
2.10	142.2	195.6	158.0	174.5	189.2	328.1	181.5	165.6
2.00	159.3	217.5	186.7	211.0	227.0	354.3	192.3	195.0
1.90	193.8	265.0	238.9	273.8	291.1	395.9	222.4	247.8
1.80	260.9	352.2	327.9	377.4	396.1	471.6	288.0	337.6
1.70	383.5	499.0	474.2	543.5	563.5	604.7	410.8	484.6

R(Fe-O)	$1\,^4A_g$	$2\,^4A_g$	$3\,^4A_g$	$4\,^4A_g$	$1\,^4B_{3u}$	$2\,^4B_{3u}$	$3\,^4B_{3u}$	$4\,^4B_{3u}$	$5\,^4B_{3u}$
9.00	46.5	46.7	88.6	88.6	20.2	46.5	88.6	88.6	88.6
8.00	53.4	53.7	95.6	95.6	27.2	53.5	95.5	95.6	95.7
7.00	61.5	61.9	103.8	103.8	35.4	61.6	103.7	103.8	103.8
6.00	70.7	71.3	113.0	113.1	44.6	70.8	112.9	113.1	113.1
5.00	80.2	81.2	122.7	122.9	54.3	80.4	122.6	122.8	122.9
4.50	84.6	85.8	127.3	127.5	58.9	84.7	127.1	127.4	127.5
4.00	88.3	89.9	131.1	131.4	62.7	88.2	130.8	131.2	131.4
3.70	90.2	92.0	133.1	133.4	64.6	89.8	132.6	133.1	133.3
3.35	96.0	96.2	98.4	140.4	71.6	94.8	96.2	98.9	139.6
3.00	43.0	106.9	108.0	109.2	43.9	47.9	104.6	108.7	109.4
2.80	21.8	84.3	85.5	87.5	16.9	28.3	83.7	86.8	96.1
2.70	10.8	73.6	74.3	76.7	6.9	18.8	73.5	76.5	85.7
2.60	-0.4	62.1	63.5	65.8	-2.8	9.7	63.5	66.4	75.6
2.50	-11.1	50.6	53.0	55.4	-11.4	1.7	54.5	57.0	66.2
2.40	-20.4	40.1	43.2	45.8	-17.7	-4.0	47.5	49.5	58.8
2.30	-26.9	31.7	34.5	37.1	-20.0	-5.5	44.4	45.4	55.0
2.20	-25.3	-5.0	-4.2	6.0	-10.7	9.3	55.2	56.1	66.2
2.10	-35.0	-29.2	-28.6	-9.5	8.5	31.7	72.2	73.3	83.9
2.00	-35.6	-32.1	-31.5	-10.5	42.3	66.9	98.9	103.3	114.5
1.90	-12.9	-10.1	-9.4	12.0	101.6	127.2	147.0	154.2	169.2
1.80	46.3	48.7	49.6	70.8	201.3	228.2	230.7	239.5	261.7
1.70	162.7	164.7	165.8	186.6	362.0	370.1	379.7	391.6	410.6

R(Fe-O)	$1\,^4B_{2u}$	$2\,^4B_{2u}$	$3\,^4B_{2u}$	$4\,^4B_{2u}$	$5\,^4B_{2u}$	$1\,^4B_{1g}$	$2\,^4B_{1g}$	$3\,^4B_{1g}$	$4\,^4B_{1g}$
9.00	20.2	46.5	88.6	88.6	88.6	46.7	88.6	88.6	88.6
8.00	27.2	53.5	95.5	95.6	95.7	53.7	95.6	95.6	95.7
7.00	35.4	61.6	103.7	103.8	103.8	61.9	103.8	103.8	103.9
6.00	44.6	70.8	112.9	113.1	113.1	71.3	113.0	113.1	113.1
5.00	54.3	80.4	122.6	122.8	122.9	81.1	122.7	122.9	122.9
4.50	58.9	84.8	127.1	127.4	127.5	85.7	127.3	127.4	127.5
4.00	62.7	88.3	130.8	131.3	131.4	89.7	131.1	131.3	131.3
3.70	64.6	89.9	132.6	133.1	133.3	91.6	132.9	133.1	133.1
3.35	71.6	94.7	97.7	139.6	140.1	95.9	97.0	139.6	140.1
3.00	45.6	104.8	107.8	108.1	108.9	43.2	106.9	108.1	109.2
2.80	24.4	82.7	85.4	86.3	92.0	22.1	84.3	85.6	87.6
2.70	13.8	71.9	74.5	75.2	81.8	11.0	73.3	74.7	76.9
2.60	3.1	61.0	63.6	63.9	71.6	-0.1	61.5	64.1	66.2
2.50	-6.8	50.6	52.9	53.1	61.8	-10.7	49.5	53.9	56.1
2.40	-15.1	41.4	43.4	43.7	53.6	-19.9	38.0	44.6	47.5
2.30	-20.0	34.1	36.8	37.3	48.9	-26.3	27.1	36.9	41.8
2.20	-9.5	41.6	43.6	44.4	58.6	-24.3	-14.0	1.2	19.6
2.10	6.8	52.8	54.2	57.6	74.1	-43.9	-34.5	-15.2	-2.4
2.00	33.6	71.8	73.5	82.4	100.3	-53.6	-37.9	-18.4	-0.7
1.90	82.7	109.6	111.9	129.3	148.0	-41.2	-20.1	0.5	26.5
1.80	168.6	179.6	182.2	212.0	231.3	4.0	28.8	56.5	89.5
1.70	300.4	302.8	311.6	349.7	370.2	100.8	127.1	171.0	207.6

R(Fe-O)	$1\,^4B_{1u}$	$2\,^4B_{1u}$	$3\,^4B_{1u}$	$4\,^4B_{1u}$	$5\,^4B_{1u}$	$6\,^4B_{1u}$	$1\,^4B_{2g}$	$2\,^4B_{2g}$	$3\,^4B_{2g}$	$4\,^4B_{2g}$
9.00	20.2	20.3	46.5	46.7	88.6	88.6	46.5	88.6	88.6	88.6
8.00	27.2	27.4	53.4	53.7	95.6	95.6	53.5	95.5	95.6	95.7
7.00	35.3	35.6	61.5	61.9	103.8	103.8	61.6	103.7	103.8	103.8
6.00	44.5	45.0	70.7	71.3	113.0	113.1	70.8	112.9	113.1	113.1
5.00	54.1	55.0	80.2	81.2	122.7	122.9	80.4	122.6	122.8	122.9
4.50	58.6	59.7	84.6	85.8	127.3	127.5	84.7	127.0	127.4	127.5
4.00	62.3	64.0	88.3	89.9	131.1	131.4	88.3	130.8	131.2	131.3
3.70	64.2	66.4	90.2	92.0	133.1	133.4	89.9	132.6	133.0	133.3
3.35	71.4	74.6	96.1	96.1	98.3	140.6	94.9	96.1	98.8	139.4
3.00	43.1	104.3	106.9	108.1	109.2	109.9	43.7	47.7	108.7	109.4
2.80	21.5	83.8	85.1	87.1	92.2	95.5	17.1	28.5	84.3	87.3
2.70	10.6	73.0	74.0	76.4	81.2	85.3	7.0	18.9	74.1	76.9
2.60	-0.5	61.5	63.3	65.8	70.3	75.3	-2.9	9.6	64.2	66.7
2.50	-10.9	50.0	53.2	55.7	60.3	65.9	-11.9	1.2	55.2	57.1
2.40	-19.7	39.5	44.5	47.3	52.3	57.9	-18.9	-5.1	47.9	49.1
2.30	-25.2	31.4	38.5	42.0	47.9	52.9	-22.5	-7.9	41.2	45.4
2.20	-15.6	37.1	47.3	50.7	57.0	63.7	-20.3	-9.6	-0.8	4.0
2.10	-0.3	46.5	60.9	65.6	71.6	79.4	-36.9	-31.5	-16.0	-9.6
2.00	25.9	64.6	83.5	91.0	96.4	105.3	-46.3	-36.2	-14.6	-8.8
1.90	74.5	101.6	125.0	138.4	143.0	153.1	-33.7	-18.7	4.4	22.2
1.80	159.8	170.5	198.2	221.6	225.7	236.8	11.6	30.6	60.6	89.8
1.70	289.8	302.2	321.4	360.7	364.6	376.0	108.2	129.9	175.1	211.2

R(Fe-O)	$1\,^4B_{3g}$	$2\,^4B_{3g}$	$3\,^4B_{3g}$	$4\,^4B_{3g}$	$1\,^4A_u$	$2\,^4A_u$	$3\,^4A_u$	$4\,^4A_u$	$5\,^4A_u$
9.00	46.5	88.6	88.6	88.6	20.3	46.7	88.6	88.6	88.6
8.00	53.5	95.5	95.6	95.7	27.4	53.7	95.6	95.6	95.7
7.00	61.6	103.7	103.8	103.8	35.6	61.9	103.8	103.8	103.9
6.00	70.8	112.9	113.1	113.1	45.0	71.3	113.0	113.1	113.1
5.00	80.4	122.6	122.8	122.9	54.9	81.1	122.7	122.9	122.9
4.50	84.8	127.0	127.4	127.5	59.7	85.7	127.3	127.5	127.5
4.00	88.3	130.8	131.2	131.3	63.8	89.6	131.1	131.3	131.3
3.70	89.9	132.6	133.1	133.3	66.0	91.6	133.0	133.2	133.2
3.35	94.8	97.6	139.4	139.9	73.4	96.0	96.9	139.8	140.3
3.00	45.5	107.7	108.1	108.9	43.3	106.9	107.8	108.1	109.2
2.80	24.7	83.3	85.8	86.7	21.8	83.8	85.1	87.2	92.2
2.70	13.9	72.5	74.9	75.5	10.9	72.9	74.1	76.5	81.3
2.60	3.1	61.7	63.7	64.2	0.0	61.4	63.4	65.8	70.4
2.50	-7.2	51.1	52.6	53.3	-10.3	50.0	53.4	55.8	60.4
2.40	-16.1	40.7	42.8	43.9	-18.9	39.5	44.6	47.4	52.5
2.30	-22.3	30.7	33.9	38.2	-24.2	31.5	38.7	41.9	47.9
2.20	-21.0	-7.5	0.0	15.8	-14.8	36.9	47.6	51.5	57.6
2.10	-39.3	-33.7	-16.4	-4.3	0.7	46.6	61.1	65.9	72.0
2.00	-48.7	-38.5	-19.8	-1.9	27.3	64.8	83.5	91.2	97.0
1.90	-36.2	-21.6	-0.3	26.3	76.3	102.0	125.0	138.3	143.7
1.80	9.0	26.8	56.3	90.6	162.0	171.4	198.2	221.3	226.7
1.70	105.8	125.2	171.1	209.5	291.4	304.9	321.6	359.8	365.7

R(Fe-O)	$1\,^2A_g$	$2\,^2A_g$	$1\,^2B_{3u}$	$2\,^2B_{3u}$	$3\,^2B_{3u}$	$4\,^2B_{3u}$	$5\,^2B_{3u}$	$6\,^2B_{3u}$	$7\,^2B_{3u}$	$8\,^2B_{3u}$	$9\,^2B_{3u}$	$10\,^2B_{3u}$
1.70	159.6	178.8	244.5	365.8	373.8	375.3	385.3	390.9	405.0	407.9	422.4	433.5
1.80	65.2	84.0	143.4	224.5	232.0	236.7	246.2	250.9	254.7	262.9	266.6	275.3
1.90	21.2	39.2	87.9	139.3	145.8	153.4	161.3	162.6	165.3	166.9	177.5	178.8
2.00	8.3	26.9	60.3	89.8	94.5	105.8	106.0	108.3	114.7	118.4	119.7	121.1
2.10	19.0	35.2	45.9	59.3	62.1	72.2	75.3	78.2	84.6	85.6	86.3	89.6
2.20	24.2	35.0	46.9	48.0	48.8	58.7	62.2	68.8	69.8	70.3	76.3	79.3
2.30	31.2	38.6	45.5	46.2	54.5	56.0	60.0	66.0	66.3	68.7	75.7	76.8
2.40	40.8	45.8	48.5	50.2	59.6	63.9	65.5	68.9	69.2	74.0	80.4	80.6
2.50	52.0	55.1	55.4	57.7	67.0	71.5	75.7	76.2	77.9	82.3	88.0	88.4
2.60	63.7	65.6	64.3	67.0	76.3	80.8	84.7	85.4	90.8	92.1	97.6	97.8
2.70	75.3	76.4	74.2	77.1	86.4	91.0	94.7	95.5	102.6	103.6	107.9	108.2
2.80	86.2	87.6	84.4	87.4	96.7	101.4	104.9	105.8	113.1	115.7	118.1	118.9

R(Fe-O)	$1\,^2B_{2u}$	$2\,^2B_{2u}$	$3\,^2B_{2u}$	$4\,^2B_{2u}$	$5\,^2B_{2u}$	$6\,^2B_{2u}$	$7\,^2B_{2u}$	$8\,^2B_{2u}$	$9\,^2B_{2u}$	$10\,^2B_{2u}$	$1\,^2B_{1g}$	$2\,^2B_{1g}$
1.70	289.7	298.2	313.6	339.4	348.8	363.6	371.4	378.9	389.1	410.4	119.2	161.9
1.80	168.0	176.0	193.4	208.6	218.1	223.2	229.1	240.5	247.9	267.5	44.0	68.0
1.90	97.4	104.4	123.9	124.2	138.7	142.9	146.0	157.7	161.0	176.2	13.7	24.4
2.00	58.7	64.7	76.0	86.1	90.1	92.9	104.1	107.6	111.1	118.6	12.3	13.7
2.10	36.6	41.8	48.5	60.9	62.6	64.6	74.1	78.1	82.0	84.4	23.9	36.4
2.20	31.7	35.8	38.6	50.5	51.5	60.1	60.7	65.9	69.2	74.3	26.3	36.1
2.30	34.9	37.9	38.5	49.5	50.4	58.5	60.6	63.9	68.4	69.3	32.1	39.4
2.40	42.2	44.2	44.6	54.3	55.1	61.9	63.1	70.1	72.0	74.5	41.2	46.4
2.50	51.5	53.6	53.8	62.4	63.2	67.6	71.4	76.4	82.5	82.6	52.1	55.6
2.60	61.8	64.3	64.5	72.2	73.2	75.9	81.6	85.1	92.3	94.0	63.8	65.8
2.70	72.6	75.1	75.7	82.4	83.9	85.7	92.5	94.9	102.7	105.8	75.4	76.5
2.80	83.4	85.9	86.8	92.6	94.7	96.2	103.5	105.1	113.2	117.2	86.3	87.6

R(Fe-O)	$3\,^2B_{1g}$	$1\,^2B_{1u}$	$2\,^2B_{1u}$	$3\,^2B_{1u}$	$4\,^2B_{1u}$	$5\,^2B_{1u}$	$6\,^2B_{1u}$	$7\,^2B_{1u}$	$1\,^2B_{2g}$	$2\,^2B_{2g}$	$3\,^2B_{2g}$	$1\,^2B_{3g}$
1.70	165.6	289.5	308.7	314.7	352.7	355.4	358.2	369.4	108.4	176.5	184.2	115.6
1.80	70.8	167.0	189.0	189.8	214.5	217.7	227.3	228.7	33.8	82.4	88.9	40.7
1.90	26.6	95.9	115.1	120.3	129.9	134.1	143.4	150.3	4.0	38.4	43.6	10.7
2.00	16.4	56.9	72.5	81.7	83.0	86.6	94.5	104.6	3.4	28.8	31.9	10.7
2.10	38.7	34.7	46.9	53.1	59.3	61.9	65.4	72.6	32.9	45.7	48.4	27.5
2.20	39.5	29.8	38.8	43.2	49.8	54.7	58.0	58.2	43.1	44.1	45.6	29.4
2.30	42.6	33.1	39.5	42.9	49.0	53.8	55.3	59.1	44.2	46.4	53.8	34.5
2.40	49.2	40.9	45.4	48.2	53.4	58.8	59.3	62.7	48.7	51.4	60.6	42.6
2.50	58.1	51.2	54.1	56.5	61.2	66.7	66.9	70.4	56.3	59.3	68.5	52.4
2.60	68.3	62.4	64.1	66.4	71.2	75.9	76.5	80.3	65.7	68.8	78.0	63.2
2.70	79.0	73.7	74.8	77.0	82.0	85.9	86.8	91.0	75.8	79.0	88.2	74.2
2.80	89.7	84.4	85.8	87.7	92.8	96.1	97.2	101.9	86.2	89.4	98.6	85.2

R(Fe-O)	$2\,^2B_{3g}$	$3\,^2B_{3g}$	$1\,^2A_u$	$2\,^2A_u$	$3\,^2A_u$	$4\,^2A_u$	$5\,^2A_u$	$6\,^2A_u$	$7\,^2A_u$	$8\,^2A_u$	$9\,^2A_u$	$10\,^2A_u$
1.70	170.5	177.6	286.2	309.1	312.2	352.6	356.8	358.2	371.1	379.9	385.5	401.2
1.80	75.6	82.4	164.6	187.6	189.6	216.2	217.8	226.9	229.8	240.1	249.1	261.0
1.90	31.0	37.7	94.0	113.9	120.3	131.6	134.3	144.5	150.3	155.2	166.2	168.4
2.00	17.4	25.2	55.5	71.8	82.6	82.9	86.6	95.0	104.7	105.5	108.6	120.0
2.10	32.0	34.0	33.7	46.4	53.3	58.6	62.0	65.6	72.2	75.2	78.7	89.6
2.20	33.1	33.4	29.1	38.6	43.4	49.3	54.8	58.0	58.1	61.5	70.0	74.8
2.30	37.1	37.7	32.6	39.5	43.0	48.7	53.9	55.5	58.6	62.1	68.3	70.6
2.40	44.7	45.6	40.6	45.4	48.2	53.2	58.8	59.5	62.3	69.3	70.7	76.7
2.50	54.8	55.4	50.9	54.1	56.4	61.1	66.8	67.1	70.2	75.1	81.5	85.7
2.60	65.8	66.3	62.2	64.2	66.4	71.1	76.0	76.5	80.2	83.7	93.3	96.2
2.70	77.0	77.6	73.6	74.8	77.0	81.9	86.0	86.8	91.0	93.7	105.3	107.2
2.80	87.9	88.7	84.4	85.8	87.7	92.8	96.1	97.2	101.8	104.1	116.9	117.8

Table S4. Fully optimized geometries (C_1 symmetry) of the $Fe^{2+}(H_2O)_6$ – $Fe^{3+}(H_2O)_6$ complex for different Fe–Fe distances (R). The optimal geometries under D_{2d} symmetry are also listed.

	x (bohr)	y (bohr)	z (bohr)	x (Å)	y (Å)	z (Å)
			R = 10.0 Å			
Atom		C_1			D_{2d}	
Fe	–9.51374	–0.00042	0.00215	0.00000	0.00000	5.00000
Fe	9.38351	–0.01165	0.00868	0.00000	0.00000	–5.00000
O	–7.33191	–0.43383	3.18482	2.13396	0.00000	5.08224
O	–7.45993	3.06656	–1.20537	0.00000	1.60579	3.62092
O	–7.35113	–2.48731	–2.05109	0.00000	–1.60579	3.62092
O	–11.85881	2.45769	1.94051	0.00000	1.48783	6.53247
O	–11.74650	–2.96044	1.24599	0.00000	–1.48783	6.53247
O	–11.86906	0.35209	–3.10069	–2.13396	0.00000	5.08224
O	11.55460	–0.55961	3.54541	0.00000	–2.13396	–5.08224
O	7.21431	–3.48489	0.72358	–1.60579	0.00000	–3.62092
O	7.04052	2.73575	2.00415	1.60579	0.00000	–3.62092
O	12.15089	–2.59580	–1.82103	–1.48783	0.00000	–6.53247
O	12.11258	3.12240	–0.86437	1.48783	0.00000	–6.53247
O	7.64016	0.82110	–3.64018	0.00000	2.13396	–5.08224
H	–6.02766	0.65968	3.78235	2.74231	0.00000	4.34896
H	–7.63374	–1.65343	4.48501	2.68407	0.00000	5.86016
H	–6.15025	3.09815	–2.44553	0.76264	2.03621	3.25128
H	–7.83591	4.78682	–0.79435	–0.76264	2.03621	3.25128
H	–5.99531	–3.51964	–1.46014	0.76264	–2.03621	3.25128
H	–7.70330	–3.00133	–3.74849	–0.76264	–2.03621	3.25128
H	–11.75179	2.96743	3.67155	0.75649	1.89055	6.94728
H	–13.35478	3.23245	1.28085	–0.75649	1.89055	6.94728
H	–13.20890	–2.81046	2.30059	0.75649	–1.89055	6.94728
H	–11.61853	–4.71049	0.81164	–0.75649	–1.89055	6.94728
H	–11.81224	1.60398	–4.40361	–2.74231	0.00000	4.34896
H	–13.32408	–0.66614	–3.44616	–2.68407	0.00000	5.86016
H	13.04632	0.36850	3.91557	0.00000	–2.74231	–4.34896
H	11.44774	–1.83293	4.80360	0.00000	–2.68407	–5.86016
H	6.38733	–3.95648	2.23964	–2.03621	–0.76264	–3.25128
H	7.72472	–5.01238	–0.06851	–2.03621	0.76264	–3.25128
H	6.39651	4.25730	1.31155	2.03621	–0.76264	–3.25128
H	7.32951	3.04693	3.74773	2.03621	0.76264	–3.25128
H	12.44929	–2.85813	–3.57046	–1.89055	–0.75649	–6.94728
H	13.47168	–3.45767	–0.96320	–1.89055	0.75649	–6.94728
H	13.59102	2.88784	–1.85485	1.89055	–0.75649	–6.94728
H	12.24804	4.77624	–0.18383	1.89055	0.75649	–6.94728
H	6.57757	–0.20533	–4.65073	0.00000	2.74231	–4.34896

H	8.36697	2.04323	–4.73554	0.00000	2.68407	–5.86016

R = 9.0 Å

Atom		C_1			D_{2d}	
Fe	–8.42800	–0.01544	0.01081	0.00000	0.00000	4.50000
Fe	8.57952	0.00076	0.00036	0.00000	0.00000	–4.50000
O	–6.78637	1.50757	–3.46427	2.13362	0.00000	4.59388
O	–6.20593	–3.54629	0.17963	0.00000	1.63055	3.15043
O	–6.19070	2.43253	2.46221	0.00000	–1.63055	3.15043
O	–11.14471	–2.30007	–2.23923	0.00000	1.47997	6.04465
O	–11.26143	3.16264	–0.36071	0.00000	–1.47997	6.04465
O	–10.60637	–1.21498	3.38360	–2.13362	0.00000	4.59388
O	10.93236	0.86882	–3.00492	0.00000	–2.13362	–4.59388
O	6.46176	3.16835	–0.74452	–1.63055	0.00000	–3.15043
O	6.50122	–2.21497	–2.41757	1.63055	0.00000	–3.15043
O	10.86569	2.20482	2.28783	–1.47997	0.00000	–6.04465
O	10.90057	–3.04833	0.79719	1.47997	0.00000	–6.04465
O	6.43418	–0.97398	3.08561	0.00000	2.13362	–4.59388
H	–5.86850	0.67251	–4.75487	2.74670	0.00000	3.86439
H	–7.56091	2.93294	–4.23474	2.68026	0.00000	5.37440
H	–5.62445	–4.34991	1.67102	0.76333	2.06688	2.78929
H	–6.67007	–4.86880	–0.94261	–0.76333	2.06688	2.78929
H	–5.71008	4.11270	2.06314	0.76333	–2.06688	2.78929
H	–6.52898	2.40842	4.22564	–0.76333	–2.06688	2.78929
H	–11.45707	–2.26561	–4.00600	0.75607	1.88049	6.46268
H	–12.45854	–3.29935	–1.53151	–0.75607	1.88049	6.46268
H	–12.72762	3.03993	–1.38985	0.75607	–1.88049	6.46268
H	–11.48048	4.66414	0.59647	–0.75607	–1.88049	6.46268
H	–10.54649	–2.70231	4.38453	–2.74670	0.00000	3.86439
H	–12.09003	–0.34540	3.90193	–2.68026	0.00000	5.37440
H	12.41159	–0.05548	–3.48668	0.00000	–2.74670	–3.86439
H	10.86044	2.30291	–4.10345	0.00000	–2.68026	–5.37440
H	5.18840	3.37313	–2.00527	–2.06688	–0.76333	–2.78929
H	6.81088	4.81250	–0.07721	–2.06688	0.76333	–2.78929
H	5.20901	–3.40037	–1.99603	2.06688	–0.76333	–2.78929
H	6.88478	–2.45574	–4.16847	2.06688	0.76333	–2.78929
H	10.76321	2.43947	4.07748	–1.88049	–0.75607	–6.46268
H	12.34067	3.10448	1.74968	–1.88049	0.75607	–6.46268
H	12.36044	–3.01129	1.86581	1.88049	–0.75607	–6.46268
H	10.83393	–4.71547	0.10094	1.88049	0.75607	–6.46268
H	5.12743	–0.01121	3.87161	0.00000	2.74670	–3.86439
H	6.79085	–2.36944	4.17918	0.00000	2.68026	–5.37440

R = 8.0 Å

Atom		C_1			D_{2d}	
Fe	–7.65607	0.00189	–0.00402	0.00000	0.00000	4.00000
Fe	7.46173	0.01674	–0.01033	0.00000	0.00000	–4.00000

O	–6.03679	–0.02060	–3.53489	2.13280	0.00000	4.10989
O	–5.60898	–3.08685	1.16127	0.00000	1.66351	2.69011
O	–5.11717	2.59456	1.38247	0.00000	–1.66351	2.69011
O	–10.40060	–2.49754	–1.27555	0.00000	1.47045	5.56030
O	–9.98493	2.92147	–1.19719	0.00000	–1.47045	5.56030
O	–9.47065	0.10779	3.46698	–2.13280	0.00000	4.10989
O	9.48799	0.10421	–3.69691	0.00000	–2.13280	–4.10989
O	5.58974	3.59430	–0.99101	–1.66351	0.00000	–2.69011
O	5.18656	–3.00899	–1.64814	1.66351	0.00000	–2.69011
O	10.42452	2.66690	1.43215	–1.47045	0.00000	–5.56030
O	10.24053	–3.01933	1.09810	1.47045	0.00000	–5.56030
O	5.98966	–0.41412	3.84134	0.00000	2.13280	–4.10989
H	–5.02037	–1.32169	–4.26450	2.75233	0.00000	3.38564
H	–6.53910	1.06377	–4.89345	2.67461	0.00000	4.89397
H	–4.29979	–3.14716	2.39973	0.76406	2.10776	2.34029
H	–6.14994	–4.79304	0.89580	–0.76406	2.10776	2.34029
H	–4.14099	3.76195	0.41373	0.76406	–2.10776	2.34029
H	–5.20367	3.25726	3.06278	–0.76406	–2.10776	2.34029
H	–10.64943	–3.11982	–2.95557	0.75553	1.86819	5.98234
H	–11.79835	–3.11956	–0.30837	–0.75553	1.86819	5.98234
H	–11.60326	2.69885	–1.97723	0.75553	–1.86819	5.98234
H	–9.78434	4.70544	–0.98357	–0.75553	–1.86819	5.98234
H	–9.42364	–1.11786	4.79572	–2.75233	0.00000	3.38564
H	–10.76891	1.28253	3.92667	–2.67461	0.00000	4.89397
H	10.96465	–0.87396	–3.99828	0.00000	–2.75233	–3.38564
H	9.37578	1.24278	–5.07966	0.00000	–2.67461	–4.89397
H	4.64363	4.05666	–2.46291	–2.10776	–0.76406	–2.34029
H	6.28497	5.11397	–0.33180	–2.10776	0.76406	–2.34029
H	4.64732	–4.49775	–0.80502	2.10776	–0.76406	–2.34029
H	5.51435	–3.47137	–3.35291	2.10776	0.76406	–2.34029
H	10.81608	3.11280	3.12659	–1.86819	–0.75553	–5.98234
H	11.73630	3.37538	0.42944	–1.86819	0.75553	–5.98234
H	11.78369	–2.62627	1.92906	1.86819	–0.75553	–5.98234
H	10.36633	–4.75617	0.66400	1.86819	0.75553	–5.98234
H	5.07185	0.71326	4.89182	0.00000	2.75233	–3.38564
H	6.83090	–1.55875	4.94184	0.00000	2.67461	–4.89397

R = 7.0 Å

Atom		C_1			D_{2d}	
Fe	6.69060	0.00204	–0.01265	0.00000	0.00000	3.50000
Fe	–6.53749	0.00276	–0.01426	0.00000	0.00000	–3.50000
O	4.94133	1.06121	–3.31245	2.13165	0.00000	3.62992
O	4.30998	2.04342	2.26991	0.00000	1.70802	2.24586
O	4.65532	–3.29111	0.27818	0.00000	–1.70802	2.24586
O	8.97231	3.18333	–0.19802	0.00000	1.45753	5.08232
O	9.35209	–1.87023	–2.20435	0.00000	–1.45753	5.08232
O	8.72061	–1.14608	3.13810	–2.13165	0.00000	3.62992

O	–9.14079	0.13929	–3.32167	0.00000	–2.13165	–3.62992
O	–4.64779	–3.33523	–1.66372	–1.70802	0.00000	–2.24586
O	–4.45298	3.15041	–1.80329	1.70802	0.00000	–2.24586
O	–9.21314	–2.88702	1.56415	–1.45753	0.00000	–5.08232
O	–9.05269	2.93040	1.69221	1.45753	0.00000	–5.08232
O	–4.43474	0.01527	3.62642	0.00000	2.13165	–3.62992
H	3.70928	2.35481	–3.55838	2.75930	0.00000	2.91241
H	5.53357	0.58716	–4.95572	2.66751	0.00000	4.41835
H	2.97789	1.42638	3.31442	0.76475	2.16319	1.91165
H	4.64607	3.74445	2.78564	–0.76475	2.16319	1.91165
H	3.57591	–4.02936	–0.96368	0.76475	–2.16319	1.91165
H	4.97667	–4.56575	1.52092	–0.76475	–2.16319	1.91165
H	9.04064	4.44031	–1.49685	0.75483	1.85128	5.50978
H	10.32655	3.57382	0.93838	–0.75483	1.85128	5.50978
H	10.87912	–1.14320	–2.85027	0.75483	–1.85128	5.50978
H	9.39922	–3.61515	–2.67752	–0.75483	–1.85128	5.50978
H	8.48611	–0.68411	4.87028	–2.75930	0.00000	2.91241
H	10.23421	–2.13849	3.09245	–2.66751	0.00000	4.41835
H	–10.64738	1.11998	–3.28677	0.00000	–2.75930	–2.91241
H	–9.25368	–0.83360	–4.82663	0.00000	–2.66751	–4.41835
H	–4.44119	–3.58734	–3.42817	–2.16319	–0.76475	–1.91165
H	–5.20368	–4.92092	–1.02222	–2.16319	0.76475	–1.91165
H	–4.30752	4.77683	–1.05796	2.16319	–0.76475	–1.91165
H	–4.90389	3.45720	–3.51701	2.16319	0.76475	–1.91165
H	–9.54821	–3.41807	3.24666	–1.85128	–0.75483	–5.50978
H	–10.55958	–3.56741	0.58608	–1.85128	0.75483	–5.50978
H	–10.38463	2.48524	2.81442	1.85128	–0.75483	–5.50978
H	–9.37619	4.64026	1.24783	1.85128	0.75483	–5.50978
H	–4.24596	–1.46675	4.62194	0.00000	2.75930	–2.91241
H	–4.97025	1.28955	4.77808	0.00000	2.66751	–4.41835

R = 6.5 Å

Atom		C_1			D_{2d}	
Fe	6.18768	–0.03589	–0.00464	0.00000	0.00000	3.25000
Fe	–6.09553	–0.02197	0.00019	0.00000	0.00000	–3.25000
O	4.37656	–3.01301	1.71033	2.13076	0.00000	3.39326
O	5.79202	–1.69780	–3.50377	0.00000	1.73498	2.03093
O	3.04977	2.18846	–0.44561	0.00000	–1.73498	2.03093
O	9.58000	–1.99490	0.32483	0.00000	1.44978	4.84624
O	6.95026	1.49169	3.50779	0.00000	–1.44978	4.84624
O	8.22812	2.88657	–1.64877	–2.13076	0.00000	3.39326
O	–5.07676	–2.55989	3.14119	0.00000	–2.13076	–3.39326
O	–2.84195	3.05393	0.50532	–1.73498	0.00000	–2.03093
O	–4.29951	–2.36724	–2.84102	1.73498	0.00000	–2.03093
O	–8.16407	2.37430	2.64876	–1.44978	0.00000	–4.84624
O	–9.60593	–2.46289	–0.29061	1.44978	0.00000	–4.84624
O	–7.80204	2.19247	–3.11730	0.00000	2.13076	–3.39326

H	3.91150	–4.56818	0.91798	2.76374	0.00000	2.68027
H	4.32866	–3.30081	3.49431	2.66260	0.00000	4.18456
H	4.62906	–1.31320	–4.82898	0.76505	2.19680	1.70643
H	6.98027	–2.87448	–4.19847	–0.76505	2.19680	1.70643
H	1.32278	1.95469	0.03795	0.76505	–2.19680	1.70643
H	3.19262	3.84354	–1.15340	–0.76505	–2.19680	1.70643
H	9.87880	–3.62294	1.05425	0.75440	1.84103	5.27700
H	11.20020	–1.39741	–0.21844	–0.75440	1.84103	5.27700
H	8.42100	1.10019	4.48914	0.75440	–1.84103	5.27700
H	6.09466	2.80969	4.39833	–0.75440	–1.84103	5.27700
H	8.70457	3.04331	–3.38738	–2.76374	0.00000	2.68027
H	9.10536	4.20676	–0.77483	–2.66260	0.00000	4.18456
H	–6.08215	–4.04638	3.28274	0.00000	–2.76374	–2.68027
H	–4.50207	–2.22705	4.80766	0.00000	–2.66260	–4.18456
H	–3.08653	4.41174	–0.65015	–2.19680	–0.76505	–1.70643
H	–3.11389	3.81050	2.11813	–2.19680	0.76505	–1.70643
H	–4.70166	–2.03072	–4.56294	2.19680	–0.76505	–1.70643
H	–4.20913	–4.15718	–2.70544	2.19680	0.76505	–1.70643
H	–9.25271	3.70941	2.12730	–1.84103	–0.75440	–5.27700
H	–8.64546	2.00501	4.34162	–1.84103	0.75440	–5.27700
H	–11.04685	–2.28858	0.77120	1.84103	–0.75440	–5.27700
H	–10.08648	–3.69284	–1.50965	1.84103	0.75440	–5.27700
H	–7.49656	3.72759	–3.99781	0.00000	2.76374	–2.68027
H	–9.43394	1.66802	–3.66657	0.00000	2.66260	–4.18456

R = 6.0 Å

Atom		C_1			D_{2d}	
Fe	–5.69587	0.02896	0.00817	0.00000	0.00000	3.00000
Fe	5.64244	0.05897	–0.00192	0.00000	0.00000	–3.00000
O	–2.59827	–1.70539	–1.47507	2.12963	0.00000	3.15964
O	–4.13369	0.84037	3.47397	0.00000	1.76587	1.82267
O	–4.79579	3.55363	–1.37718	0.00000	–1.76587	1.82267
O	–7.03001	–3.34575	1.47598	0.00000	1.44092	4.61300
O	–7.55039	–0.80794	–3.35317	0.00000	–1.44092	4.61300
O	–9.06738	1.64672	1.25068	–2.12963	0.00000	3.15964
O	7.52463	–2.63467	–2.51385	0.00000	–2.12963	–3.15964
O	4.20998	2.22723	–3.28180	–1.76587	0.00000	–1.82267
O	2.47147	–3.24283	0.08530	1.76587	0.00000	–1.82267
O	9.01110	2.64008	–0.25336	–1.44092	0.00000	–4.61300
O	7.67317	–1.85975	3.12604	1.44092	0.00000	–4.61300
O	3.98074	2.51994	2.83218	0.00000	2.12963	–3.15964
H	–0.98677	–2.12681	–0.74320	2.76907	0.00000	2.45224
H	–2.70126	–2.52770	–3.07882	2.65646	0.00000	3.95446
H	–3.57319	2.45929	4.04374	0.76532	2.23537	1.50965
H	–4.33928	–0.18659	4.94849	–0.76532	2.23537	1.50965
H	–3.50730	4.03372	–2.54337	0.76532	–2.23537	1.50965
H	–5.86641	5.00022	–1.17662	–0.76532	–2.23537	1.50965

H	–6.35348	–5.01455	1.33092	0.75389	1.82916	5.04761
H	–8.62314	–3.52975	2.31718	–0.75389	1.82916	5.04761
H	–8.57052	–2.27006	–3.66707	0.75389	–1.82916	5.04761
H	–7.79325	0.27710	–4.78015	–0.75389	–1.82916	5.04761
H	–9.45159	2.35786	2.86883	–2.76907	0.00000	2.45224
H	–10.60053	1.75492	0.29431	–2.65646	0.00000	3.95446
H	8.76599	–3.77499	–1.87833	0.00000	–2.76907	–2.45224
H	7.86344	–2.51844	–4.27704	0.00000	–2.65646	–3.95446
H	3.89211	1.62758	–4.94443	–2.23537	–0.76532	–1.50965
H	5.00620	3.82518	–3.52196	–2.23537	0.76532	–1.50965
H	2.45204	–4.19580	1.61299	2.23537	–0.76532	–1.50965
H	3.05958	–4.41675	–1.15345	2.23537	0.76532	–1.50965
H	9.63112	3.85618	0.91709	–1.82916	–0.75389	–5.04761
H	10.30467	2.51285	–1.49741	–1.82916	0.75389	–5.04761
H	9.29988	–1.23055	3.57345	1.82916	–0.75389	–5.04761
H	7.50120	–3.37713	4.07327	1.82916	0.75389	–5.04761
H	3.93416	4.31027	2.66570	0.00000	2.76907	–2.45224
H	4.48101	2.21449	4.53552	0.00000	2.65646	–3.95446

R = 5.5 Å

Atom		C_1			D_{2d}	
Fe	–5.16103	–0.04822	0.00509	0.00000	0.00000	2.75000
Fe	5.23243	–0.02151	0.00558	0.00000	0.00000	–2.75000
O	–2.43124	3.60068	0.06101	2.12791	0.00000	2.92988
O	–8.24960	–2.95188	–0.31732	0.00000	1.80166	1.62282
O	–3.41984	–2.15618	–3.21670	0.00000	–1.80166	1.62282
O	–3.42424	–2.34361	2.96645	0.00000	1.43078	4.38336
O	–7.25735	2.40486	–2.59749	0.00000	–1.43078	4.38336
O	–7.42854	1.73750	3.04380	–2.12791	0.00000	2.92988
O	8.35406	–2.01929	1.35121	0.00000	–2.12791	–2.92988
O	2.43638	2.06690	–1.57497	–1.80166	0.00000	–1.62282
O	3.87897	–3.44628	–1.23724	1.80166	0.00000	–1.62282
O	3.59086	–0.39528	3.51045	–1.43078	0.00000	–4.38336
O	7.23242	0.43713	–3.34929	1.43078	0.00000	–4.38336
O	7.00688	3.21506	1.33945	0.00000	2.12791	–2.92988
H	–2.41783	4.59233	1.56564	2.77521	0.00000	2.22946
H	–3.13455	4.70665	–1.18237	2.64845	0.00000	3.72903
H	–8.85437	–4.15409	0.87642	0.76557	2.28001	1.32355
H	–9.50370	–2.94082	–1.60856	–0.76557	2.28001	1.32355
H	–4.16168	–3.78439	–3.43917	0.76557	–2.28001	1.32355
H	–3.26075	–1.51156	–4.88768	–0.76557	–2.28001	1.32355
H	–3.45367	–4.14248	2.90636	0.75329	1.81540	4.82244
H	–3.98298	–1.92762	4.62952	–0.75329	1.81540	4.82244
H	–7.55427	2.26938	–4.36747	0.75329	–1.81540	4.82244
H	–8.60601	3.43188	–1.98527	–0.75329	–1.81540	4.82244
H	–9.02543	1.01580	3.46059	–2.77521	0.00000	2.22946

H	–7.37560	3.27403	3.97603	–2.64845	0.00000	3.72903
H	8.65897	–2.66750	3.01212	0.00000	–2.77521	–2.22946
H	9.85937	–2.37095	0.40875	0.00000	–2.64845	–3.72903
H	0.85632	2.64861	–0.87591	–2.28001	–0.76557	–1.32355
H	2.69322	2.91406	–3.14925	–2.28001	0.76557	–1.32355
H	2.57803	–3.77667	–2.43959	2.28001	–0.76557	–1.32355
H	4.76580	–5.00556	–0.98980	2.28001	0.76557	–1.32355
H	3.96360	0.70075	4.90084	–1.81540	–0.75329	–4.82244
H	2.85042	–1.88524	4.20780	–1.81540	0.75329	–4.82244
H	7.34190	–0.69874	–4.75274	1.81540	–0.75329	–4.82244
H	8.44100	1.74375	–3.68164	1.81540	0.75329	–4.82244
H	6.53481	4.94846	1.14204	0.00000	2.77521	–2.22946
H	8.62079	3.23583	2.16080	0.00000	2.64845	–3.72903

R = 5.0 Å

Atom		C_1			D_{2d}	
Fe	4.67812	–0.01563	0.03435	0.00000	0.00000	2.50000
Fe	–4.77046	0.00942	0.01587	0.00000	0.00000	–2.50000
O	3.14517	0.58522	3.80658	2.12542	0.00000	2.70659
O	6.62588	–0.83636	–3.48676	0.00000	1.84157	1.43137
O	2.46395	–3.82857	–1.02216	0.00000	–1.84157	1.43137
O	2.39664	3.26253	–1.96801	0.00000	1.42022	4.15800
O	7.51078	–2.48286	1.87227	0.00000	–1.42022	4.15800
O	7.31676	3.30082	0.62461	–2.12542	0.00000	2.70659
O	–6.58147	1.27109	–3.24092	0.00000	–2.12542	–2.70659
O	–3.43853	–1.45877	3.36983	–1.84157	0.00000	–1.43137
O	–2.34720	–1.92107	–2.24956	1.84157	0.00000	–1.43137
O	–2.59229	3.16659	0.18937	–1.42022	0.00000	–4.15800
O	–7.27534	–3.03223	–0.04010	1.42022	0.00000	–4.15800
O	–7.51017	1.99194	2.03346	0.00000	2.12542	–2.70659
H	3.16279	2.18816	4.62876	2.78278	0.00000	2.01536
H	3.81069	–0.55661	5.03701	2.63736	0.00000	3.51147
H	6.61497	–0.10691	–5.13260	0.76585	2.32974	1.14810
H	8.15330	–1.79457	–3.42318	–0.76585	2.32974	1.14810
H	3.20737	–4.49785	–2.52728	0.76585	–2.32974	1.14810
H	2.48682	–5.21773	0.12828	–0.76585	–2.32974	1.14810
H	2.27941	3.35458	–3.76507	0.75257	1.80067	4.60215
H	3.29827	4.76473	–1.51914	–0.75257	1.80067	4.60215
H	7.73553	–4.26167	2.02576	0.75257	–1.80067	4.60215
H	9.03528	–1.78403	2.53179	–0.75257	–1.80067	4.60215
H	8.57950	3.74704	–0.58115	–2.78278	0.00000	2.01536
H	7.86033	4.10719	2.14017	–2.63736	0.00000	3.51147
H	–6.33673	2.81139	–4.15497	0.00000	–2.78278	–2.01536
H	–8.01569	0.47169	–4.00432	0.00000	–2.63736	–3.51147
H	–2.57877	–0.58671	4.69303	–2.32974	–0.76585	–1.14810
H	–4.11186	–2.97175	4.10076	–2.32974	0.76585	–1.14810
H	–0.86727	–2.87624	–1.79114	2.32974	–0.76585	–1.14810

H	–2.73007	–2.27134	–3.98048	2.32974	0.76585	–1.14810
H	–3.18266	4.74196	0.85239	–1.80067	–0.75257	–4.60215
H	–0.99796	3.44978	–0.63236	–1.80067	0.75257	–4.60215
H	–7.11196	–4.64105	–0.84912	1.80067	–0.75257	–4.60215
H	–8.93194	–3.02113	0.69149	1.80067	0.75257	–4.60215
H	–7.83579	1.98051	3.81272	0.00000	2.78278	–2.01536
H	–8.83619	2.98555	1.30399	0.00000	2.63736	–3.51147

$R = 4.5$ Å

Atom		C_1			D_{2d}	
Fe	–4.33971	–0.00319	0.00607	0.00000	0.00000	2.25000
Fe	4.16401	0.01672	0.02626	0.00000	0.00000	–2.25000
O	–2.37917	3.30136	0.18180	2.12032	0.00000	2.49952
O	–6.74707	–3.10907	–0.32865	0.00000	1.88262	1.24392
O	–2.36279	–1.46382	–2.94411	0.00000	–1.88262	1.24392
O	–2.32108	–1.80632	2.73919	0.00000	1.41019	3.93460
O	–6.77624	1.84763	–2.48446	0.00000	–1.41019	3.93460
O	–6.73178	1.22858	2.88980	–2.12032	0.00000	2.49952
O	6.60372	–1.04265	3.30906	0.00000	–2.12032	–2.49952
O	2.35209	0.76799	–3.96020	–1.88262	0.00000	–1.24392
O	2.40284	–3.80309	1.16325	1.88262	0.00000	–1.24392
O	2.42442	3.09675	2.56849	–1.41019	0.00000	–3.93460
O	6.69609	–2.27685	–2.42854	1.41019	0.00000	–3.93460
O	6.73834	3.22455	–0.78019	0.00000	2.12032	–2.49952
H	–0.97043	3.67688	1.25737	2.79284	0.00000	1.82289
H	–3.01741	4.85416	–0.49232	2.61739	0.00000	3.31379
H	–6.68839	–4.70136	0.52652	0.76620	2.38064	0.97777
H	–8.26533	–3.14427	–1.31507	–0.76620	2.38064	0.97777
H	–2.99242	–2.80095	–3.98702	0.76620	–2.38064	0.97777
H	–0.94217	–0.69948	–3.77586	–0.76620	–2.38064	0.97777
H	–0.93759	–2.94683	2.47770	0.75174	1.78635	4.38396
H	–2.92328	–2.00953	4.43303	–0.75174	1.78635	4.38396
H	–6.75893	1.87117	–4.29272	0.75174	–1.78635	4.38396
H	–8.28709	2.72209	–2.00270	–0.75174	–1.78635	4.38396
H	–8.22279	0.36232	3.44288	–2.79284	0.00000	1.82289
H	–6.70477	2.78400	3.81186	–2.61739	0.00000	3.31379
H	6.71049	–0.51576	5.02804	0.00000	–2.79284	–1.82289
H	8.17662	–1.87296	3.00908	0.00000	–2.61739	–3.31379
H	2.22828	2.40527	–4.70855	–2.38064	–0.76620	–0.97777
H	3.32358	–0.18124	–5.15504	–2.38064	0.76620	–0.97777
H	2.24942	–5.22195	0.05937	2.38064	–0.76620	–0.97777
H	3.38220	–4.42873	2.55057	2.38064	0.76620	–0.97777
H	3.36634	4.61991	2.30739	–1.78635	–0.75174	–4.38396
H	2.34213	2.94247	4.36493	–1.78635	0.75174	–4.38396
H	6.92423	–4.04380	–2.69300	1.78635	–0.75174	–4.38396
H	8.19442	–1.53302	–3.10251	1.78635	0.75174	–4.38396
H	6.95449	4.32328	–2.19113	0.00000	2.79284	–1.82289

H	8.23158	3.46605	0.20290	0.00000	2.61739	–3.31379
			R = 4.0 Å			
Atom		C_1			D_{2d}	
Fe	–3.91278	–0.00042	–0.00061	0.00000	0.00000	2.00000
Fe	3.64612	0.00235	–0.00556	0.00000	0.00000	–2.00000
O	–2.01587	2.31925	–2.39422	2.11205	0.00000	2.32855
O	–6.39891	–2.25938	2.10553	0.00000	1.92006	1.06105
O	–2.06632	–3.26513	–0.79965	0.00000	–1.92006	1.06105
O	–2.05419	0.89842	3.22993	0.00000	1.40463	3.71642
O	–6.35261	–0.68053	–3.05042	0.00000	–1.40463	3.71642
O	–6.35362	2.99012	0.90058	–2.11205	0.00000	2.32855
O	6.26547	1.49441	2.97800	0.00000	–2.11205	–2.32855
O	2.21435	–2.22576	–3.50524	–1.92006	0.00000	–1.06105
O	2.21642	–1.97466	3.66252	1.92006	0.00000	–1.06105
O	2.21935	4.16668	–0.10195	–1.40463	0.00000	–3.71642
O	6.28817	–3.32123	–0.19469	1.40463	0.00000	–3.71642
O	6.23713	1.85296	–2.81392	0.00000	2.11205	–2.32855
H	–0.78382	3.55484	–1.88909	2.81050	0.00000	1.67875
H	–2.68088	2.78452	–4.01232	2.58010	0.00000	3.15981
H	–6.42538	–2.59715	3.88218	0.76661	2.42787	0.81272
H	–7.90348	–3.02533	1.45009	–0.76661	2.42787	0.81272
H	–2.75707	–4.88896	–0.39566	0.76661	–2.42787	0.81272
H	–0.81653	–3.46693	–2.10117	–0.76661	–2.42787	0.81272
H	–0.80543	–0.14317	4.03904	0.75069	1.77662	4.17099
H	–2.73075	2.05411	4.44794	–0.75069	1.77662	4.17099
H	–6.38078	–2.06101	–4.21863	0.75069	–1.77662	4.17099
H	–7.84211	0.28384	–3.41310	–0.75069	–1.77662	4.17099
H	–7.86217	2.82380	1.88890	–2.81050	0.00000	1.67875
H	–6.35864	4.69764	0.30453	–2.58010	0.00000	3.15981
H	6.44199	3.07769	3.81883	0.00000	–2.81050	–1.67875
H	7.81361	0.63671	3.32594	0.00000	–2.58010	–3.15981
H	1.97409	–1.58930	–5.17641	–2.42787	–0.76661	–0.81272
H	3.34211	–3.62432	–3.72305	–2.42787	0.76661	–0.81272
H	1.97384	–3.74268	3.92820	2.42787	–0.76661	–0.81272
H	3.33925	–1.47790	4.99178	2.42787	0.76661	–0.81272
H	3.34317	5.07506	–1.19126	–1.77662	–0.75069	–4.17099
H	1.96859	5.27614	1.29860	–1.77662	0.75069	–4.17099
H	6.46876	–4.83929	0.75823	1.77662	–0.75069	–4.17099
H	7.83257	–3.19591	–1.11815	1.77662	0.75069	–4.17099
H	6.39139	1.80541	–4.60810	0.00000	2.81050	–1.67875
H	7.79608	2.57074	–2.25872	0.00000	2.58010	–3.15981