

Terms & Conditions

Electronic Supporting Information files are available without a subscription to ACS Web Editions. The American Chemical Society holds a copyright ownership interest in any copyrightable Supporting Information. Files available from the ACS website may be downloaded for personal use only. Users are not otherwise permitted to reproduce, republish, redistribute, or sell any Supporting Information from the ACS website, either in whole or in part, in either machine-readable form or any other form without permission from the American Chemical Society. For permission to reproduce, republish and redistribute this material, requesters must process their own requests via the RightsLink permission system. Information about how to use the RightsLink permission system can be found at <http://pubs.acs.org/page/copyright/permissions.html>



ACS Publications

MOST TRUSTED. MOST CITED. MOST READ.

Copyright © 1997 American Chemical Society

TABLE S26: Orbital Energies/Mn_{III}Mn_{IV}(μ-O)₂(Oac)(TACN)₂ BS ACCINT=3.5

S121

Mn_{III}Mn_{IV}(μ-O)₂(Oac)(TACN)₂ BS ACCINT=3.5 Orbital Energies and Descriptions for β- A''

Orbital	Energy (eV)	Occupancy	Primary Contributors SFO(%)
1	-29.0780	1.0	N _t 1S(61.3), C ₁ 1S(14.1), H ₄ 1S(11.1),
2	-28.9820	1.0	N' _t 1S(61.7), C ₂ 1S(13.8), H ₁₂ 1S(11.2),
3	-27.9340	1.0	O 1S(94.0),
4	-25.1480	1.0	N _c 1P-Z(8.2), N _t 1S(5.2), N _t 1P-Y(5.1), C' ₁ 1S(34.7), C ₁ 1S(17.7), H ₅ 1S(8.5),
5	-24.9730	1.0	N' _c 1P-Z(7.8), N' _t 1S(5.1), N _t 1P-Y(5.4), C ₃ 1S(34.0), C ₂ 1S(18.5), H ₁₃ 1S(8.4),
6	-21.9770	1.0	N _c 1P-Z(8.5), N _t 1P-Y(8.1), C' ₁ 1S(12.6), C ₁ 1S(13.8), C ₃ 1S(12.5), H ₅ 1S(6.2), H ₇ 1S(6.6), H ₁₀ 1S(5.4),
7	-21.8210	1.0	N' _c 1P-Z(7.9), N' _t 1P-Y(7.8), C' ₃ 1S(13.0), C ₂ 1S(12.5), C' ₂ 1S(13.3), H ₁₃ 1S(6.4), H ₁₅ 1S(6.3), H ₁₈ 1S(5.8),
8	-20.8060	1.0	N _t 1P-X(17.5), C ₁ 1S(7.1), C ₃ 1S(15.4), H ₄ 1S(6.3), H ₈ 1S(9.4), H ₉ 1S(11.0), H ₁₀ 1S(6.0),
9	-20.6850	1.0	N' _t 1P-X(17.5), C ₂ 1S(7.7), C' ₂ 1S(14.5), H ₁₂ 1S(6.4), H ₁₆ 1S(9.8), H ₁₇ 1S(10.8), H ₁₈ 1S(5.6),
10	-18.7440	1.0	N _c 1P-Z(5.1), N _t 1P-X(5.1), N _t 1P-Y(25.8), C' ₁ 1P-Z(5.4), C ₁ 1P-Z(12.6), H ₄ 1S(7.8), H ₇ 1S(6.2),
11	-18.5940	1.0	N' _t 1P-X(5.2), N' _c 1P-Y(26.1), C ₂ 1P-Z(13.6), H ₁₂ 1S(7.8), H ₁₅ 1S(7.2),
12	-17.9560	1.0	N _c 1P-Z(12.4), C' ₁ 1P-X(18.8), C ₁ 1P-X(11.4), H ₆ 1S(11.2), H ₇ 1S(9.4),
13	-17.7730	1.0	N' _c 1P-Z(12.7), C' ₃ 1P-X(19.0), C ₂ 1P-X(12.4), H ₁₄ 1S(11.1), H ₁₅ 1S(8.4),
14	-16.7370	1.0	O ^a 1P-Z(19.7), O ^{a'} 1P-Z(23.2), C _a 1P-Z(30.0), C _b 1P-Z(13.1), H ₂ 1S(7.9),
15	-16.4340	1.0	N _c 1P-Z(8.4), N _t 1P-X(6.4), N _t 1P-Z(6.4), C' ₁ 1P-Y(7.1), C' ₁ 1P-Z(7.6), C ₁ 1P-X(14.5), C ₁ 1P-Y(7.6), C ₁ 1P-Z(7.0), H ₈ 1S(13.0),
16	-16.2550	1.0	N' _c 1P-Z(8.9), N' _t 1P-X(6.9), N' _t 1P-Z(6.2), C' ₃ 1P-Y(7.6), C' ₃ 1P-Z(7.2), C ₂ 1P-X(13.5), C ₂ 1P-Y(7.9), C ₂ 1P-Z(7.5), H ₁₆ 1S(12.6),
17	-16.1920	1.0	N _t 1P-X(5.1), N _t 1P-Z(20.8), C' ₁ 1P-X(6.3), C ₃ 1P-X(11.4), H ₆ 1S(7.3), H ₉ 1S(8.6),
18	-16.0710	1.0	N' _t 1P-X(5.2), N' _c 1P-Z(21.0), C' ₃ 1P-X(6.8), C' ₂ 1P-X(11.3), H ₁₄ 1S(7.4), H ₁₇ 1S(8.4),
19	-15.9720	1.0	N _c 1P-Z(6.8), N _t 1P-Y(5.7), C' ₁ 1P-Y(18.7), C' ₁ 1P-Z(5.8), C ₁ 1P-X(5.3), H ₅ 1S(20.7), H ₈ 1S(5.5),
20	-15.7950	1.0	N' _c 1P-Z(8.0), N' _t 1P-Y(5.8), C ₃ 1P-Y(19.1), C ₃ 1P-Z(5.9), C ₂ 1P-X(5.5), H ₁₃ 1S(20.4), H ₁₆ 1S(6.0),
21	-14.9480	1.0	Mn _{III} 1D-XZ(8.5), Mn _{IV} 1D-XZ(21.7), O 1P-X(51.7),
22	-14.6740	1.0	O 1P-Y(5.3), O ^a 1P-Z(6.7), O ^{a'} 1P-Z(8.9), C _b 1P-Z(31.4), H ₂ 1S(31.9),
23	-14.3590	1.0	Mn _{III} 1D-XZ(11.7), Mn _{IV} 1D-XZ(7.5), O 1P-Z(22.5), H ₉ 1S(6.4),
24	-14.1400	1.0	C' ₁ 1P-X(6.2), C' ₁ 1P-Z(7.4), H ₆ 1S(8.6), H ₇ 1S(7.6), H ₉ 1S(7.0),
25	-14.0270	1.0	C' ₂ 1P-X(5.3), C' ₂ 1P-Y(6.4), H ₇ 1S(5.7), H ₁₇ 1S(9.7), H ₁₈ 1S(5.3),
26	-13.9330	1.0	C ₃ 1P-Y(10.0), H ₉ 1S(5.5), H ₁₀ 1S(8.9), H ₁₄ 1S(5.9), H ₁₅ 1S(5.9),
27	-13.8390	1.0	C' ₂ 1P-Y(12.7), H ₁₃ 1S(5.9), H ₁₅ 1S(8.0), H ₁₇ 1S(6.4), H ₁₈ 1S(11.2),
28	-13.5180	1.0	Mn _{IV} 1D-YZ(31.4), O 1P-Y(25.3), O ^a 1P-Z(15.0),
29	-13.2180	1.0	O 1P-X(5.1), O ^a 1P-Z(13.5), O ^{a'} 1P-Z(18.6), N _t 1P-Z(9.6),
30	-12.9670	1.0	Mn _{III} 1D-YZ(4.5), O 1P-X(7.6), O 1P-Y(11.7), O ^a 1P-Z(15.8), O ^{a'} 1P-Z(22.7), N _t 1P-X(5.7), N _t 1P-Z(6.2),
31	-12.4410	1.0	O 1P-Z(41.9), N _t 1P-X(8.4), N _t 1P-Z(10.0), N' _t 1P-X(9.0), N' _t 1P-Z(10.5),
32	-11.3520	1.0	Mn _{III} 1D-YZ(5.6), Mn _{IV} 1D-YZ(49.9), O 1P-Y(28.3),
33	-8.7200	0.0	Mn _{III} 1D-YZ(75.9), O 1P-Y(11.9),
34	-7.8870	0.0	Mn _{IV} 1D-XZ(50.1), O 1P-X(14.7), O 1P-Z(8.1), N _t 1P-Z(5.3),
35	-6.8730	0.0	Mn _{III} 1D-XZ(61.6), O 1P-X(5.2), O 1P-Z(11.7),

TABLE S26: Orbital Energies/Mn_{III}Mn_{IV}(μ-O)₂(Oac)(TACN)₂ BS ACCINT=3.5

S122

Orbital	Energy (eV)	Occupancy	Primary Contributors SFO(%)
36	-6.2120	0.0	O ^a 1P-Z(17.7), O ^{a'} 1P-Z(14.9), C ₄ 1P-Z(53.3), H ₂ 1S(9.1),
37	-5.1550	0.0	H ₄ 1S(11.8), H ₄ 2S(6.6), H ₅ 1S(8.1), H ₅ 2S(5.7), H ₇ 1S(16.7), H ₇ 2S(12.8), H ₁₂ 1S(7.5), H ₁₃ 1S(6.1), H ₁₅ 1S(12.6), H ₁₅ 2S(10.4),
38	-4.6410	0.0	H ₄ 1S(17.9), H ₇ 1S(8.2), H ₁₂ 1S(17.8), H ₁₂ 2S(5.3), H ₁₃ 1S(6.8), H ₁₅ 1S(12.8), H ₁₅ 2S(6.1),
39	-4.3190	0.0	H ₄ 1S(11.5), H ₅ 1S(5.9), H ₅ 2S(10.1), H ₆ 1S(8.6), H ₁₂ 1S(12.9), H ₁₃ 2S(7.0),
40	-4.0470	0.0	C ₁ 1P-Z(5.1), H ₆ 1S(10.9), H ₈ 1S(24.2), H ₈ 2S(13.9), H ₁₂ 1S(5.7), H ₁₄ 1S(6.5), H ₁₆ 1S(8.2), H ₁₆ 2S(5.3),
41	-3.9220	0.0	H ₅ 1S(7.2), H ₈ 1S(9.8), H ₁₄ 1S(8.5), H ₁₆ 1S(29.0), H ₁₆ 2S(16.1), H ₁₇ 2S(5.4),
42	-3.6320	0.0	N _c 1P-Z(10.6), N _t 1P-Y(8.8), C ₁ ' 1P-Z(5.6), C ₁ 1P-Y(19.8), C ₁ 1P-Z(5.4), C ₃ 1P-X(5.0), H ₄ 1S(5.5), H ₈ 1S(5.9), H ₉ 1S(10.7), H ₁₃ 1S(5.9),

TABLE S27: Orbital Energies/ $\text{Mn}_{\text{III}}\text{Mn}_{\text{IV}}(\mu-\text{O})_2(\text{Oac})(\text{TACN})_2$ HS ACCINT=3.5

S123

 $\text{Mn}_{\text{III}}\text{Mn}_{\text{IV}}(\mu-\text{O})_2(\text{Oac})(\text{TACN})_2$ HS ACCINT=3.5 Fragment Types

Atom types	Indices	Charges	Alpha Spin	Beta Spin	Net Spin
Mn _{III}	1	1.059	4.572	1.368	3.2040
Mn _{IV}	2	1.066	4.653	1.281	3.3720
O	3 5	-0.783	3.512	3.272	0.2400
O ^a	4	-0.632	3.321	3.312	0.0090
O ^{a'}	6	-0.637	3.329	3.307	0.0220
N _c	7	-0.373	2.692	2.682	0.0100
N _t	8 9	-0.424	2.691	2.732	-0.0410
N _{c'}	10	-0.372	2.685	2.687	-0.0020
N _{t'}	11 12	-0.421	2.692	2.729	-0.0370
C ^a	13	0.974	1.513	1.514	-0.0010
C ^{a'}	14	0.235	1.879	1.886	-0.0070
C ₁	15 20	0.415	1.795	1.791	0.0040
C ₁	16 19	0.422	1.792	1.786	0.0060
C ₃	17 18	0.399	1.802	1.800	0.0020
C _{3'}	21 26	0.415	1.795	1.790	0.0050
C ₂	22 25	0.418	1.794	1.788	0.0060
C _{2'}	23 24	0.397	1.803	1.800	0.0030
H ₁	27	-0.071	0.536	0.535	0.0010
H ₂	28 29	-0.056	0.528	0.528	0.0000
H ₃	30	0.102	0.453	0.446	0.0070
H ₄	31 32	0.165	0.419	0.415	0.0040
H ₅	33 43	-0.075	0.537	0.538	-0.0010
H ₆	34 44	-0.071	0.536	0.535	0.0010
H ₇	35 41	-0.078	0.539	0.539	0.0000
H ₈	36 42	-0.073	0.535	0.538	-0.0030
H ₉	37 40	-0.073	0.537	0.537	0.0000
H ₁₀	38 39	-0.055	0.527	0.527	0.0000
H ₁₁	45	0.109	0.450	0.442	0.0080
H ₁₂	46 47	0.164	0.420	0.415	0.0050
H ₁₃	48 58	-0.073	0.536	0.537	-0.0010
H ₁₄	49 59	-0.070	0.535	0.535	0.0000
H ₁₅	50 56	-0.075	0.538	0.537	0.0010
H ₁₆	51 57	-0.072	0.535	0.537	-0.0020
H ₁₇	52 55	-0.073	0.536	0.537	-0.0010
H ₁₈	53 54	-0.053	0.526	0.526	0.0000

TABLE S27: Orbital Energies/ $\text{Mn}_{\text{III}}\text{Mn}_{\text{IV}}(\mu-\text{O})_2(\text{Oac})(\text{TACN})_2$ HS ACCINT=3.5 **$\text{Mn}_{\text{III}}\text{Mn}_{\text{IV}}(\mu-\text{O})_2(\text{Oac})(\text{TACN})_2$ HS ACCINT=3.5 Orbital Energies and Descriptions for $\alpha - \text{A}'$**

Orbital	Energy (eV)	Occupancy	Primary Contributors SFO(%)
1	-32.6460	1.0	O ^a 1S(35.3), O ^{a'} 1S(33.6), C _a 1S(18.1),
2	-30.3190	1.0	O ^a 1S(37.3), O ^{a'} 1S(38.7), C _a 1P-X(12.6),
3	-30.0570	1.0	N _c 1S(5.7), N _t 1S(5.6), N _c ' 1S(24.6), N _t ' 1S(22.1), C ₃ ' 1S(11.2), C ₂ 1S(6.9),
4	-29.9760	1.0	N _c 1S(23.5), N _t 1S(22.5), N _c ' 1S(5.4), C ₁ ' 1S(11.0), C ₁ 1S(7.0),
5	-29.1950	1.0	N _c ' 1S(29.0), N _t ' 1S(30.5), C ₃ ' 1S(6.1), C ₂ ' 1S(10.3), H ₁₁ 1S(6.3), H ₁₂ 1S(5.4),
6	-29.1380	1.0	N _c 1S(29.8), N _t 1S(29.7), C ₁ ' 1S(6.4), C ₃ 1S(10.2), H ₃ 1S(6.3), H ₄ 1S(5.1),
7	-28.4370	1.0	O 1S(89.7),
8	-25.1010	1.0	N _t ' 1P-Y(5.8), C ₂ 1S(20.5), C ₂ ' 1S(33.9), H ₁₈ 1S(6.0),
9	-25.0610	1.0	N _t 1P-Y(5.8), C ₁ 1S(20.5), C ₃ 1S(34.0), H ₁₀ 1S(6.1),
10	-23.4520	1.0	N _t ' 1S(7.8), C ₃ ' 1S(12.4), C ₂ 1S(8.8), C ₂ ' 1S(14.1), H ₁₄ 1S(5.0), H ₁₇ 1S(5.1),
11	-23.4080	1.0	N _t 1S(7.8), C ₁ ' 1S(12.2), C ₁ 1S(8.9), C ₃ 1S(13.8), H ₆ 1S(5.0), H ₉ 1S(5.1),
12	-23.2390	1.0	C _a 1S(8.2), C _a 1P-Y(9.0), C _b 1S(42.6), H ₁ 1S(9.2), H ₂ 1S(20.0),
13	-21.1020	1.0	N _c ' 1P-X(11.3), C ₃ ' 1S(8.3), C ₂ 1S(8.0), H ₁₁ 1S(5.1), H ₁₄ 1S(9.5),
14	-21.0010	1.0	N _c 1P-X(10.3), C ₁ ' 1S(8.7), C ₁ 1S(7.8), H ₆ 1S(10.1),
15	-19.8290	1.0	N _c ' 1P-X(5.7), N _c 1P-Y(5.5), N _t ' 1P-Y(12.0), C ₃ ' 1P-Y(5.7), C ₂ ' 1P-Z(5.2), C ₂ ' 1P-Y(5.8), H ₁₃ 1S(7.1),
16	-19.7470	1.0	N _c 1P-X(5.5), N _c 1P-Y(5.4), N _t 1P-Y(12.1), C ₁ ' 1P-Y(5.6), C ₃ 1P-Y(6.3), H ₅ 1S(6.9),
17	-19.1460	1.0	O ^a 1S(7.2), O ^a ' 1P-X(12.0), O ^a ' 1P-Y(6.4), O ^{a'} 1S(6.7), O ^{a'} 1P-X(10.9), O ^{a'} 1P-Y(5.5), C _a 1S(10.1), H ₂ 1S(5.8),
18	-18.8200	1.0	N _c ' 1P-X(8.4), N _t ' 1P-X(8.4), N _t ' 1P-Z(10.1), C ₂ ' 1P-X(6.3), C ₂ ' 1P-Y(8.6), H ₁₈ 1S(5.5),
19	-18.7450	1.0	N _c 1P-X(8.3), N _t 1P-X(10.6), N _t 1P-Z(6.3), C ₃ 1P-X(5.0), C ₃ 1P-Y(8.8), H ₁₀ 1S(5.3),
20	-18.4230	1.0	N _t ' 1P-Z(8.1), N _t ' 1P-Z(9.0),
21	-18.1720	1.0	N _t 1P-Z(5.4), C ₁ 1P-X(5.7), C ₂ 1P-X(5.3),
22	-17.8250	1.0	O ^a 1P-X(5.0), O ^a ' 1P-Y(7.6), O ^{a'} 1P-X(5.8), O ^{a'} 1P-Y(8.2), C _a 1P-X(5.1), H ₈ 1S(5.5), H ₁₆ 1S(5.8),
23	-17.5590	1.0	N _t ' 1P-Y(6.4), C ₃ 1P-X(5.3), C ₂ ' 1P-X(8.7), H ₈ 1S(5.8), H ₁₆ 1S(6.9),
24	-17.4300	1.0	O ^a 1P-Y(5.6), O ^{a'} 1P-Y(6.3), C ₃ 1P-X(8.7), H ₉ 1S(6.0),
25	-16.8140	1.0	O ^a 1P-X(14.7), O ^{a'} 1P-X(13.8), O ^{a'} 1P-Y(5.1), C _a 1P-Y(14.0), C _a 2P-Y(5.2), C _b 1P-Y(14.6),
26	-16.5230	1.0	N _c ' 1P-X(5.3), C ₂ 1P-Z(12.8), C ₂ ' 1P-Y(7.9), C ₂ ' 1P-Z(12.2), H ₁₅ 1S(9.9), H ₁₈ 1S(8.0),
27	-16.4710	1.0	C ₁ 1P-Z(11.9), C ₃ 1P-Y(7.8), C ₃ 1P-Z(14.3), H ₇ 1S(8.6), H ₁₀ 1S(8.1),
28	-16.3000	1.0	N _t ' 1P-X(5.5), N _t ' 1P-Y(5.7), C ₃ ' 1P-X(9.3), C ₂ ' 1P-Y(6.5), C ₂ ' 1P-Z(12.2), H ₁₄ 1S(6.7),
29	-16.2500	1.0	N _t 1P-X(5.3), C ₁ ' 1P-X(10.9), C ₃ 1P-Y(6.0), C ₃ 1P-Z(9.4), H ₆ 1S(7.1),
30	-16.0790	1.0	O 1P-X(5.3), N _t ' 1P-Y(6.2), C ₂ 1P-Y(5.3), C ₂ ' 1P-Y(7.2), H ₁₇ 1S(5.7),
31	-16.0000	1.0	N _t 1P-X(7.0), C ₃ 1P-Y(7.5),
32	-15.6520	1.0	Mn _{III} 1D-Z2(7.6), Mn _{III} 1D(X2-Y2)(10.3), Mn _{IV} 1D-Z2(7.8), Mn _{IV} 1D(X2-Y2)(10.3), O 1P-Z(43.3),
33	-15.0330	1.0	Mn _{III} 1D-Z2(11.8), Mn _{IV} 1D-Z2(12.1), O 1P-X(38.8),
34	-14.9130	1.0	Mn _{III} 1D-XY(14.3), Mn _{IV} 1D-XY(14.3), O 1P-Y(35.7),
35	-14.7960	1.0	O ^{a'} 1P-X(5.5), C _b 1P-X(39.5), H ₁ 1S(28.2), H ₂ 1S(12.5),

TABLE S27: Orbital Energies/Mn_{III}Mn_{IV}(μ-O)₂(Oac)(TACN)₂ HS ACCINT=3.5

S125

Orbital	Energy (eV)	Occupancy	Primary Contributors SFO(%)
36	-14.3650	1.0	C ₃ ' 1P-X(9.8), C ₂ ' 1P-X(14.2), H ₁₄ 1S(12.2), H ₁₅ 1S(11.3), H ₁₆ 1S(7.8),
37	-14.3260	1.0	Mn _{III} 1D-XY(4.4), C ₁ ' 1P-X(8.9), C ₁ 1P-X(12.0), H ₆ 1S(12.3), H ₇ 1S(10.2), H ₈ 1S(6.6),
38	-14.2020	1.0	Mn _{III} 1D-Z2(5.1), Mn _{III} 1D(X2-Y2)(5.0), Mn _{IV} 1D-Z2(5.1), N _c 1P-Y(5.7), N _c ' 1P-Y(8.4),
39	-13.9880	1.0	Mn _{III} 1D(X2-Y2)(5.5), Mn _{III} 1D-XY(4.9), Mn _{IV} 1D(X2-Y2)(7.4), Mn _{IV} 1D-XY(5.4), N _c 1P-Y(11.7), N _c ' 1P-Y(9.5), C ₁ ' 1P-Y(5.0),
40	-13.3710	1.0	Mn _{III} 1D-Z2(5.0), Mn _{III} 1D(X2-Y2)(7.2), Mn _{IV} 1D-Z2(6.2), Mn _{IV} 1D(X2-Y2)(6.7), N _t 1P-Z(6.0), N _t ' 1P-Z(8.8),
41	-13.1650	1.0	N _t 1P-Z(11.0), N _t ' 1P-Z(8.3),
42	-12.8910	1.0	Mn _{III} 1D-XY(5.3), Mn _{IV} 1D-XY(4.8), O ^a 1P-Y(17.8), O ^{a'} 1P-Y(16.9), C _b 1P-Y(9.1),
43	-12.5530	1.0	Mn _{III} 1D-XY(19.1), Mn _{IV} 1D-XY(18.6), O ^a 1P-X(7.2), O ^a 1P-Y(10.5), O ^{a'} 1P-X(7.1), O ^{a'} 1P-Y(10.5), N _c 1P-Y(5.0), N _c ' 1P-Y(5.0),
44	-12.3330	1.0	Mn _{III} 1D-XY(18.1), Mn _{IV} 1D-XY(18.6), O ^a 1P-X(13.2), O ^a 1P-Y(7.0), O ^{a'} 1P-X(13.6), O ^{a'} 1P-Y(7.8),
45	-12.0360	1.0	Mn _{III} 1D-Z2(25.6), Mn _{IV} 1D-Z2(24.9), O 1P-Z(30.6),
46	-11.3400	1.0	Mn _{III} 1D-Z2(11.5), Mn _{III} 1D(X2-Y2)(16.1), Mn _{IV} 1D-Z2(11.3), Mn _{IV} 1D(X2-Y2)(15.6), O 1P-X(20.0),
47	-10.9240	1.0	Mn _{III} 1D-XY(16.9), Mn _{IV} 1D-XY(17.6), O 1P-Y(46.1),
48	-9.2800	1.0	Mn _{III} 1D-Z2(10.9), Mn _{III} 1D(X2-Y2)(10.7), Mn _{IV} 1D-Z2(11.4), Mn _{IV} 1D(X2-Y2)(12.2), O 1P-X(14.5), N _c 1P-Y(5.8), N _c ' 1P-Y(5.1),
49	-9.2430	0.0	Mn _{III} 1D(X2-Y2)(20.9), Mn _{IV} 1D(X2-Y2)(19.2), O 1P-Z(8.9), O ^a 1P-Y(6.6), O ^{a'} 1P-Y(6.0),
50	-6.8450	0.0	H ₃ 1S(18.7), H ₃ 2S(8.8), H ₅ 1S(7.0), H ₁₁ 1S(18.2), H ₁₁ 2S(8.1), H ₁₃ 1S(7.4),
51	-5.9410	0.0	C ₂ ' 1P-X(5.5), H ₁₄ 1S(5.2),
52	-5.8010	0.0	C ₃ 1P-X(6.0), H ₃ 1S(8.1), H ₁₁ 1S(8.9),
53	-5.4250	0.0	C ₃ ' 1P-X(5.5), H ₄ 1S(8.0), H ₆ 1S(5.4), H ₁₂ 1S(15.5), H ₁₂ 2S(5.8), H ₁₄ 1S(9.9), H ₁₈ 1S(9.4),
54	-5.3020	0.0	C ₁ ' 1P-X(6.0), H ₄ 1S(15.3), H ₆ 1S(9.2), H ₁₀ 1S(12.3), H ₁₂ ' 1S(8.7), H ₁₄ 1S(5.0), H ₁₈ 1S(7.2),
55	-4.6110	0.0	H ₆ 1S(5.3), H ₆ 2S(7.8), H ₁₄ 1S(7.8), H ₁₄ 2S(10.9),
56	-4.4940	0.0	H ₅ 1S(9.7), H ₅ 2S(7.7), H ₆ 1S(6.7), H ₆ 2S(10.6), H ₁₃ 1S(7.7), H ₁₃ 2S(5.7), H ₁₄ 1S(5.7), H ₁₄ 2S(8.6),
57	-4.2470	0.0	H ₃ 1S(9.2), H ₅ 1S(10.1), H ₁₀ 1S(10.0), H ₁₀ 2S(5.7), H ₁₁ 1S(7.0), H ₁₃ 1S(11.3), H ₁₈ 1S(13.8), H ₁₈ 2S(8.0),
58	-4.1860	0.0	H ₇ 1S(11.1), H ₇ 2S(10.4), H ₉ 1S(6.0), H ₁₀ 1S(10.2), H ₁₀ 2S(8.5), H ₁₅ 1S(9.7), H ₁₅ 2S(10.0), H ₁₇ 1S(6.6), H ₁₈ 1S(7.0), H ₁₈ 2S(6.2),

TABLE S27: Orbital Energies/ $\text{Mn}_{\text{III}}\text{Mn}_{\text{IV}}(\mu-\text{O})_2(\text{Oac})(\text{TACN})_2$ HS ACCINT=3.5

S126

 $\text{Mn}_{\text{III}}\text{Mn}_{\text{IV}}(\mu-\text{O})_2(\text{Oac})(\text{TACN})_2$ HS ACCINT=3.5 Orbital Energies and Descriptions for $\alpha - \text{A}''$

Orbital	Energy (eV)	Occupancy	Primary Contributors SFO(%)
1	-29.1050	1.0	$\text{N}_t^{'}$ 1S(61.7), C_2 1S(13.7), H_{12} 1S(11.2),
2	-29.0660	1.0	$\text{N}_t^{'}$ 1S(61.8), C_1 1S(13.7), H_4 1S(11.2),
3	-28.0290	1.0	O 1S(93.2),
4	-25.0700	1.0	$\text{N}_c^{'}$ 1P-Z(7.8), $\text{N}_t^{'}$ 1P-Y(5.4), $\text{C}_3^{'}$ 1S(34.0), C_2 1S(18.7), H_{13} 1S(8.3),
5	-25.0230	1.0	$\text{N}_c^{'}$ 1P-Z(7.7), $\text{N}_t^{'}$ 1P-Y(5.5), $\text{C}_1^{'}$ 1S(33.9), C_1 1S(18.8), H_5 1S(8.2),
6	-21.9250	1.0	$\text{N}_c^{'}$ 1P-Z(8.0), $\text{N}_t^{'}$ 1P-Y(7.8), $\text{N}_t^{'}$ 1P-Z(5.0), $\text{C}_3^{'}$ 1S(13.0), C_2 1S(12.3), $\text{C}_2^{'}$ 1S(13.5), H_{13} 1S(6.3), H_{15} 1S(6.2), H_{18} 1S(5.8),
7	-21.8800	1.0	$\text{N}_c^{'}$ 1P-Z(7.9), $\text{N}_t^{'}$ 1P-Y(7.8), $\text{N}_t^{'}$ 1P-Z(5.0), $\text{C}_1^{'}$ 1S(13.1), C_1 1S(12.2), C_3 1S(13.5), H_5 1S(6.3), H_7 1S(6.2), H_{10} 1S(5.9),
8	-20.8060	1.0	$\text{N}_t^{'}$ 1P-X(17.3), C_2 1S(7.8), $\text{C}_2^{'}$ 1S(14.3), H_{12} 1S(6.3), H_{16} 1S(9.7), H_{17} 1S(10.5), H_{18} 1S(5.4),
9	-20.7660	1.0	$\text{N}_t^{'}$ 1P-X(17.3), C_1 1S(7.8), C_3 1S(14.1), H_4 1S(6.3), H_8 1S(9.7), H_9 1S(10.5), H_{10} 1S(5.4),
10	-18.7230	1.0	$\text{N}_t^{'}$ 1P-Y(25.1), C_2 1P-Z(12.7), H_{12} 1S(7.6), H_{15} 1S(6.5),
11	-18.6790	1.0	$\text{N}_t^{'}$ 1P-Y(25.2), C_1 1P-Z(12.8), H_4 1S(7.5), H_7 1S(6.7),
12	-17.8830	1.0	$\text{N}_c^{'}$ 1P-Z(12.1), $\text{C}_3^{'}$ 1P-X(18.1), C_2 1P-X(11.8), H_{14} 1S(10.6), H_{15} 1S(8.3),
13	-17.8340	1.0	$\text{N}_c^{'}$ 1P-Z(12.0), $\text{C}_1^{'}$ 1P-X(18.2), C_1 1P-X(12.0), H_6 1S(10.5), H_7 1S(8.4),
14	-16.7260	1.0	O ^a 1P-Z(21.5), O ^{a'} 1P-Z(21.4), C_b 1P-Z(29.3), C_b 1P-Z(12.4), H_2 1S(7.3),
15	-16.4030	1.0	Mn_{III} 1D-XZ(4.9), $\text{N}_c^{'}$ 1P-Z(7.2), $\text{N}_t^{'}$ 1P-X(6.3), $\text{N}_t^{'}$ 1P-Z(9.3), $\text{C}_3^{'}$ 1P-Y(7.7), $\text{C}_3^{'}$ 1P-Z(7.2), C_2 1P-X(12.2), C_2 1P-Y(8.8), C_2 1P-Z(5.5), H_{16} 1S(9.8),
16	-16.3610	1.0	Mn_{IV} 1D-XZ(5.6), $\text{N}_c^{'}$ 1P-Z(6.8), $\text{N}_t^{'}$ 1P-X(6.3), $\text{N}_t^{'}$ 1P-Z(9.9), $\text{C}_1^{'}$ 1P-Y(7.9), $\text{C}_1^{'}$ 1P-Z(7.1), C_1 1P-X(12.0), C_1 1P-Y(8.9), C_1 1P-Z(5.2), H_8 1S(9.4),
17	-16.1910	1.0	$\text{N}_t^{'}$ 1P-X(5.8), $\text{N}_t^{'}$ 1P-Z(17.2), $\text{C}_3^{'}$ 1P-X(7.1), $\text{C}_2^{'}$ 1P-X(10.3), H_{14} 1S(6.9), H_{17} 1S(7.7),
18	-16.1480	1.0	$\text{N}_t^{'}$ 1P-X(5.8), $\text{N}_t^{'}$ 1P-Z(17.6), $\text{C}_1^{'}$ 1P-X(7.0), C_3 1P-X(10.4), H_6 1S(6.9), H_9 1S(7.8),
19	-15.8940	1.0	$\text{N}_c^{'}$ 1P-Z(8.3), $\text{N}_t^{'}$ 1P-Y(5.2), $\text{C}_3^{'}$ 1P-Y(17.0), $\text{C}_3^{'}$ 1P-Z(6.8), C_2 1P-X(6.7), H_{13} 1S(19.8), H_{16} 1S(6.8),
20	-15.8470	1.0	$\text{N}_c^{'}$ 1P-Z(8.4), $\text{N}_t^{'}$ 1P-Y(5.2), $\text{C}_1^{'}$ 1P-Y(16.8), $\text{C}_1^{'}$ 1P-Z(7.0), C_1 1P-X(6.9), H_5 1S(19.7), H_8 1S(7.0),
21	-15.3840	1.0	Mn_{III} 1D-XZ(16.6), Mn_{IV} 1D-XZ(16.7), O 1P-X(43.0),
22	-14.8020	1.0	Mn_{III} 1D-XZ(10.4), Mn_{IV} 1D-XZ(10.0), O 1P-Y(11.2), O 1P-Z(13.8), C_b 1P-Z(10.8), H_2 1S(10.7),
23	-14.7090	1.0	Mn_{III} 1D-XZ(4.9), Mn_{IV} 1D-XZ(4.8), O 1P-Z(10.2), C_b 1P-Z(17.2), H_2 1S(17.0),
24	-14.1510	1.0	C_3 1P-Y(5.7), $\text{C}_2^{'}$ 1P-X(5.5), $\text{C}_2^{'}$ 1P-Y(8.2), H_9 1S(7.3), H_{17} 1S(10.8), H_{18} 1S(6.5),
25	-14.0710	1.0	O 1P-Y(5.4), C_3 1P-Y(5.0), H_9 1S(6.8),
26	-13.9550	1.0	$\text{C}_3^{'}$ 1P-X(6.7), $\text{C}_3^{'}$ 1P-Z(7.8), C_2 1P-X(6.0), $\text{C}_2^{'}$ 1P-Y(7.8), H_{13} 1S(7.5), H_{14} 1S(8.0), H_{15} 1S(12.7), H_{18} 1S(6.4),
27	-13.9170	1.0	$\text{C}_1^{'}$ 1P-X(7.3), $\text{C}_1^{'}$ 1P-Z(8.9), C_1 1P-X(6.2), C_1 1P-Z(5.2), C_3 1P-Y(5.9), H_3 1S(7.5), H_6 1S(9.2), H_7 1S(13.5),
28	-13.7790	1.0	Mn_{III} 1D-YZ(10.3), Mn_{IV} 1D-YZ(10.7), O 1P-Y(16.7), C_3 1P-Y(5.7), H_{10} 1S(5.5),
29	-13.4620	1.0	Mn_{III} 1D-YZ(19.3), Mn_{IV} 1D-YZ(17.5), O ^a 1P-Z(24.4), O ^{a'} 1P-Z(28.1),
30	-13.2810	1.0	O 1P-X(14.5), $\text{N}_t^{'}$ 1P-X(6.3), $\text{N}_t^{'}$ 1P-Z(9.7), $\text{N}_t^{'}$ 1P-X(6.7), $\text{N}_t^{'}$ 1P-Z(10.2),
31	-12.5120	1.0	O 1P-Z(38.3), $\text{N}_t^{'}$ 1P-X(9.2), $\text{N}_t^{'}$ 1P-Z(11.0), $\text{N}_t^{'}$ 1P-X(8.8), $\text{N}_t^{'}$ 1P-Z(10.6),
32	-12.1230	1.0	Mn_{III} 1D-YZ(25.4), Mn_{IV} 1D-YZ(25.2), O ^a 1P-Z(17.4), O ^{a'} 1P-Z(18.5),
33	-10.9850	1.0	Mn_{III} 1D-YZ(21.4), Mn_{IV} 1D-YZ(22.7), O 1P-Y(51.6),
34	-8.5370	0.0	Mn_{III} 1D-XZ(22.1), Mn_{IV} 1D-XZ(24.3), O 1P-X(25.1),
35	-8.2520	0.0	Mn_{III} 1D-XZ(27.5), Mn_{IV} 1D-XZ(25.0), O 1P-Z(28.0),

TABLE S27: Orbital Energies/ $\text{Mn}_{\text{III}}\text{Mn}_{\text{IV}}(\mu-\text{O})_2(\text{Oac})(\text{TACN})_2$ HS ACCINT=3.5

S127

Orbital	Energy (eV)	Occupancy	Primary Contributors SFO(%)
36	-6.2310	0.0	O ^a 1P-Z(16.4), O ^{a'} 1P-Z(15.7), C _a 1P-Z(54.4), H ₂ 1S(9.2),
37	-5.2030	0.0	H ₄ 1S(9.3), H ₄ 2S(5.5), H ₅ 1S(5.9), H ₇ 1S(13.9), H ₇ 2S(11.6), H ₁₂ 1S(12.7), H ₁₂ 2S(7.5), H ₁₃ 1S(6.7), H ₁₅ 1S(15.9), H ₁₅ 2S(12.7),
38	-4.6850	0.0	H ₄ 1S(18.8), H ₄ 2S(5.6), H ₅ 1S(5.7), H ₇ 1S(12.1), H ₇ 2S(5.5), H ₁₂ 1S(20.4), H ₁₂ 2S(5.8), H ₁₅ 1S(8.8),
39	-4.3310	0.0	H ₄ 1S(13.4), H ₅ 2S(9.1), H ₆ 1S(5.4), H ₁₂ 1S(11.3), H ₁₃ 1S(6.1), H ₁₃ 2S(9.8), H ₁₄ 1S(6.1),
40	-4.0320	0.0	H ₆ 1S(8.9), H ₈ 1S(15.0), H ₈ 2S(9.2), H ₁₄ 1S(10.1), H ₁₆ 1S(18.1), H ₁₆ 2S(10.8),
41	-3.9100	0.0	H ₅ 1S(5.9), H ₆ 1S(5.5), H ₈ 1S(20.6), H ₈ 2S(10.4), H ₁₃ 1S(6.8), H ₁₆ 1S(17.0), H ₁₆ 2S(8.2),
42	-3.5850	0.0	N _c 1P-Z(10.0), N _t 1P-Y(8.7), C ₂ 1P-Y(21.2), C ₂ 1P-Z(5.7), C ₂ ' 1P-X(5.6), H ₅ 1S(6.2), H ₁₆ 1S(5.8), H ₁₇ 1S(11.3),
43	-3.5660	0.0	N _c 1P-Z(9.7), N _t 1P-Y(7.8), C ₁ 1P-Y(20.1), C ₃ 1P-X(5.2), H ₈ 1S(5.5), H ₉ 1S(11.5), H ₁₃ 1S(8.0),

TABLE S27: Orbital Energies/Mn_{III}Mn_{IV}(μ-O)₂(Oac)(TACN)₂ HS ACCINT=3.5

S128

Mn_{III}Mn_{IV}(μ-O)₂(Oac)(TACN)₂ HS ACCINT=3.5 Orbital Energies and Descriptions for β - A'

Orbital	Energy (eV)	Occupancy	Primary Contributors SFO(%)
1	-32.5970	1.0	O ^A 1S(35.6), O ^{A'} 1S(33.2), C _a 1S(18.3),
2	-30.2620	1.0	O ^A 1S(36.4), O ^{A'} 1S(38.4), C _a 1P-X(12.9),
3	-30.0340	1.0	N _c ' 1S(25.0), N _t ' 1S(24.1), C ₃ ' 1S(11.6), C ₂ 1S(7.3), C ₂ ' 1S(5.2),
4	-29.9560	1.0	N _c 1S(23.3), N _t 1S(25.0), C ₁ 1S(11.2), C ₁ ' 1S(7.5), C ₃ 1S(5.4),
5	-29.1830	1.0	N _c ' 1S(30.3), N _t ' 1S(30.5), C ₃ ' 1S(6.5), C ₂ ' 1S(10.3), H ₁₁ 1S(6.5), H ₁₂ 1S(5.4),
6	-29.1200	1.0	N _c 1S(31.6), N _t 1S(29.0), C ₁ ' 1S(7.1), C ₃ 1S(10.0), H ₃ 1S(6.7), H ₄ 1S(5.0),
7	-28.0500	1.0	O 1S(91.5),
8	-25.0960	1.0	N _t 1P-Y(5.9), C ₂ 1S(20.4), C ₂ ' 1S(34.0), H ₁₈ 1S(6.1),
9	-25.0540	1.0	N _t 1P-Y(5.9), C ₁ 1S(20.3), C ₃ 1S(34.1), H ₁₀ 1S(6.1),
10	-23.4420	1.0	N _t ' 1S(7.9), C ₃ ' 1S(12.3), C ₂ 1S(8.9), C ₂ ' 1S(14.1), H ₁₄ 1S(5.0), H ₁₇ 1S(5.1),
11	-23.3970	1.0	N _t 1S(7.8), C ₁ ' 1S(12.1), C ₁ 1S(9.0), C ₃ 1S(13.8), H ₆ 1S(5.0), H ₉ 1S(5.1),
12	-23.2370	1.0	C _a 1S(8.0), C _a 1P-Y(9.3), C _b 1S(42.9), H ₁ 1S(9.2), H ₂ 1S(20.1),
13	-21.0800	1.0	N _c ' 1P-X(11.6), C ₃ ' 1S(8.5), C ₂ 1S(8.1), H ₁₁ 1S(5.2), H ₁₄ 1S(9.9),
14	-20.9800	1.0	N _c 1P-X(10.7), C ₁ ' 1S(8.9), C ₁ 1S(7.9), H ₆ 1S(10.5),
15	-19.7930	1.0	N _c ' 1P-X(5.9), N _c 1P-Y(5.6), N _t ' 1P-Y(12.8), C ₃ ' 1P-Y(5.9), C ₃ ' 1P-Z(5.5), C ₂ ' 1P-Y(6.2), H ₁₃ 1S(7.5),
16	-19.7150	1.0	N _c 1P-X(5.7), N _c 1P-Y(5.4), N _t 1P-Y(13.0), C ₁ ' 1P-Y(5.8), C ₁ ' 1P-Z(5.2), C ₃ 1P-Y(6.7), H ₄ 1S(5.0), H ₅ 1S(7.2),
17	-19.0470	1.0	O ^A 1S(7.5), O ^A 1P-X(12.3), O ^A 1P-Y(6.4), O ^{A'} 1S(6.9), O ^{A'} 1P-X(10.8), O ^{A'} 1P-Y(5.3), C _a 1S(10.1), H ₂ 1S(5.8),
18	-18.7850	1.0	N _c ' 1P-X(8.9), N _t ' 1P-X(8.6), N _t ' 1P-Z(10.7), C ₂ ' 1P-X(6.6), C ₂ ' 1P-Y(9.0), H ₁₈ 1S(5.7),
19	-18.7150	1.0	N _c 1P-X(9.2), N _t 1P-X(10.7), N _t 1P-Z(7.3), C ₃ 1P-X(5.6), C ₃ 1P-Y(9.2), H ₁₀ 1S(5.7),
20	-18.3540	1.0	N _t 1P-Z(7.6), N _t ' 1P-Z(9.1),
21	-18.1420	1.0	N _t 1P-Z(6.0), C ₁ 1P-X(6.1), C ₂ ' 1P-X(5.1),
22	-17.7240	1.0	O ^A 1P-Y(6.2), O ^{A'} 1P-X(5.2), O ^{A'} 1P-Y(6.8), H ₈ 1S(5.9), H ₁₆ 1S(7.2),
23	-17.5450	1.0	N _t ' 1P-Y(5.1), N _t ' 1P-Y(5.7), C ₃ 1P-X(6.6), C ₂ ' 1P-X(8.1), H ₈ 1S(6.7), H ₁₆ 1S(6.0),
24	-17.3770	1.0	O ^A 1P-Y(8.3), O ^{A'} 1P-X(5.1), O ^{A'} 1P-Y(8.9), C ₃ 1P-X(7.1), H ₉ 1S(5.2),
25	-16.7290	1.0	O ^A 1P-X(15.8), O ^{A'} 1P-X(14.4), C _a 1P-Y(15.4), C _a 2P-Y(5.7), C _b 1P-Y(16.0), H ₂ 1S(5.3),
26	-16.4830	1.0	N _c ' 1P-X(5.9), C ₂ 1P-Z(13.8), C ₂ ' 1P-Y(10.3), C ₂ ' 1P-Z(9.2), H ₁₅ 1S(10.8), H ₁₈ 1S(9.2),
27	-16.4200	1.0	N _c 1P-X(5.2), C ₁ 1P-Z(13.4), C ₂ ' 1P-Y(10.2), C ₃ 1P-Z(11.1), H ₇ 1S(10.3), H ₁₀ 1S(9.5),
28	-16.2460	1.0	N _c ' 1P-Y(5.5), N _t ' 1P-X(6.1), N _t ' 1P-Y(6.2), C ₃ ' 1P-X(9.3), C ₂ ' 1P-Z(19.5), H ₁₄ 1S(7.6), H ₁₇ 1S(5.1),
29	-16.1920	1.0	N _c 1P-Y(5.1), N _t 1P-X(6.0), N _t 1P-Y(6.2), C ₁ ' 1P-X(10.0), C ₃ 1P-Z(18.4), H ₆ 1S(8.0),
30	-16.0100	1.0	N _t ' 1P-X(8.6), N _t ' 1P-Y(6.5), C ₃ ' 1P-X(5.1), C ₂ 1P-Y(6.6), C ₂ ' 1P-X(5.8), C ₂ ' 1P-Y(8.3), H ₁₇ 1S(6.0),
31	-15.9600	1.0	N _t 1P-X(9.2), N _t 1P-Y(6.5), C ₁ 1P-X(5.0), C ₁ 1P-Y(6.6), C ₃ 1P-X(6.0), C ₃ 1P-Y(8.6), H ₉ 1S(6.1),
32	-14.7860	1.0	O ^A 1P-X(5.5), C _b 1P-X(40.3), H ₁ 1S(28.6), H ₂ 1S(13.0),
33	-14.7200	1.0	Mn _{III} 1D(X2-Y2)(7.0), Mn _{IV} 1D(X2-Y2)(6.1), O 1P-Z(60.5),
34	-14.4310	1.0	C ₃ ' 1P-X(6.5), C ₂ 1P-X(11.8), H ₁₄ 1S(8.0), H ₁₅ 1S(9.0), H ₁₆ 1S(6.3),
35	-14.3420	1.0	Mn _{III} 1D-Z2(4.1), O 1P-X(41.9), C ₃ 1P-Z(7.5), C ₂ ' 1P-Z(5.5),

TABLE S27: Orbital Energies/ $\text{Mn}_{\text{III}}\text{Mn}_{\text{IV}}(\mu-\text{O})_2(\text{Oac})(\text{TACN})_2$ HS ACCINT=3.5

S129

Orbital	Energy (eV)	Occupancy	Primary Contributors SFO(%)
36	-14.3320	1.0	O 1P-X(14.5), C ₁ 1P-X(7.1), C ₁ 1P-X(9.7), H ₆ 1S(6.1), H ₇ 1S(5.2), H ₈ 1S(6.9),
37	-13.7620	1.0	O 1P-Y(24.0), N _c 1P-Y(7.1), N _c 1P-Y(16.1),
38	-13.6490	1.0	Mn _{III} 1D-XY(7.7), Mn _{IV} 1D-XY(4.0), O 1P-Y(17.5), O ^a 1P-Y(9.8), O ^a 1P-Y(6.7), N _c 1P-Y(9.0), C _b 1P-Y(8.7),
39	-13.5390	1.0	Mn _{IV} 1D(X2-Y2)(5.0), N _c 1P-Y(26.4), N _c 1P-Y(8.3), C ₁ 1P-Y(6.6),
40	-13.0500	1.0	N _t 1P-Z(10.6), N _t 1P-X(6.3), N _t 1P-Z(14.8), C ₂ 1P-Z(5.4),
41	-12.8750	1.0	O 1P-X(16.0), N _t 1P-X(7.0), N _t 1P-Z(13.2), N _t 1P-Z(8.9),
42	-12.3760	1.0	O ^a 1P-X(20.9), O ^a 1P-Y(34.1), O ^a 1P-X(12.6), N _c 1P-Y(5.2),
43	-12.3300	1.0	Mn _{III} 1D-XY(4.3), O 1P-Y(16.3), O ^a 1P-X(9.5), O ^a 1P-Y(33.0), N _c 1P-Y(6.6), C _b 1P-Y(5.7),
44	-9.2580	0.0	Mn _{III} 1D-Z2(33.9), Mn _{III} 1D(X2-Y2)(6.3), Mn _{IV} 1D-Z2(31.5), Mn _{IV} 1D(X2-Y2)(4.6), O 1P-Z(11.3),
45	-9.0470	0.0	Mn _{III} 1D-Z2(7.4), Mn _{III} 1D-XY(46.7), Mn _{IV} 1D-XY(34.7),
46	-8.4630	0.0	Mn _{III} 1D(X2-Y2)(25.8), Mn _{III} 1D-XY(9.2), Mn _{IV} 1D-Z2(22.1), Mn _{IV} 1D(X2-Y2)(12.7), Mn _{IV} 1D-XY(9.5), O 1P-Y(7.2),
47	-8.4440	0.0	Mn _{III} 1D-Z2(13.1), Mn _{III} 1D(X2-Y2)(5.7), Mn _{III} 1D-XY(13.4), Mn _{IV} 1D(X2-Y2)(17.0), Mn _{IV} 1D-XY(27.7), O 1P-Y(14.0),
48	-7.3290	0.0	Mn _{III} 1D-Z2(16.6), Mn _{III} 1D(X2-Y2)(35.0), Mn _{III} 1D-XY(6.9), Mn _{IV} 1D(X2-Y2)(9.4), O ^a 1P-Y(5.1), N _c 1P-Y(5.3),
49	-7.1060	0.0	Mn _{III} 1D-Z2(7.6), Mn _{IV} 1D-Z2(24.5), Mn _{IV} 1D(X2-Y2)(29.5), Mn _{IV} 1D-XY(7.8), O 1P-X(7.7), N _c 1P-Y(5.4),
50	-6.8120	0.0	H ₃ 1S(18.1), H ₃ 2S(8.9), H ₅ 1S(6.8), H ₁₁ 1S(17.5), H ₁₁ 2S(8.1), H ₁₃ 1S(7.2),
51	-5.9350	0.0	C ₂ 1P-X(5.1), H ₁₄ 1S(5.1),
52	-5.7760	0.0	C ₃ 1P-X(5.2), H ₃ 1S(8.2), H ₁₁ 1S(8.7),
53	-5.4050	0.0	H ₄ 1S(11.2), H ₆ 1S(8.1), H ₁₀ 1S(7.1), H ₁₂ 1S(11.6), H ₁₄ 1S(7.7), H ₁₈ 1S(7.8),

TABLE S27: Orbital Energies/ $\text{Mn}_{\text{III}}\text{Mn}_{\text{IV}}(\mu-\text{O})_2(\text{Oac})(\text{TACN})_2$ HS ACCINT=3.5

S130

 $\text{Mn}_{\text{III}}\text{Mn}_{\text{IV}}(\mu-\text{O})_2(\text{Oac})(\text{TACN})_2$ HS ACCINT=3.5 Orbital Energies and Descriptions for $\beta - \text{A}''$

Orbital	Energy (eV)	Occupancy	Primary Contributors SFO(%)
1	-29.1110	1.0	$\text{N}_t^{'}$ 1S(62.1), C_2 1S(13.7), H_{12} 1S(11.2),
2	-29.0740	1.0	$\text{N}_t^{'}$ 1S(62.1), C_1 1S(13.6), H_4 1S(11.2),
3	-27.6220	1.0	O 1S(93.9),
4	-25.0650	1.0	$\text{N}_c^{'}$ 1P-Z(7.8), $\text{N}_t^{'}$ 1P-Y(5.5), $\text{C}_3^{'}$ 1S(34.0), C_2 1S(18.7), H_{13} 1S(8.3),
5	-25.0170	1.0	$\text{N}_c^{'}$ 1P-Z(7.7), $\text{N}_t^{'}$ 1P-Y(5.5), $\text{C}_1^{'}$ 1S(33.9), C_1 1S(18.8), H_5 1S(8.3),
6	-21.9200	1.0	$\text{N}_c^{'}$ 1P-Z(7.9), $\text{N}_t^{'}$ 1P-Y(7.8), $\text{N}_t^{'}$ 1P-Z(5.0), $\text{C}_3^{'}$ 1S(13.1), C_2 1S(12.3), $\text{C}_2^{'}$ 1S(13.5), H_{13} 1S(6.3), H_{15} 1S(6.2), H_{18} 1S(5.8),
7	-21.8750	1.0	$\text{N}_c^{'}$ 1P-Z(7.8), $\text{N}_t^{'}$ 1P-Y(7.8), $\text{N}_t^{'}$ 1P-Z(5.1), $\text{C}_1^{'}$ 1S(13.1), C_1 1S(12.1), C_3 1S(13.6), H_5 1S(6.4), H_7 1S(6.2), H_{10} 1S(5.9),
8	-20.7920	1.0	$\text{N}_t^{'}$ 1P-X(17.6), C_2 1S(7.8), $\text{C}_2^{'}$ 1S(14.3), H_{12} 1S(6.3), H_{16} 1S(9.7), H_{17} 1S(10.7), H_{18} 1S(5.5),
9	-20.7520	1.0	$\text{N}_t^{'}$ 1P-X(17.6), C_1 1S(7.9), C_3 1S(14.1), H_4 1S(6.3), H_8 1S(9.8), H_9 1S(10.6), H_{10} 1S(5.4),
10	-18.7010	1.0	$\text{N}_t^{'}$ 1P-X(5.1), $\text{N}_t^{'}$ 1P-Y(25.9), C_2 1P-Z(13.3), H_{12} 1S(7.7), H_{15} 1S(7.0),
11	-18.6580	1.0	$\text{N}_t^{'}$ 1P-X(5.1), $\text{N}_t^{'}$ 1P-Y(25.9), C_1 1P-Z(13.5), H_4 1S(7.7), H_7 1S(7.2),
12	-17.8630	1.0	$\text{N}_c^{'}$ 1P-Z(12.6), $\text{C}_3^{'}$ 1P-X(18.6), C_2 1P-X(12.2), H_{14} 1S(10.9), H_{15} 1S(8.1),
13	-17.8130	1.0	$\text{N}_c^{'}$ 1P-Z(12.5), $\text{C}_1^{'}$ 1P-X(18.6), C_1 1P-X(12.3), H_6 1S(10.9), H_7 1S(8.1),
14	-16.6550	1.0	O^{α} 1P-Z(21.3), $\text{O}^{\alpha'}$ 1P-Z(21.0), C_k 1P-Z(30.1), C_b 1P-Z(13.7), H_2 1S(8.2),
15	-16.3520	1.0	$\text{N}_c^{'}$ 1P-Z(8.7), $\text{N}_t^{'}$ 1P-X(6.8), $\text{N}_t^{'}$ 1P-Z(6.6), $\text{C}_3^{'}$ 1P-Y(7.3), $\text{C}_3^{'}$ 1P-Z(7.3), C_2 1P-X(13.2), C_2 1P-Y(7.8), C_2 1P-Z(7.0), H_{16} 1S(12.0),
16	-16.3040	1.0	$\text{N}_c^{'}$ 1P-Z(8.6), $\text{N}_t^{'}$ 1P-X(6.9), $\text{N}_t^{'}$ 1P-Z(6.6), $\text{C}_1^{'}$ 1P-Y(7.6), $\text{C}_1^{'}$ 1P-Z(7.2), C_1 1P-X(13.0), C_1 1P-Y(8.0), C_1 1P-Z(7.1), H_8 1S(11.9),
17	-16.1810	1.0	$\text{N}_t^{'}$ 1P-X(5.2), $\text{N}_t^{'}$ 1P-Z(20.7), $\text{C}_3^{'}$ 1P-X(6.9), $\text{C}_2^{'}$ 1P-X(11.3), H_{14} 1S(7.5), H_{17} 1S(8.4),
18	-16.1400	1.0	$\text{N}_c^{'}$ 1P-X(5.2), $\text{N}_t^{'}$ 1P-Z(20.8), $\text{C}_1^{'}$ 1P-X(7.0), C_3 1P-X(11.3), H_6 1S(7.5), H_9 1S(8.4),
19	-15.8820	1.0	$\text{N}_c^{'}$ 1P-Z(7.9), $\text{N}_t^{'}$ 1P-Y(5.6), $\text{C}_3^{'}$ 1P-Y(18.8), $\text{C}_3^{'}$ 1P-Z(6.0), C_2 1P-X(5.6), H_{13} 1S(20.2), H_{16} 1S(5.9),
20	-15.8330	1.0	$\text{N}_c^{'}$ 1P-Z(8.1), $\text{N}_t^{'}$ 1P-Y(5.6), $\text{C}_1^{'}$ 1P-Y(18.8), $\text{C}_1^{'}$ 1P-Z(6.1), C_1 1P-X(5.7), H_5 1S(20.1), H_8 1S(6.1),
21	-14.6240	1.0	Mn_{III} 1D-XZ(15.4), Mn_{IV} 1D-XZ(13.2), O 1P-X(55.9),
22	-14.5750	1.0	O^{α} 1P-Z(11.3), $\text{O}^{\alpha'}$ 1P-Z(7.8), C_b 1P-Z(32.2), H_2 1S(33.3),
23	-14.2560	1.0	Mn_{III} 1D-XZ(5.9), Mn_{IV} 1D-XZ(7.1), O 1P-Z(14.3), $\text{C}_2^{'}$ 1P-Y(5.9), H_2 1S(6.3), H_{17} 1S(8.9),
24	-14.1220	1.0	$\text{C}_3^{'}$ 1P-Y(7.6), $\text{C}_2^{'}$ 1P-Y(6.2), H_9 1S(10.0), H_{10} 1S(5.9), H_{17} 1S(8.3), H_{18} 1S(5.1),
25	-14.0010	1.0	$\text{C}_3^{'}$ 1P-X(6.2), $\text{C}_3^{'}$ 1P-Z(7.5), H_{14} 1S(8.7), H_{15} 1S(9.8),
26	-13.9260	1.0	$\text{C}_1^{'}$ 1P-X(5.9), $\text{C}_1^{'}$ 1P-Z(6.6), H_6 1S(7.8), H_7 1S(9.9),
27	-13.7980	1.0	O 1P-Z(9.8), C_3 1P-Y(8.5), $\text{C}_2^{'}$ 1P-Y(6.1), H_{10} 1S(8.2), H_{18} 1S(6.1),
28	-13.2190	1.0	O 1P-X(8.5), O^{α} 1P-Z(13.3), $\text{O}^{\alpha'}$ 1P-Z(14.8), $\text{N}_t^{'}$ 1P-Z(8.8), $\text{N}_t^{'}$ 1P-Z(8.7),
29	-12.9190	1.0	O 1P-X(6.6), O^{α} 1P-Z(30.4), $\text{O}^{\alpha'}$ 1P-Z(32.1),
30	-12.6600	1.0	Mn_{III} 1D-YZ(7.2), Mn_{IV} 1D-YZ(6.0), O 1P-Y(58.9),
31	-12.3250	1.0	O 1P-Y(10.5), O 1P-Z(48.2), $\text{N}_t^{'}$ 1P-X(6.0), $\text{N}_t^{'}$ 1P-Z(6.3), $\text{N}_t^{'}$ 1P-X(5.6), $\text{N}_t^{'}$ 1P-Z(5.8),
32	-9.1830	0.0	Mn_{III} 1D-YZ(49.5), Mn_{IV} 1D-YZ(37.7),
33	-8.3510	0.0	Mn_{III} 1D-YZ(30.3), Mn_{IV} 1D-YZ(42.6), O 1P-Y(21.7),
34	-7.1290	0.0	Mn_{III} 1D-XZ(34.8), Mn_{IV} 1D-XZ(22.7), O 1P-X(18.8),
35	-6.7670	0.0	Mn_{III} 1D-XZ(25.6), Mn_{IV} 1D-XZ(38.0), O 1P-Z(17.8),

TABLE S27: Orbital Energies/ $\text{Mn}_{\text{III}}\text{Mn}_{\text{IV}}(\mu - \text{O})_2(\text{Oac})(\text{TACN})_2$ HS ACCINT=3.5

S131

Orbital	Energy (eV)	Occupancy	Primary Contributors SFO(%)
36	-6.1210	0.0	O ²⁻ 1P-Z(16.4), O ²⁻ 1P-Z(15.7), C ₆ 1P-Z(51.6), H ₂ 1S(9.2),
37	-5.1430	0.0	H ₄ 1S(10.4), H ₄ 2S(6.2), H ₅ 1S(6.8), H ₅ 2S(5.1), H ₇ 1S(14.8), H ₇ 2S(12.0), H ₁₂ 1S(9.6), H ₁₂ 2S(5.6), H ₁₃ 1S(6.8), H ₁₃ 2S(5.1), H ₁₅ 1S(13.8), H ₁₅ 2S(10.9),
38	-4.6530	0.0	H ₄ 1S(18.7), H ₄ 2S(5.5), H ₇ 1S(10.3), H ₁₂ 1S(18.8), H ₁₂ 2S(5.3), H ₁₃ 1S(5.3), H ₁₅ 1S(10.7),
39	-4.3110	0.0	H ₄ 1S(12.1), H ₅ 1S(5.9), H ₅ 2S(9.8), H ₆ 1S(5.3), H ₁₂ 1S(12.8), H ₁₃ 1S(5.4), H ₁₃ 2S(9.5), H ₁₄ 1S(5.9),
40	-4.0320	0.0	H ₆ 1S(8.2), H ₈ 1S(14.9), H ₈ 2S(9.3), H ₁₄ 1S(10.0), H ₁₆ 1S(19.2), H ₁₆ 2S(11.5),
41	-3.9240	0.0	H ₅ 1S(5.9), H ₆ 1S(5.2), H ₈ 1S(21.7), H ₈ 2S(11.3), H ₁₃ 1S(6.6), H ₁₆ 1S(16.8), H ₁₆ 2S(8.3),

TABLE S27: Orbital Energies/ $\text{Mn}_{\text{III}}\text{Mn}_{\text{IV}}(\mu - \text{O})_2(\text{Oac})(\text{TACN})_2$ S=5/2 ACCINT=3.5

S132

 $\text{Mn}_{\text{III}}\text{Mn}_{\text{IV}}(\mu - \text{O})_2(\text{Oac})(\text{TACN})_2$ S=5/2 ACCINT=3.5 Fragment Types

Atom types	Indices	Charges	Alpha Spin	Beta Spin	Net Spin
MnIII	1	1.008	4.197	1.794	2.4030
MnIV	2	1.000	4.202	1.798	2.4040
O	3 5	-0.761	3.474	3.286	0.1880
O ^a	4	-0.624	3.307	3.317	-0.0100
O ^{a'}	6	-0.626	3.309	3.317	-0.0080
N _c	7	-0.361	2.658	2.703	-0.0450
N _t	8 9	-0.414	2.695	2.719	-0.0240
N _{c'}	10	-0.361	2.658	2.703	-0.0450
N _{t'}	11 12	-0.413	2.694	2.719	-0.0250
C ^a	13	0.977	1.511	1.512	-0.0010
C ^b	14	0.235	1.879	1.886	-0.0070
C ₁	15 20	0.417	1.794	1.789	0.0050
C ₁	16 19	0.423	1.790	1.787	0.0030
C ₃	17 18	0.397	1.801	1.802	-0.0010
C ₃	21 26	0.417	1.794	1.789	0.0050
C ₂	22 25	0.420	1.791	1.789	0.0020
C ₂	23 24	0.397	1.801	1.802	-0.0010
H ₁	27	-0.067	0.533	0.534	-0.0010
H ₂	28 29	-0.053	0.527	0.527	0.0000
H ₃	30	0.105	0.451	0.444	0.0070
H ₄	31 32	0.161	0.420	0.419	0.0010
H ₅	33 43	-0.073	0.535	0.537	-0.0020
H ₆	34 44	-0.068	0.533	0.534	-0.0010
H ₇	35 41	-0.077	0.539	0.538	0.0010
H ₈	36 42	-0.075	0.537	0.538	-0.0010
H ₉	37 40	-0.075	0.537	0.537	0.0000
H ₁₀	38 39	-0.056	0.528	0.528	0.0000
H ₁₁	45	0.106	0.450	0.444	0.0060
H ₁₂	46 47	0.160	0.421	0.419	0.0020
H ₁₃	48 58	-0.073	0.536	0.537	-0.0010
H ₁₄	49 59	-0.068	0.533	0.534	-0.0010
H ₁₅	50 56	-0.076	0.538	0.538	0.0000
H ₁₆	51 57	-0.074	0.536	0.538	-0.0020
H ₁₇	52 55	-0.075	0.537	0.538	-0.0010
H ₁₈	53 54	-0.055	0.528	0.527	0.0010

TABLE S27: Orbital Energies/Mn_{III}Mn_{IV}(μ -O)₂(Oac)(TACN)₂ S=5/2 ACCINT=3.5

S133

Mn_{III}Mn_{IV}(μ -O)₂(Oac)(TACN)₂ S=5/2 ACCINT=3.5 Orbital Energies and Descriptions for α - A'

Orbital	Energy (eV)	Occupancy	Primary Contributors SFO(%)
1	-32.8530	1.0	O ^a 1S(34.8), O ^{a'} 1S(34.2), C _a 1S(18.0),
2	-30.5180	1.0	O ^a 1S(39.1), O ^{a'} 1S(39.6), C _a 1P-X(13.0),
3	-30.0880	1.0	N _c 1S(19.6), N _t 1S(10.2), N _c ' 1S(19.2), N _t ' 1S(10.1), C ₁ ' 1S(8.1), C ₃ ' 1S(7.9),
4	-30.0370	1.0	N _c 1S(19.0), N _t 1S(9.8), N _c ' 1S(19.3), N _t ' 1S(10.0), C ₁ ' 1S(8.1), C ₃ ' 1S(8.2),
5	-29.1850	1.0	N _c 1S(11.1), N _t 1S(18.9), N _c ' 1S(11.9), N _t ' 1S(20.1), C ₃ 1S(6.1), C ₂ ' 1S(6.5),
6	-29.1620	1.0	N _c 1S(11.5), N _t 1S(20.5), N _c ' 1S(10.9), N _t ' 1S(19.3), C ₃ 1S(6.7), C ₂ ' 1S(6.2),
7	-28.2570	1.0	O 1S(90.3),
8	-25.0470	1.0	C ₁ 1S(9.4), C ₃ 1S(14.5), C ₂ 1S(11.9), C ₂ ' 1S(18.4),
9	-25.0390	1.0	C ₁ 1S(11.9), C ₃ 1S(18.7), C ₂ 1S(9.3), C ₂ ' 1S(14.8),
10	-23.4420	1.0	C _b 1S(14.5), C ₃ 1S(5.3), C ₂ ' 1S(5.3), H ₂ 1S(6.6),
11	-23.4130	1.0	C ₁ ' 1S(6.6), C ₃ 1S(7.6), C ₃ ' 1S(6.5), C ₂ ' 1S(7.6),
12	-23.3620	1.0	C _a 1S(5.6), C _a 1P-Y(6.2), C _b 1S(29.7), H ₁ 1S(6.4), H ₂ 1S(13.9),
13	-21.1380	1.0	N _c 1P-X(8.2), N _c ' 1P-X(8.1), C ₁ ' 1S(5.0), C ₁ 1S(5.7), C ₂ 1S(5.6), H ₆ 1S(6.0), H ₁₄ 1S(5.9),
14	-21.0480	1.0	N _c 1P-X(7.1), N _c ' 1P-X(7.2), C ₁ ' 1S(5.4), C ₁ 1S(5.5), C ₃ ' 1S(5.5), C ₂ 1S(5.6), H ₆ 1S(6.6), H ₁₄ 1S(6.7),
15	-19.8310	1.0	N _t 1P-Y(7.2), N _t ' 1P-Y(7.2), H ₁₃ 1S(5.0),
16	-19.7520	1.0	N _t 1P-Y(7.5), N _t ' 1P-Y(7.4), H ₅ 1S(5.1), H ₁₃ 1S(5.1),
17	-19.2820	1.0	O ^a 1S(7.2), O ^{a'} 1P-X(11.9), O ^a 1P-Y(6.1), O ^{a'} 1S(7.1), O ^{a'} 1P-X(11.5), O ^{a'} 1P-Y(5.9), C _a 1S(10.2), H ₂ 1S(5.8),
18	-18.7820	1.0	N _t 1P-X(5.3), N _t 1P-Z(7.3), N _t ' 1P-X(5.6), N _t ' 1P-Z(7.5), C ₃ 1P-Y(6.3), C ₂ ' 1P-Y(6.6),
19	-18.7390	1.0	N _t 1P-X(7.9), N _t ' 1P-X(7.6), C ₃ 1P-Y(6.8), C ₂ ' 1P-Y(6.5),
20	-18.4240	1.0	N _t 1P-Z(8.5), N _t ' 1P-Z(8.4),
21	-18.1580	1.0	C ₁ 1P-X(5.4), C ₂ 1P-X(5.5),
22	-17.8840	1.0	O ^a 1P-X(5.7), O ^a 1P-Y(8.9), O ^{a'} 1P-X(6.1), O ^{a'} 1P-Y(8.9), C _a 1P-X(5.6), H ₈ 1S(5.3), H ₁₆ 1S(5.1),
23	-17.5330	1.0	N _t 1P-Y(5.5), N _t ' 1P-Y(5.8), C ₃ 1P-X(7.1), C ₂ ' 1P-X(7.5), H ₈ 1S(6.5), H ₁₆ 1S(6.8),
24	-17.4460	1.0	C ₃ 1P-X(8.1), C ₂ ' 1P-X(7.6), H ₉ 1S(5.1),
25	-16.9390	1.0	O ^a 1P-X(14.9), O ^{a'} 1P-X(14.1), O ^{a'} 1P-Y(5.2), C _a 1P-Y(14.5), C _a 2P-Y(5.4), C _b 1P-Y(15.0), H ₂ 1S(5.1),
26	-16.5050	1.0	C ₁ 1P-Z(7.7), C ₂ 1P-Z(7.7), H ₇ 1S(6.4), H ₁₅ 1S(6.4),
27	-16.4470	1.0	C ₁ 1P-Z(7.2), C ₃ 1P-Z(7.7), C ₂ 1P-Z(7.2), C ₂ ' 1P-Z(7.7), H ₇ 1S(5.9), H ₁₅ 1S(5.9),
28	-16.2570	1.0	C ₃ 1P-Z(10.4), C ₂ ' 1P-Z(11.1),
29	-16.2380	1.0	C ₁ 1P-X(7.0), C ₃ 1P-Z(8.3), C ₃ ' 1P-X(6.5), C ₂ ' 1P-Z(7.5),
30	-16.0210	1.0	C ₃ 1P-Y(6.1), C ₂ ' 1P-Y(6.0),
31	-15.9660	1.0	N _t 1P-X(5.8), N _t ' 1P-X(5.8), C ₃ 1P-Y(6.5), C ₂ ' 1P-Y(6.4),
32	-15.2430	1.0	Mn _{III} 1D-Z2(5.1), Mn _{III} 1D(X2-Y2)(10.7), Mn _{IV} 1D-Z2(5.1), Mn _{IV} 1D(X2-Y2)(10.8), O 1P-Z(49.9),
33	-14.9280	1.0	O ^{a'} 1P-X(5.1), C _b 1P-X(40.5), H ₁ 1S(28.3), H ₂ 1S(12.9),
34	-14.7970	1.0	Mn _{III} 1D-XY(11.4), Mn _{IV} 1D-XY(11.4), O 1P-Y(34.2),
35	-14.6920	1.0	Mn _{III} 1D-Z2(9.2), Mn _{IV} 1D-Z2(9.1), O 1P-X(44.6),

TABLE S27: Orbital Energies/Mn_{III}Mn_{IV}(μ-O)₂(OAc)(TACN)₂ S=5/2 ACCINT=3.5

S134

Orbital	Energy (eV)	Occupancy	Primary Contributors SFO(%)
36	-14.3600	1.0	C ₁ 1P-X(8.7), C ₂ 1P-X(8.6), H ₆ 1S(5.8), H ₇ 1S(6.7), H ₁₄ 1S(5.8), H ₁₅ 1S(6.6),
37	-14.2820	1.0	Mn _{III} 1D-XY(4.5), Mn _{IV} 1D-XY(4.6), O 1P-Y(9.5), C ₁ 1P-X(6.4), C ₂ 1P-X(6.4), H ₇ 1S(5.1), H ₁₅ 1S(5.2),
38	-14.1220	1.0	Mn _{III} 1D-ZZ(4.5), Mn _{IV} 1D-ZZ(4.5), N _c 1P-Y(9.8), N _{c'} 1P-Y(9.5), C _{1'} 1P-Y(5.1),
39	-13.9520	1.0	Mn _{III} 1D(X2-Y2)(4.5), Mn _{IV} 1D(X2-Y2)(4.4), N _c 1P-Y(12.1), N _{c'} 1P-Y(12.5), C _{1'} 1P-Y(5.3), C _{3'} 1P-Y(5.4),
40	-13.0930	1.0	O ^a 1P-Y(7.4), O ^{a'} 1P-Y(8.1), N _t 1P-Z(5.6),
41	-13.0730	1.0	Mn _{III} 1D-ZZ(4.0), Mn _{III} 1D(X2-Y2)(5.6), Mn _{IV} 1D-ZZ(4.5), Mn _{IV} 1D(X2-Y2)(5.1), O 1P-X(6.7), N _t 1P-Z(7.8), N _{t'} 1P-X(5.1), N _{t'} 1P-Z(9.2),
42	-12.9000	1.0	O ^a 1P-Y(10.1), O ^{a'} 1P-Y(11.0), N _t 1P-Z(8.3), N _{t'} 1P-Z(7.9), C _b 1P-Y(5.0),
43	-12.6290	1.0	O ^a 1P-X(17.8), O ^{a'} 1P-Y(18.6), O ^{a'} 1P-X(17.2), O ^{a'} 1P-Y(17.1),
44	-12.1130	1.0	Mn _{III} 1D-ZZ(4.3), Mn _{III} 1D-XY(36.4), Mn _{IV} 1D-ZZ(4.3), Mn _{IV} 1D-XY(36.5),
45	-11.1430	1.0	Mn _{III} 1D-ZZ(30.6), Mn _{IV} 1D-ZZ(30.7), O 1P-Z(24.1),
46	-10.7560	1.0	Mn _{III} 1D-XY(19.2), Mn _{IV} 1D-XY(19.2), O 1P-Y(44.8),
47	-10.6800	1.0	Mn _{III} 1D-ZZ(12.3), Mn _{III} 1D(X2-Y2)(22.4), Mn _{IV} 1D-ZZ(12.3), Mn _{IV} 1D(X2-Y2)(22.3), O 1P-X(10.7),
48	-8.9230	0.0	Mn _{III} 1D(X2-Y2)(20.4), Mn _{IV} 1D-ZZ(4.1), Mn _{IV} 1D(X2-Y2)(21.1), O 1P-Z(8.2), O ^a 1P-Y(5.3), O ^{a'} 1P-Y(5.4),
49	-8.7720	0.0	Mn _{III} 1D-ZZ(17.0), Mn _{III} 1D(X2-Y2)(8.8), Mn _{III} 1D-XY(4.4), Mn _{IV} 1D-ZZ(16.5), Mn _{IV} 1D(X2-Y2)(8.0), Mn _{IV} 1D-XY(4.2), O 1P-X(15.8),
50	-6.8930	0.0	H ₃ 1S(20.0), H ₃ 2S(8.9), H ₅ 1S(7.2), H ₁₁ 1S(19.6), H ₁₁ 2S(8.7), H ₁₃ 1S(7.2),
51	-5.9270	0.0	
52	-5.7990	0.0	H ₃ 1S(7.9), H ₁₁ 1S(7.8),
53	-5.4050	0.0	H ₄ 1S(11.8), H ₆ 1S(7.9), H ₁₀ 1S(7.3), H ₁₂ 1S(11.3), H ₁₄ 1S(7.8), H ₁₈ 1S(6.9),
54	-5.2830	0.0	C ₃ ' 1P-X(5.1), H ₄ 1S(11.6), H ₆ 1S(7.2), H ₁₀ 1S(9.6), H ₁₂ 1S(12.1), H ₁₃ 1S(5.0), H ₁₄ 1S(7.6), H ₁₈ 1S(9.8),
55	-4.6100	0.0	H ₆ 1S(6.5), H ₆ 2S(9.8), H ₁₄ 1S(6.6), H ₁₄ 2S(9.6),
56	-4.4970	0.0	H ₃ 1S(9.2), H ₅ 2S(6.9), H ₆ 1S(5.8), H ₆ 2S(9.4), H ₁₃ 1S(9.4), H ₁₃ 2S(7.1), H ₁₄ 1S(6.2), H ₁₄ 2S(10.0),
57	-4.2650	0.0	H ₃ 1S(8.4), H ₅ 1S(9.6), H ₁₀ 1S(11.2), H ₁₀ 2S(6.6), H ₁₁ 1S(8.4), H ₁₃ 1S(9.7), H ₁₈ 1S(11.9), H ₁₈ 2S(6.7),

TABLE S27: Orbital Energies/Mn_{III}Mn_{IV}(μ-O)₂(Oac)(TACN)₂ S=5/2 ACCINT=3.5

S135

Mn_{III}Mn_{IV}(μ-O)₂(Oac)(TACN)₂ S=5/2 ACCINT=3.5 Orbital Energies and Descriptions for α - A''

Orbital	Energy (eV)	Occupancy	Primary Contributors SFO(%)
1	-28.9990	1.0	N _t ' 1S(57.3), C ₂ 1S(13.2), H ₁₂ 1S(10.3),
2	-28.9970	1.0	N _t 1S(57.4), C ₁ 1S(13.2), H ₄ 1S(10.4),
3	-27.8370	1.0	O 1S(93.5),
4	-25.0710	1.0	N _c 1P-Z(6.3), C ₁ ' 1S(27.0), C ₁ 1S(13.8), C ₃ ' 1S(7.7), H ₅ 1S(6.6),
5	-25.0690	1.0	N _c ' 1P-Z(6.4), C ₁ ' 1S(7.6), C ₃ 1S(26.9), C ₂ 1S(13.8), H ₁₃ 1S(6.6),
6	-21.9000	1.0	N _c 1P-Z(6.2), N _t 1P-Y(5.9), C ₃ ' 1S(9.2), C ₂ 1S(10.0), C ₂ ' 1S(9.2),
7	-21.8980	1.0	N _c 1P-Z(6.1), N _t 1P-Y(5.9), C ₁ ' 1S(9.2), C ₁ 1S(10.0), C ₃ 1S(9.2),
8	-20.7340	1.0	N _t 1P-X(7.0), N _t ' 1P-X(10.4), C ₃ 1S(6.2), C ₂ ' 1S(9.3), H ₁₆ 1S(5.6), H ₁₇ 1S(6.6),
9	-20.7280	1.0	N _t 1P-X(10.5), N _t ' 1P-X(7.0), C ₃ 1S(9.3), C ₂ ' 1S(6.2), H ₈ 1S(5.7), H ₉ 1S(6.6),
10	-18.6740	1.0	N _t 1P-Y(12.7), N _t ' 1P-Y(12.9), C ₁ 1P-Z(6.2), C ₂ 1P-Z(6.3),
11	-18.6550	1.0	N _t 1P-Y(13.2), N _t ' 1P-Y(12.9), C ₁ 1P-Z(6.5), C ₂ 1P-Z(6.4),
12	-17.8830	1.0	N _c 1P-Z(6.2), N _c ' 1P-Z(6.3), C ₁ ' 1P-X(9.3), C ₁ 1P-X(5.6), C ₃ ' 1P-X(9.4), C ₂ 1P-X(5.7), H ₆ 1S(5.6), H ₁₄ 1S(5.6),
13	-17.8710	1.0	N _c 1P-Z(6.1), N _c ' 1P-Z(6.1), C ₁ ' 1P-X(9.6), C ₁ 1P-X(5.8), C ₃ ' 1P-X(9.5), C ₂ 1P-X(5.8), H ₆ 1S(5.6), H ₁₄ 1S(5.6),
14	-16.8720	1.0	O ^a 1P-Z(21.9), O ^{a'} 1P-Z(22.2), C _a 1P-Z(30.1), C _b 1P-Z(12.5), H ₂ 1S(7.2),
15	-16.3680	1.0	C ₁ 1P-X(7.4), C ₂ 1P-X(6.6), H ₈ 1S(6.6), H ₁₆ 1S(5.9),
16	-16.3500	1.0	C ₁ 1P-X(7.0), C ₂ 1P-X(7.8), H ₈ 1S(6.1), H ₁₆ 1S(6.7),
17	-16.1220	1.0	N _t 1P-Z(8.6), N _t ' 1P-Z(11.5), C ₂ ' 1P-X(6.3),
18	-16.1100	1.0	N _t 1P-Z(12.1), N _t ' 1P-Z(9.2), C ₃ 1P-X(6.7), C ₂ ' 1P-X(5.1),
19	-15.9010	1.0	C ₁ ' 1P-Y(9.9), C ₃ ' 1P-Y(8.9), H ₅ 1S(10.9), H ₁₃ 1S(9.9),
20	-15.8930	1.0	C ₁ ' 1P-Y(8.6), C ₃ ' 1P-Y(9.5), H ₅ 1S(9.8), H ₁₃ 1S(10.8),
21	-15.0220	1.0	Mn _{III} 1D-XZ(16.8), Mn _{IV} 1D-XZ(16.7), O 1P-X(47.8),
22	-14.8050	1.0	Mn _{III} 1D-YZ(4.2), O 1P-Y(6.8), O ^a 1P-Z(7.9), O ^{a'} 1P-Z(5.4), C _b 1P-Z(31.3), H ₂ 1S(31.2),
23	-14.4390	1.0	Mn _{III} 1D-XZ(13.1), Mn _{IV} 1D-XZ(13.1), O 1P-Z(22.1),
24	-14.1090	1.0	H ₉ 1S(7.8), H ₁₇ 1S(6.9),
25	-14.0500	1.0	H ₆ 1S(5.1), H ₁₄ 1S(5.8), H ₁₅ 1S(5.1),
26	-13.9260	1.0	C ₃ 1P-Y(6.7), C ₂ ' 1P-Y(6.5), H ₇ 1S(6.3), H ₁₀ 1S(5.4), H ₁₅ 1S(6.1), H ₁₈ 1S(5.3),
27	-13.9020	1.0	Mn _{III} 1D-YZ(5.2), Mn _{IV} 1D-YZ(5.8), O 1P-Y(12.2), C ₃ 1P-Y(5.2), C ₂ ' 1P-Y(5.9), H ₁₈ 1S(5.0),
28	-13.6700	1.0	Mn _{III} 1D-YZ(10.8), Mn _{IV} 1D-YZ(13.1), O 1P-Y(21.5), O 1P-Z(6.4),
29	-13.4900	1.0	Mn _{III} 1D-YZ(11.0), Mn _{IV} 1D-YZ(7.9), O ^a 1P-Z(31.3), O ^{a'} 1P-Z(36.3),
30	-13.1350	1.0	Mn _{III} 1D-YZ(4.1), Mn _{IV} 1D-YZ(4.1), O 1P-X(13.9), N _t 1P-X(8.0), N _t ' 1P-Z(10.6), N _t ' 1P-X(8.0), N _t ' 1P-Z(10.6),
31	-12.3350	1.0	O 1P-Z(42.0), N _t 1P-X(8.7), N _t 1P-Z(10.3), N _t ' 1P-X(8.7), N _t ' 1P-Z(10.4),
32	-11.9710	1.0	Mn _{III} 1D-YZ(31.7), Mn _{IV} 1D-YZ(31.8), O ^a 1P-Z(11.3), O ^{a'} 1P-Z(11.9),
33	-10.7950	1.0	Mn _{III} 1D-YZ(23.8), Mn _{IV} 1D-YZ(23.8), O 1P-Y(48.6),
34	-8.0260	0.0	Mn _{III} 1D-XZ(25.4), Mn _{IV} 1D-XZ(25.5), O 1P-X(23.1),
35	-7.7030	0.0	Mn _{III} 1D-XZ(28.2), Mn _{IV} 1D-XZ(28.1), O 1P-Z(25.2),

TABLE S27: Orbital Energies/ $\text{Mn}_{\text{III}}\text{Mn}_{\text{IV}}(\mu - \text{O})_2(\text{Oac})(\text{TACN})_2$ S=5/2 ACCINT=3.5

S136

Orbital	Energy (eV)	Occupancy	Primary Contributors SFO(%)
36	-6.3780	0.0	O ^a 1P-Z(16.9), O ^{a'} 1P-Z(16.1), C _a 1P-Z(55.6), H ₂ 1S(9.1),
37	-5.1640	0.0	H ₄ 1S(10.4), H ₄ 2S(6.2), H ₅ 1S(7.0), H ₅ 2S(5.1), H ₇ 1S(14.8), H ₇ 2S(11.9), H ₁₂ 1S(11.1), H ₁₂ 2S(6.6), H ₁₃ 1S(7.0), H ₁₃ 2S(5.1), H ₁₅ 1S(14.8), H ₁₅ 2S(11.7),
38	-4.6450	0.0	H ₄ 1S(18.5), H ₄ 2S(5.5), H ₅ 1S(5.1), H ₇ 1S(10.7), H ₁₂ 1S(19.8), H ₁₂ 2S(5.8), H ₁₅ 1S(10.3),
39	-4.3240	0.0	H ₄ 1S(12.5), H ₅ 1S(5.2), H ₅ 2S(9.2), H ₆ 1S(6.0), H ₁₂ 1S(12.0), H ₁₃ 1S(5.5), H ₁₃ 2S(9.2), H ₁₄ 1S(6.0),
40	-4.0230	0.0	H ₆ 1S(10.6), H ₈ 1S(17.1), H ₈ 2S(10.4), H ₁₄ 1S(9.6), H ₁₆ 1S(14.2), H ₁₆ 2S(8.8),
41	-3.8950	0.0	H ₅ 1S(7.4), H ₈ 1S(17.3), H ₈ 2S(8.5), H ₁₃ 1S(6.3), H ₁₄ 1S(5.9), H ₁₆ 1S(19.3), H ₁₆ 2S(9.8),
42	-3.5760	0.0	N _c 1P-Z(8.8), N _t 1P-Y(7.2), C ₁ 1P-Z(6.0), C ₁ 1P-Y(15.7), H ₉ 1S(8.6),
43	-3.5610	0.0	N _c 1P-Z(7.0), N _t 1P-Y(5.1), C ₂ 1P-Y(14.9), H ₅ 1S(5.5), H ₁₆ 1S(8.1), H ₁₇ 1S(9.3),

TABLE S27: Orbital Energies/Mn_{III}Mn_{IV}(μ-O)₂(Oac)(TACN)₂ S=5/2 ACCINT=3.5

S137

Mn_{III}Mn_{IV}(μ-O)₂(Oac)(TACN)₂ S=5/2 ACCINT=3.5 Orbital Energies and Descriptions for β - A'

Orbital	Energy (eV)	Occupancy	Primary Contributors SFO(%)
1	-32.8420	1.0	O ^A 1S(34.9), O ^{A'} 1S(34.2), C _a 1S(18.2),
2	-30.5040	1.0	O ^A 1S(39.1), O ^{A'} 1S(39.6), C _a 1P-X(13.3),
3	-30.0900	1.0	N _c 1S(20.2), N _t 1S(10.1), N _c ' 1S(19.6), N _t ' 1S(9.9), C ₁ ' 1S(8.2), C ₃ ' 1S(8.0),
4	-30.0450	1.0	N _c 1S(19.2), N _t 1S(9.6), N _c ' 1S(19.7), N _t ' 1S(9.9), C ₁ ' 1S(8.1), C ₃ ' 1S(8.3),
5	-29.1900	1.0	N _c 1S(10.8), N _t 1S(19.4), N _c ' 1S(11.6), N _t ' 1S(20.7), C ₃ 1S(6.2), C ₂ ' 1S(6.6),
6	-29.1700	1.0	N _c 1S(11.4), N _t 1S(20.9), N _c ' 1S(10.7), N _t ' 1S(19.4), C ₃ 1S(6.7), C ₂ ' 1S(6.2),
7	-27.9500	1.0	O 1S(91.5),
8	-25.0460	1.0	C ₁ 1S(9.4), C ₃ 1S(14.5), C ₂ 1S(11.9), C ₂ ' 1S(18.4),
9	-25.0380	1.0	C ₁ 1S(11.9), C ₃ 1S(18.7), C ₂ 1S(9.3), C ₂ ' 1S(14.8),
10	-23.4400	1.0	C _b 1S(15.8), C ₃ 1S(5.1), C ₂ ' 1S(5.1), H ₂ 1S(7.2),
11	-23.4110	1.0	C ₁ ' 1S(6.6), C ₃ 1S(7.6), C ₃ ' 1S(6.6), C ₂ ' 1S(7.6),
12	-23.3670	1.0	C _a 1S(5.3), C _a 1P-Y(6.1), C _b 1S(28.5), H ₁ 1S(6.1), H ₂ 1S(13.3),
13	-21.1320	1.0	N _c 1P-X(8.3), N _c ' 1P-X(8.2), C ₁ ' 1S(5.0), C ₁ 1S(5.7), C ₂ 1S(5.6), H ₆ 1S(6.0), H ₁₄ 1S(6.0),
14	-21.0450	1.0	N _c 1P-X(7.2), N _c ' 1P-X(7.3), C ₁ ' 1S(5.4), C ₁ 1S(5.5), C ₃ ' 1S(5.4), C ₂ 1S(5.6), H ₆ 1S(6.6), H ₁₄ 1S(6.7),
15	-19.8120	1.0	N _t 1P-Y(7.3), N _t ' 1P-Y(7.4), H ₅ 1S(5.1), H ₁₃ 1S(5.1),
16	-19.7400	1.0	N _t 1P-Y(7.6), N _t ' 1P-Y(7.5), H ₅ 1S(5.2), H ₁₃ 1S(5.1),
17	-19.2290	1.0	O ^A 1S(7.5), O ^A 1P-X(12.1), O ^A ' 1P-Y(6.3), O ^{A'} 1S(7.3), O ^{A'} 1P-X(11.7), O ^{A'} ' 1P-Y(6.0), C _a 1S(10.3), H ₂ 1S(6.0),
18	-18.7670	1.0	N _t 1P-X(5.4), N _t ' 1P-Z(7.2), N _c ' 1P-X(5.0), N _t ' 1P-X(5.7), N _t ' 1P-Z(7.5), C ₃ 1P-Y(6.3), C ₂ ' 1P-Y(6.6),
19	-18.7280	1.0	N _t 1P-X(7.7), N _t ' 1P-X(7.4), C ₃ 1P-Y(6.9), C ₂ ' 1P-Y(6.6),
20	-18.3780	1.0	N _t 1P-Z(8.5), N _t ' 1P-Z(8.3),
21	-18.1450	1.0	N _t 1P-Z(5.0), N _t ' 1P-Z(5.1), C ₁ 1P-X(5.4), C ₂ 1P-X(5.5),
22	-17.8290	1.0	O ^A 1P-X(6.0), O ^A 1P-Y(9.5), O ^A ' 1P-X(6.4), O ^{A'} ' 1P-Y(9.4), C _a 1P-X(5.6), H ₈ 1S(5.5), H ₁₆ 1S(5.3),
23	-17.5270	1.0	N _t 1P-Y(5.6), N _t ' 1P-Y(5.9), C ₃ 1P-X(7.3), C ₂ ' 1P-X(7.8), H ₈ 1S(6.5), H ₁₆ 1S(6.8),
24	-17.4350	1.0	C ₃ 1P-X(7.8), C ₂ ' 1P-X(7.4),
25	-16.9060	1.0	O ^A ' 1P-X(15.7), O ^{A'} ' 1P-X(14.8), O ^{A'} ' 1P-Y(5.1), C _a 1P-Y(15.2), C _a 2P-Y(5.7), C _b 1P-Y(15.5), H ₂ 1S(5.2),
26	-16.4880	1.0	C ₁ 1P-Z(7.9), C ₃ 1P-Y(5.2), C ₂ 1P-Z(8.0), C ₂ ' 1P-Y(5.3), H ₇ 1S(6.6), H ₁₅ 1S(6.6),
27	-16.4310	1.0	C ₁ 1P-Z(7.6), C ₃ 1P-Z(6.8), C ₂ 1P-Z(7.6), C ₂ ' 1P-Z(6.8), H ₇ 1S(6.4), H ₁₅ 1S(6.4),
28	-16.2320	1.0	C ₃ 1P-Z(11.8), C ₂ ' 1P-Z(13.0),
29	-16.2160	1.0	C ₁ 1P-X(6.4), C ₃ 1P-Z(10.2), C ₃ ' 1P-X(5.8), C ₂ ' 1P-Z(9.0),
30	-15.9930	1.0	C ₃ 1P-Y(5.7), C ₂ ' 1P-Y(5.7),
31	-15.9520	1.0	N _t 1P-X(5.8), N _t ' 1P-X(5.8), C ₃ 1P-Y(6.4), C ₂ ' 1P-Y(6.2),
32	-14.9200	1.0	O ^{A'} ' 1P-X(5.5), C _b 1P-X(40.4), H ₁ 1S(28.4), H ₂ 1S(12.9),
33	-14.6550	1.0	Mn _{III} 1D(X ₂ -Y ₂)(6.9), Mn _{IV} 1D(X ₂ -Y ₂)(6.9), O 1P-Z(53.8),
34	-14.4250	1.0	O 1P-Z(10.6), C ₁ 1P-X(7.7), C ₂ 1P-X(7.6), H ₇ 1S(6.2), H ₁₅ 1S(6.1),
35	-14.3920	1.0	Mn _{III} 1D-Z ₂ (5.2), Mn _{IV} 1D-Z ₂ (5.2), O 1P-X(36.2),

TABLE S27: Orbital Energies/Mn_{III}Mn_{IV}(μ-O)₂(Oac)(TACN)₂ S=5/2 ACCINT=3.5

Orbital	Energy (eV)	Occupancy	Primary Contributors SFO(%)
36	-14.3450	1.0	O 1P-X(16.8), C ₁ 1P-X(5.7), C ₃ 1P-Z(6.8), C ₂ 1P-X(5.7), C ₂ ' 1P-Z(6.8), H ₇ 1S(5.4), H ₁₅ 1S(5.4),
37	-13.9210	1.0	N _c 1P-Y(13.8), N _c ' 1P-Y(13.5), C ₁ ' 1P-Y(5.2), C ₃ ' 1P-Y(5.1),
38	-13.7600	1.0	N _c 1P-Y(15.6), N _c ' 1P-Y(16.9), C ₁ ' 1P-Y(5.5), C ₃ ' 1P-Y(5.7),
39	-13.7490	1.0	Mn _{III} 1D-XY(6.7), Mn _{IV} 1D-XY(5.9), O 1P-Y(35.1), O ^a 1P-Y(8.4), O ^{a'} 1P-Y(7.8), C _b 1P-Y(8.6),
40	-12.9720	1.0	N _t 1P-Z(12.3), N _t ' 1P-Z(12.4),
41	-12.8020	1.0	O 1P-X(13.8), N _t 1P-X(5.7), N _t 1P-Z(10.4), N _t ' 1P-X(5.7), N _t ' 1P-Z(10.5),
42	-12.6050	1.0	O ^a 1P-X(19.2), O ^a ' 1P-Y(17.1), O ^{a'} 1P-X(19.8), O ^{a'} ' 1P-Y(19.8),
43	-12.4860	1.0	Mn _{III} 1D-XY(5.1), Mn _{IV} 1D-XY(5.3), O 1P-Y(24.9), O ^a 1P-Y(16.0), O ^{a'} 1P-Y(13.0), C _b 1P-Y(5.8),
44	-9.6660	1.0	Mn _{III} 1D-Z2(34.2), Mn _{IV} 1D-Z2(34.3), O 1P-Z(9.4),
45	-9.2750	0.0	Mn _{III} 1D-XY(41.6), Mn _{IV} 1D-XY(41.5),
46	-8.6640	0.0	Mn _{III} 1D-Z2(16.4), Mn _{III} 1D(X2-Y2)(26.9), Mn _{IV} 1D-Z2(16.8), Mn _{IV} 1D(X2-Y2)(26.7), O 1P-X(5.6),
47	-8.6230	0.0	Mn _{III} 1D-Z2(5.8), Mn _{III} 1D-XY(27.3), Mn _{IV} 1D-Z2(5.4), Mn _{IV} 1D-XY(27.3), O 1P-Y(23.3),
48	-7.8510	0.0	Mn _{III} 1D-Z2(18.8), Mn _{III} 1D(X2-Y2)(9.9), Mn _{III} 1D-XY(4.0), Mn _{IV} 1D-Z2(19.1), Mn _{IV} 1D(X2-Y2)(11.3), Mn _{IV} 1D-XY(4.3), O 1P-X(12.8),
49	-7.7590	0.0	Mn _{III} 1D(X2-Y2)(29.1), Mn _{IV} 1D(X2-Y2)(27.6), O 1P-Z(8.6),
50	-6.8680	0.0	H ₃ 1S(18.8), H ₃ 2S(8.3), H ₅ 1S(7.4), H ₁₁ 1S(19.2), H ₁₁ 2S(8.6), H ₁₃ 1S(7.3),
51	-5.9230	0.0	H ₆ 1S(5.0),
52	-5.7770	0.0	C ₂ ' 1P-X(5.0), H ₃ 1S(7.7), H ₁₁ 1S(7.8), H ₁₄ 1S(5.2),
53	-5.3840	0.0	Mn _{III} 2S(4.3), H ₄ 1S(13.0), H ₄ 2S(5.2), H ₆ 1S(8.5), H ₁₀ 1S(8.4), H ₁₂ 1S(10.2), H ₁₄ 1S(6.8), H ₁₈ 1S(6.9),
54	-5.2600	0.0	C ₃ ' 1P-X(5.3), H ₄ 1S(10.0), H ₅ 1S(5.1), H ₆ 1S(6.9), H ₁₀ 1S(8.7), H ₁₂ 1S(12.3), H ₁₃ 1S(5.3), H ₁₄ 1S(8.3), H ₁₈ 1S(10.8),

TABLE S27: Orbital Energies/Mn_{III}Mn_{IV}(μ-O)₂(Oac)(TACN)₂ S=5/2 ACCINT=3.5Mn_{III}Mn_{IV}(μ-O)₂(Oac)(TACN)₂ S=5/2 ACCINT=3.5 Orbital Energies and Descriptions for β - A"

Orbital	Energy (eV)	Occupancy	Primary Contributors SFO(%)
1	-29.0020	1.0	N _t 1S(58.1), C ₂ 1S(13.3), H ₁₂ 1S(10.5),
2	-29.0000	1.0	N _t 1S(58.2), C ₁ 1S(13.3), H ₄ 1S(10.5), O 1S(93.9),
3	-27.5160	1.0	O 1S(93.9),
4	-25.0690	1.0	N _c 1P-Z(6.2), C ₁ ' 1S(26.5), C ₁ 1S(13.6), C ₃ ' 1S(8.2), H ₅ 1S(6.5),
5	-25.0670	1.0	N _c ' 1P-Z(6.3), C ₁ ' 1S(8.1), C ₃ ' 1S(26.5), C ₂ 1S(13.6), H ₁₃ 1S(6.5),
6	-21.8990	1.0	N _c 1P-Z(6.1), N _t 1P-Y(5.9), C ₃ ' 1S(9.1), C ₂ 1S(9.9), C ₂ ' 1S(9.1),
7	-21.8980	1.0	N _c 1P-Z(6.1), N _t 1P-Y(5.8), C ₁ ' 1S(9.2), C ₁ 1S(9.9), C ₃ 1S(9.1),
8	-20.7260	1.0	N _t 1P-X(6.3), N _t ' 1P-X(11.2), C ₃ 1S(5.5), C ₂ ' 1S(9.9), H ₁₆ 1S(6.0), H ₁₇ 1S(7.1),
9	-20.7220	1.0	N _t 1P-X(11.3), N _t ' 1P-X(6.3), C ₃ 1S(9.8), C ₂ ' 1S(5.5), H ₈ 1S(6.1), H ₉ 1S(7.1),
10	-18.6530	1.0	N _t 1P-Y(12.9), N _t ' 1P-Y(13.0), C ₁ 1P-Z(6.4), C ₂ 1P-Z(6.5),
11	-18.6400	1.0	N _t 1P-Y(13.2), N _t ' 1P-Y(13.1), C ₁ 1P-Z(6.6), C ₂ 1P-Z(6.5),
12	-17.8740	1.0	N _c 1P-Z(6.4), N _c ' 1P-Z(6.4), C ₁ ' 1P-X(9.4), C ₁ 1P-X(5.7), C ₃ ' 1P-X(9.4), C ₂ 1P-X(5.7), H ₆ 1S(5.7), H ₁₄ 1S(5.7),
13	-17.8630	1.0	N _c 1P-Z(6.3), N _c ' 1P-Z(6.3), C ₁ ' 1P-X(9.6), C ₁ 1P-X(5.8), C ₃ ' 1P-X(9.6), C ₂ 1P-X(5.8), H ₆ 1S(5.7), H ₁₄ 1S(5.7),
14	-16.8220	1.0	O ^a 1P-Z(21.8), O ^{a'} 1P-Z(22.0), C _a 1P-Z(30.7), C _b 1P-Z(13.4), H ₂ 1S(7.9),
15	-16.3460	1.0	C ₁ 1P-X(7.9), C ₂ 1P-X(6.9), H ₈ 1S(7.4), H ₁₆ 1S(6.5),
16	-16.3300	1.0	C ₁ 1P-X(7.0), C ₂ 1P-X(8.0), H ₈ 1S(6.7), H ₁₆ 1S(7.6),
17	-16.1140	1.0	N _t 1P-Z(7.7), N _t ' 1P-Z(13.8), C ₂ ' 1P-X(7.3), H ₁₇ 1S(5.5),
18	-16.1080	1.0	N _t 1P-Z(14.0), N _t ' 1P-Z(7.9), C ₃ 1P-X(7.5), H ₉ 1S(5.6),
19	-15.8970	1.0	C ₁ ' 1P-Y(10.4), C ₃ ' 1P-Y(9.4), H ₅ 1S(11.1), H ₁₃ 1S(10.0),
20	-15.8880	1.0	C ₁ ' 1P-Y(9.1), C ₃ 1P-Y(10.1), H ₅ 1S(9.9), H ₁₃ 1S(11.0),
21	-14.7010	1.0	O ^a 1P-Z(11.2), O ^{a'} 1P-Z(7.9), C _b 1P-Z(33.4), H ₂ 1S(34.2),
22	-14.5070	1.0	Mn _{III} 1D-XZ(14.0), Mn _{IV} 1D-XZ(14.0), O 1P-X(57.4),
23	-14.1540	1.0	Mn _{III} 1D-XZ(5.0), Mn _{IV} 1D-XZ(5.0), O 1P-Z(10.8), C ₃ 1P-Y(5.3), C ₂ ' 1P-Y(5.4), H ₉ 1S(8.6), H ₁₇ 1S(8.7),
24	-14.0900	1.0	H ₉ 1S(7.3), H ₁₇ 1S(7.3),
25	-14.0050	1.0	C ₁ ' 1P-Z(5.6), C ₃ ' 1P-Z(5.8), H ₆ 1S(6.5), H ₇ 1S(7.7), H ₁₄ 1S(6.7), H ₁₅ 1S(7.9),
26	-13.9220	1.0	C ₃ 1P-Y(7.1), C ₂ ' 1P-Y(7.1), H ₇ 1S(5.8), H ₁₀ 1S(5.8), H ₁₅ 1S(5.9), H ₁₈ 1S(5.8),
27	-13.7220	1.0	Mn _{III} 1D-XZ(5.2), Mn _{IV} 1D-XZ(5.2), O 1P-Z(13.5), C ₃ 1P-Y(6.5), C ₂ ' 1P-Y(6.4), H ₁₀ 1S(6.6), H ₁₈ 1S(6.6),
28	-13.2870	1.0	O ^a 1P-Z(33.6), O ^{a'} 1P-Z(35.9),
29	-12.9470	1.0	O 1P-X(12.8), O ^a 1P-Z(10.0), O ^{a'} 1P-Z(10.5), N _t 1P-X(8.5), N _t ' 1P-Z(9.4), N _t ' 1P-X(8.7), N _t ' 1P-Z(9.7),
30	-12.6070	1.0	Mn _{III} 1D-YZ(8.3), Mn _{IV} 1D-YZ(7.9), O 1P-Y(62.9),
31	-12.2230	1.0	O 1P-Y(5.8), O 1P-Z(50.0), N _t 1P-X(6.5), N _t ' 1P-Z(7.0), N _t ' 1P-X(6.6), N _t ' 1P-Z(7.0),
32	-9.2840	0.0	Mn _{III} 1D-YZ(44.7), Mn _{IV} 1D-YZ(44.3),
33	-8.4570	0.0	Mn _{III} 1D-YZ(35.4), Mn _{IV} 1D-YZ(35.9), O 1P-Y(23.0),
34	-6.9860	0.0	Mn _{III} 1D-XZ(29.7), Mn _{IV} 1D-XZ(29.7), O 1P-X(18.1),
35	-6.6050	0.0	Mn _{III} 1D-XZ(31.4), Mn _{IV} 1D-XZ(31.5), O 1P-Z(17.0),

TABLE S27: Orbital Energies/ $Mn_{III}Mn_{IV}(\mu - O)_2(Oac)(TACN)_2$ S=5/2 ACCINT=3.5**S140**

Orbital	Energy (eV)	Occupancy	Primary Contributors SFO(%)
36	-6.2790	0.0	O* 1P-Z(16.7), O* 1P-Z(15.8), C _a 1P-Z(52.7), H ₂ 1S(9.0),
37	-5.1180	0.0	H ₄ 1S(10.2), H ₄ 2S(6.0), H ₅ 1S(8.0), H ₅ 2S(5.9), H ₇ 1S(14.6), H ₇ 2S(11.4), H ₁₂ 1S(9.1), H ₁₂ 2S(5.4), H ₁₃ 1S(7.5), H ₁₃ 2S(5.7), H ₁₅ 1S(13.6), H ₁₅ 2S(10.6),
38	-4.6180	0.0	H ₄ 1S(18.2), H ₄ 2S(5.3), H ₇ 1S(9.9), H ₁₂ 1S(18.0), H ₁₂ 2S(5.1), H ₁₃ 1S(6.0), H ₁₅ 1S(11.2),
39	-4.3100	0.0	H ₄ 1S(12.2), H ₅ 1S(6.1), H ₅ 2S(10.0), H ₆ 1S(5.8), H ₁₂ 1S(13.1), H ₁₃ 1S(5.0), H ₁₃ 2S(9.1), H ₁₄ 1S(5.5),
40	-4.0270	0.0	H ₆ 1S(9.3), H ₈ 1S(16.0), H ₈ 2S(10.0), H ₁₄ 1S(9.7), H ₁₆ 1S(16.4), H ₁₆ 2S(10.3),
41	-3.9140	0.0	H ₅ 1S(7.1), H ₈ 1S(19.5), H ₈ 2S(10.0), H ₁₃ 1S(6.4), H ₁₆ 1S(19.1), H ₁₆ 2S(9.8),

TABLE S28: Orbital Energies Mn(IV)Mn(IV)(μ -O)₂(μ -O₂) (TACN)₂ BS ACCINT=3.5

Indices	Atoms	Charges	Alpha Spin	Beta Spin	Net Spin
1	Mn _{IV'}	1.1001	1.6647	4.2353	-2.5706
2	Mn _{IV}	1.1031	4.2298	1.6670	2.5628
3	O _{p1}	-0.3491	3.1814	3.1677	0.0137
4	O _{p2}	-0.3481	3.1686	3.1794	-0.0108
5	O _{μ}	-0.7127	3.3577	3.3551	0.0026
6	O _{μ}	-0.7127	3.3577	3.3551	0.0026
7	N	-0.3959	2.6966	2.6992	-0.0026
8	N	-0.3995	2.6760	2.7235	-0.0475
9	N	-0.3995	2.6760	2.7235	-0.0475
10	N	-0.3959	2.6992	2.6967	0.0025
11	N	-0.4010	2.7241	2.6770	0.0471
12	N	-0.4010	2.7241	2.6770	0.0471
13	C	0.4196	1.7901	1.7903	-0.0002
14	C	0.4203	1.7924	1.7873	0.0051
15	C	0.4042	1.7996	1.7962	0.0034
16	C	0.4042	1.7996	1.7962	0.0034
17	C	0.4203	1.7924	1.7873	0.0051
18	C	0.4196	1.7901	1.7903	-0.0002
19	C	0.4204	1.7899	1.7897	0.0002
20	C	0.4196	1.7880	1.7924	-0.0044
21	C	0.4071	1.7950	1.7980	-0.0030
22	C	0.4071	1.7950	1.7980	-0.0030
23	C	0.4196	1.7880	1.7924	-0.0044
24	C	0.4204	1.7899	1.7897	0.0002
25	H	0.1220	0.4412	0.4367	0.0045
26	H	0.1785	0.4123	0.4092	0.0031
27	H	0.1785	0.4123	0.4092	0.0031
28	H	-0.0610	0.5307	0.5303	0.0004
29	H	-0.0685	0.5343	0.5341	0.0002
30	H	-0.0729	0.5361	0.5368	-0.0007
31	H	-0.0766	0.5369	0.5397	-0.0028

Indices	Atoms	Charges	Alpha Spin	Beta Spin	Net Spin
32	H	-0.0789	0.5386	0.5403	-0.0017
33	H	-0.0484	0.5236	0.5248	-0.0012
34	H	-0.0484	0.5236	0.5248	-0.0012
35	H	-0.0789	0.5386	0.5403	-0.0017
36	H	-0.0729	0.5361	0.5368	-0.0007
37	H	-0.0766	0.5369	0.5397	-0.0028
38	H	-0.0610	0.5307	0.5303	0.0004
39	H	-0.0685	0.5343	0.5341	0.0002
40	H	0.1218	0.4368	0.4414	-0.0046
41	H	0.1798	0.4085	0.4117	-0.0032
42	H	0.1798	0.4085	0.4117	-0.0032
43	H	-0.0618	0.5306	0.5311	-0.0005
44	H	-0.0690	0.5345	0.5346	-0.0001
45	H	-0.0741	0.5374	0.5367	0.0007
46	H	-0.0741	0.5382	0.5360	0.0022
47	H	-0.0796	0.5408	0.5388	0.0020
48	H	-0.0502	0.5257	0.5246	0.0011
49	H	-0.0502	0.5257	0.5246	0.0011
50	H	-0.0796	0.5408	0.5388	0.0020
51	H	-0.0741	0.5374	0.5367	0.0007
52	H	-0.0741	0.5382	0.5360	0.0022
53	H	-0.0618	0.5306	0.5311	-0.0005
54	H	-0.0690	0.5345	0.5346	-0.0001

TABLE S28: Orbital Energies Mn(IV)Mn(IV)(μ -O)₂(μ -O₂) (TACN)₂ BS ACCINT=3.5

Orbital Energies and SFO Contributions

Orb.	Energy(eV)	Occ.	Primary Contributors SFO (percent)
Symmetry Representation for Spin-1-AA			
1	-32.575	1.0	O ₃ (S)(46.0), O ₄ (S)(46.0),
2	-30.192	1.0	N ₇ (S)(31.0), N ₈ (S)(28.0), C ₁₃ (S)(14.0), C ₁₄ (S)(8.0), C ₁₅ (S)(6.0),
3	-30.156	1.0	N ₁₀ (S)(31.0), N ₁₁ (S)(27.0), C ₁₉ (S)(14.0), C ₂₀ (S)(9.0), C ₂₁ (S)(6.0),
4	-29.350	1.0	N ₈ (S)(31.0), N ₇ (S)(30.0), C ₁₅ (S)(10.0), C ₁₃ (S)(6.0), H ₂₅ (S)(6.0),
5	-29.303	1.0	N ₁₁ (S)(32.0), N ₁₀ (S)(29.0), C ₂₁ (S)(11.0), C ₁₉ (S)(6.0), H ₄₀ (S)(6.0),
6	-28.664	1.0	O ₅ (S)(90.0),
7	-26.265	1.0	O ₃ (S)(43.0), O ₄ (S)(42.0),
8	-25.216	1.0	C ₂₁ (S)(19.0), C ₁₅ (S)(16.0), C ₂₀ (S)(11.0), C ₁₄ (S)(10.0),
9	-25.179	1.0	C ₁₅ (S)(19.0), C ₂₁ (S)(17.0), C ₁₄ (S)(10.0), C ₂₀ (S)(8.0),
10	-23.551	1.0	C ₁₅ (S)(14.0), C ₁₃ (S)(13.0), C ₁₄ (S)(9.0), N ₈ (S)(8.0),
11	-23.507	1.0	C ₁₉ (S)(13.0), C ₂₁ (S)(13.0), C ₂₀ (S)(9.0), N ₁₁ (S)(8.0),
12	-21.177	1.0	N ₇ (P:X)(12.0), H ₂₉ (S)(12.0), C ₁₃ (S)(10.0), C ₁₄ (S)(9.0),
13	-21.128	1.0	N ₁₀ (P:X)(12.0), H ₄₄ (S)(12.0), C ₁₉ (S)(10.0), C ₂₀ (S)(9.0),
14	-19.926	1.0	N ₇ (P:Y)(11.0), N ₈ (P:X)(10.0), N ₈ (P:Y)(7.0), C ₁₃ (P:Y)(7.0), H ₂₈ (S)(7.0), C ₁₅ (P:Y)(6.0), C ₁₃ (P:Z)(6.0),
15	-19.826	1.0	N ₁₀ (P:Y)(12.0), N ₁₁ (P:X)(10.0), N ₁₁ (P:Y)(8.0), H ₄₃ (S)(8.0), C ₁₉ (P:Y)(7.0), C ₁₉ (P:Z)(6.0),
16	-18.905	1.0	C ₁₅ (P:Y)(17.0), N ₈ (P:Z)(11.0), N ₇ (P:Y)(10.0), N ₈ (P:X)(10.0), H ₃₃ (S)(7.0), N ₇ (P:X)(6.0),
17	-18.872	1.0	C ₂₁ (P:Y)(17.0), N ₁₁ (P:X)(12.0), N ₁₁ (P:Z)(10.0), N ₁₀ (P:Y)(10.0), H ₄₈ (S)(7.0),
18	-18.625	1.0	O ₃ (P:X)(8.0), O ₄ (P:X)(8.0), N ₈ (P:Z)(6.0),
19	-18.398	1.0	N ₁₁ (P:Z)(8.0), C ₂₀ (P:Y)(6.0),
20	-17.879	1.0	H ₃₁ (S)(10.0), H ₄₆ (S)(7.0), C ₁₄ (P:X)(6.0), O ₃ (P:X)(6.0), O ₄ (P:X)(6.0),
21	-17.688	1.0	C ₂₁ (P:X)(12.0), C ₁₅ (P:X)(9.0), N ₁₁ (P:Y)(8.0), H ₄₆ (S)(7.0),
22	-17.278	1.0	O ₃ (P:X)(12.0), O ₄ (P:X)(12.0), O ₄ (P:Y)(9.0), C ₁₅ (P:X)(9.0), O ₃ (P:Y)(8.0), C ₂₁ (P:X)(8.0),
23	-16.769	1.0	O ₄ (P:Y)(12.0), O ₃ (P:Y)(11.0), Mn ₂ (D:XY)(10.0), C ₁₅ (P:Z)(10.0),
24	-16.589	1.0	C ₂₁ (P:Z)(12.0), C ₂₀ (P:Z)(9.0), H ₄₅ (S)(7.0), N ₁₀ (P:X)(6.0), H ₄₈ (S)(6.0),
25	-16.552	1.0	C ₁₄ (P:Z)(10.0), C ₁₅ (P:Y)(7.0), C ₂₀ (P:Z)(7.0), H ₃₀ (S)(7.0), C ₂₁ (P:Y)(6.0),

Orb.	Energy(eV)	Occ.	Primary Contributors SFO (percent)
			H ₃₃ (S)(6.0),
26	-16.384	1.0	C ₂₁ (P:Z)(9.0), C ₁₉ (P:X)(7.0), N ₁₁ (P:Y)(7.0),
27	-16.239	1.0	C ₁₅ (P:X)(7.0), H ₃₂ (S)(7.0),
28	-16.220	1.0	N ₈ (P:X)(8.0), C ₁₅ (P:Z)(7.0), C ₁₃ (P:X)(6.0), H ₄₇ (S)(6.0),
29	-15.944	1.0	N ₁₁ (P:X)(9.0),
30	-15.608	1.0	O ₅ (P:Z)(47.0), Mn ₂ (D:Z2)(11.0), Mn ₂ (D:X2-Y2)(7.0), Mn ₂ (D:XY)(6.0),
31	-15.014	1.0	O ₅ (P:X)(41.0), Mn ₂ (D:Z2)(9.0), C ₁₅ (P:Z)(7.0), Mn ₂ (D:XY)(6.0),
32	-14.619	1.0	O ₅ (P:Y)(17.0), C ₁₄ (P:X)(7.0), H ₃₀ (S)(6.0),
33	-14.477	1.0	C ₂₀ (P:X)(10.0), H ₄₄ (S)(9.0), H ₄₅ (S)(9.0), H ₄₆ (S)(6.0),
34	-14.240	1.0	O ₅ (P:Y)(25.0), Mn ₂ (D:X2-Y2)(8.0),
35	-14.115	1.0	N ₇ (P:Y)(12.0), O ₅ (P:X)(10.0), Mn ₂ (D:XY)(8.0), O ₃ (P:Y)(8.0), C ₁₃ (P:Y)(8.0), N ₇ (P:X)(6.0),
36	-13.782	1.0	N ₁₀ (P:Y)(14.0), N ₁₀ (P:X)(10.0), O ₄ (P:Y)(10.0), Mn ₂ (D:X2-Y2)(6.0), Mn ₁ (D:XY)(6.0),
37	-13.254	1.0	N ₁₁ (P:Z)(15.0), Mn ₂ (D:Z2)(7.0), N ₁₁ (P:Y)(6.0), C ₂₁ (P:Z)(6.0),
38	-13.204	1.0	N ₈ (P:Z)(17.0), N ₈ (P:Y)(7.0), C ₁₅ (P:Z)(7.0), N ₁₁ (P:Z)(6.0),
39	-12.916	1.0	O ₃ (P:Y)(30.0), O ₄ (P:Y)(18.0), Mn ₂ (D:X2-Y2)(10.0), Mn ₁ (D:X2-Y2)(8.0), O ₅ (P:Y)(6.0),
40	-11.934	1.0	Mn ₂ (D:Z2)(42.0), O ₅ (P:Z)(15.0), O ₅ (P:X)(10.0), Mn ₂ (D:XY)(9.0),
41	-11.667	1.0	Mn ₂ (D:X2-Y2)(22.0), Mn ₂ (D:XY)(18.0), O ₅ (P:Y)(16.0), O ₄ (P:Y)(6.0), N ₇ (P:Y)(6.0),
42	-9.568	0.0	Mn ₁ (D:Z2)(31.0), Mn ₁ (D:X2-Y2)(31.0), O ₄ (P:Y)(8.0), Mn ₂ (D:X2-Y2)(7.0),
43	-9.389	0.0	Mn ₁ (D:XY)(34.0), Mn ₁ (D:Z2)(24.0), O ₅ (P:Y)(17.0), Mn ₁ (D:X2-Y2)(10.0),
44	-8.690	0.0	Mn ₂ (D:XY)(17.0), Mn ₁ (D:X2-Y2)(14.0), Mn ₂ (D:X2-Y2)(11.0), O ₄ (P:Y)(11.0), Mn ₂ (D:Z2)(9.0), O ₅ (P:Z)(7.0),
45	-7.717	0.0	Mn ₁ (D:XY)(27.0), Mn ₁ (D:Z2)(17.0), Mn ₁ (D:X2-Y2)(14.0), O ₃ (P:Y)(13.0), O ₅ (P:X)(6.0),
46	-6.493	0.0	O ₃ (P:X)(24.0), O ₄ (P:X)(24.0),
47	-6.493	0.0	Mn ₂ (S)(7.0), H ₂₅ (S)(6.0),
48	-5.959	0.0	O ₃ (P:X)(12.0), O ₄ (P:X)(12.0), H ₂₈ (S)(6.0),
49	-5.635	0.0	H ₂₉ (S)(11.0), H ₄₄ (S)(9.0), H ₃₂ (S)(8.0), H ₄₇ (S)(7.0), H ₃₁ (S)(6.0), H ₂₅ (S)(6.0),
50	-5.469	0.0	H ₄₁ (S)(14.0), H ₂₅ (S)(13.0), H ₄₀ (S)(10.0), H ₂₆ (S)(10.0), H ₄₈ (S)(10.0), H ₃₃ (S)(9.0), H ₄₁ (S)(7.0), H ₂₅ (S)(7.0), H ₄₀ (S)(6.0), H ₂₆ (S)(6.0), H ₄₈ (S)(6.0),
51	-5.423	0.0	H ₄₄ (S)(10.0), H ₄₃ (S)(9.0), H ₂₉ (S)(9.0), H ₄₀ (S)(8.0), H ₂₆ (S)(6.0), H ₂₈ (S)(6.0), H ₄₆ (S)(6.0),
52	-4.937	0.0	H ₃₃ (S)(17.0), H ₄₈ (S)(15.0), H ₄₀ (S)(11.0), H ₂₅ (S)(10.0), H ₂₆ (S)(7.0),

Orb.	Energy(eV)	Occ.	Primary Contributors SFO (percent)
53	-4.706	0.0	H ₄₁ (S)(7.0), H ₃₃ (S)(7.0), H ₄₈ (S)(6.0), H ₂₉ (S)(9.0), H ₃₂ (S)(6.0), H ₄₄ (S)(6.0),
54	-4.571	0.0	H ₄₄ (S)(10.0), H ₂₉ (S)(8.0), H ₄₇ (S)(7.0), H ₄₄ (S)(6.0),
55	-4.232	0.0	H ₃₂ (S)(16.0), H ₃₂ (S)(9.0), H ₄₇ (S)(9.0),
56	-4.145	0.0	H ₃₂ (S)(10.0), H ₄₇ (S)(8.0), H ₃₂ (S)(6.0), C ₁₅ (P:Y)(6.0), H ₄₇ (S)(6.0),
57	-4.123	0.0	H ₄₅ (S)(17.0), H ₃₀ (S)(16.0), H ₃₀ (S)(11.0), H ₃₃ (S)(10.0), H ₄₅ (S)(9.0), H ₄₈ (S)(9.0), H ₄₇ (S)(7.0), C ₂₁ (P:Y)(7.0),
58	-4.035	0.0	C ₁₃ (P:X)(13.0), C ₁₅ (P:X)(10.0), C ₁₉ (P:X)(9.0), H ₃₂ (S)(7.0), H ₂₈ (S)(6.0), H ₂₉ (S)(6.0), C ₂₁ (P:X)(6.0), H ₄₇ (S)(6.0),
59	-3.960	0.0	H ₄₇ (S)(16.0), C ₁₉ (P:X)(12.0), H ₄₄ (S)(11.0), H ₃₂ (S)(11.0), C ₂₁ (P:X)(9.0), H ₂₉ (S)(8.0), C ₁₃ (P:X)(8.0), C ₁₅ (P:X)(6.0),
60	-3.701	0.0	H ₄₅ (S)(14.0), H ₃₀ (S)(13.0), H ₄₅ (S)(8.0), H ₃₀ (S)(7.0), H ₄₈ (S)(7.0),
61	-3.449	0.0	H ₃₁ (S)(18.0), H ₄₆ (S)(15.0), H ₃₁ (S)(7.0), H ₄₆ (S)(6.0), Symmetry Representation for Spin-1-AAA
1	-29.243	1.0	N ₈ (S)(62.0), C ₁₄ (S)(14.0), H ₂₆ (S)(11.0),
2	-29.202	1.0	N ₁₁ (S)(62.0), C ₂₀ (S)(14.0), H ₄₁ (S)(11.0),
3	-28.126	1.0	O ₅ (S)(94.0),
4	-25.188	1.0	C ₁₃ (S)(34.0), C ₁₄ (S)(19.0), N ₇ (P:Z)(8.0), H ₂₈ (S)(8.0),
5	-25.143	1.0	C ₁₉ (S)(34.0), C ₂₀ (S)(18.0), N ₁₀ (P:Z)(8.0), H ₄₃ (S)(8.0),
6	-22.032	1.0	C ₁₃ (S)(13.0), C ₁₅ (S)(13.0), C ₁₄ (S)(12.0), N ₈ (P:Y)(11.0), N ₇ (P:Z)(8.0), H ₂₈ (S)(6.0), H ₃₀ (S)(6.0), H ₃₃ (S)(6.0),
7	-22.028	1.0	C ₂₁ (S)(14.0), C ₁₉ (S)(13.0), C ₂₀ (S)(12.0), N ₁₁ (P:Y)(11.0), N ₁₀ (P:Z)(8.0), H ₄₃ (S)(6.0), H ₄₅ (S)(6.0), H ₄₈ (S)(6.0),
8	-20.933	1.0	N ₈ (P:X)(18.0), C ₁₅ (S)(14.0), H ₃₂ (S)(10.0), H ₃₁ (S)(9.0), C ₁₄ (S)(7.0), H ₂₆ (S)(6.0),
9	-20.899	1.0	N ₁₁ (P:X)(17.0), C ₂₁ (S)(13.0), H ₄₆ (S)(10.0), H ₄₇ (S)(10.0), C ₂₀ (S)(8.0), H ₄₁ (S)(6.0),
10	-18.875	1.0	N ₈ (P:X)(15.0), N ₈ (P:Y)(14.0), C ₁₄ (P:Z)(12.0), H ₂₆ (S)(7.0), H ₃₀ (S)(6.0),
11	-18.794	1.0	N ₁₁ (P:X)(16.0), N ₁₁ (P:Y)(14.0), C ₂₀ (P:Z)(12.0), H ₄₁ (S)(7.0), H ₄₅ (S)(7.0),
12	-17.991	1.0	C ₁₃ (P:X)(17.0), C ₁₄ (P:X)(13.0), N ₇ (P:Z)(11.0), H ₂₉ (S)(10.0), H ₃₀ (S)(8.0),
13	-17.970	1.0	C ₁₉ (P:X)(17.0), C ₂₀ (P:X)(13.0), N ₁₀ (P:Z)(11.0), H ₄₄ (S)(10.0), H ₄₅ (S)(8.0),
14	-16.558	1.0	C ₁₄ (P:Y)(15.0), H ₃₁ (S)(10.0), C ₁₃ (P:Y)(9.0), N ₈ (P:Z)(8.0), N ₇ (P:Z)(6.0), C ₁₄ (P:Z)(6.0), C ₁₃ (P:Z)(6.0),
15	-16.506	1.0	C ₂₀ (P:Y)(14.0), H ₄₆ (S)(12.0), C ₁₉ (P:Y)(9.0), C ₂₀ (P:Z)(8.0), N ₁₀ (P:Z)(8.0),

Orb.	Energy(eV)	Occ.	Primary Contributors SFO (percent)
16	-16.293	1.0	C ₁₉ (P:Z)(6.0), N ₁₁ (P:Z)(6.0), N ₈ (P:Z)(12.0), N ₁₁ (P:Z)(8.0),
17	-16.280	1.0	N ₁₁ (P:Z)(14.0), N ₈ (P:Z)(8.0),
18	-16.125	1.0	O ₄ (P:Z)(10.0), H ₂₈ (S)(10.0), C ₁₃ (P:Y)(9.0), O ₃ (P:Z)(8.0), N ₇ (P:Z)(6.0),
19	-15.982	1.0	C ₁₉ (P:Y)(13.0), H ₄₃ (S)(13.0), H ₂₈ (S)(7.0), C ₁₃ (P:Y)(7.0),
20	-15.627	1.0	O ₄ (P:Z)(22.0), O ₃ (P:Z)(17.0), O ₅ (P:Y)(9.0), Mn ₂ (D:YZ)(8.0),
21	-15.395	1.0	O ₅ (P:X)(45.0), Mn ₂ (D:XZ)(19.0), Mn ₂ (D:YZ)(6.0), Mn ₁ (D:XZ)(6.0),
22	-14.653	1.0	O ₅ (P:Z)(21.0), Mn ₁ (D:XZ)(13.0), Mn ₂ (D:XZ)(9.0),
23	-14.250	1.0	C ₂₁ (P:X)(10.0), H ₃₂ (S)(10.0), H ₄₇ (S)(10.0), C ₁₅ (P:X)(9.0), H ₄₈ (S)(7.0), H ₃₃ (S)(6.0),
24	-14.100	1.0	H ₂₉ (S)(6.0),
25	-14.025	1.0	H ₄₅ (S)(11.0), H ₄₄ (S)(8.0), C ₁₉ (P:Z)(7.0), C ₁₉ (P:X)(6.0), H ₄₃ (S)(6.0),
26	-14.004	1.0	H ₃₃ (S)(8.0), H ₃₀ (S)(6.0), C ₁₅ (P:Y)(6.0),
27	-13.341	1.0	O ₃ (P:Z)(15.0), Mn ₂ (D:YZ)(14.0), O ₅ (P:X)(11.0), N ₈ (P:Z)(10.0), N ₈ (P:Y)(7.0), O ₅ (P:Y)(6.0),
28	-13.267	1.0	Mn ₂ (D:YZ)(19.0), O ₅ (P:Y)(11.0), N ₁₁ (P:Z)(11.0), O ₃ (P:Z)(9.0), N ₁₁ (P:Y)(8.0),
29	-12.647	1.0	O ₅ (P:Z)(17.0), Mn ₂ (D:YZ)(13.0), O ₅ (P:Y)(12.0), O ₄ (P:Z)(9.0), N ₈ (P:Z)(8.0), N ₈ (P:X)(6.0),
30	-12.304	1.0	O ₅ (P:Z)(31.0), O ₅ (P:Y)(24.0), O ₄ (P:Z)(10.0), Mn ₁ (D:YZ)(9.0),
31	-10.890	1.0	O ₄ (P:Z)(30.0), O ₃ (P:Z)(23.0), Mn ₂ (D:YZ)(19.0), O ₅ (P:Y)(17.0),
32	-9.410	0.0	Mn ₁ (D:YZ)(50.0), Mn ₁ (D:XZ)(12.0), O ₃ (P:Z)(11.0), Mn ₂ (D:XZ)(6.0), O ₅ (P:Y)(6.0),
33	-8.432	0.0	Mn ₂ (D:XZ)(34.0), O ₅ (P:X)(16.0), Mn ₁ (D:YZ)(11.0), O ₅ (P:Z)(9.0), Mn ₂ (D:YZ)(7.0),
34	-7.572	0.0	Mn ₁ (D:XZ)(51.0), O ₅ (P:Z)(12.0), Mn ₁ (D:YZ)(10.0), O ₅ (P:X)(7.0),
35	-5.351	0.0	H ₄₁ (S)(18.0), H ₂₆ (S)(16.0), H ₃₀ (S)(13.0), H ₄₅ (S)(13.0), H ₃₀ (S)(11.0), H ₄₅ (S)(11.0), H ₂₆ (S)(10.0), H ₄₁ (S)(10.0),
36	-4.789	0.0	H ₃₀ (S)(14.0), H ₄₅ (S)(13.0), H ₄₁ (S)(10.0), H ₂₆ (S)(9.0), H ₂₈ (S)(8.0), H ₃₀ (S)(8.0), H ₄₃ (S)(7.0), H ₄₅ (S)(7.0),
37	-4.392	0.0	H ₃₁ (S)(11.0), H ₄₆ (S)(10.0), H ₂₆ (S)(9.0), H ₂₉ (S)(9.0), H ₄₁ (S)(7.0), H ₄₄ (S)(7.0), H ₃₁ (S)(7.0), H ₄₆ (S)(7.0),
38	-4.189	0.0	H ₄₆ (S)(15.0), H ₃₁ (S)(14.0), H ₄₄ (S)(9.0), H ₄₁ (S)(9.0), H ₄₆ (S)(9.0), H ₂₉ (S)(8.0), H ₃₁ (S)(8.0), H ₂₆ (S)(6.0),
39	-4.025	0.0	H ₃₁ (S)(12.0), H ₄₆ (S)(12.0), H ₂₈ (S)(9.0), H ₄₃ (S)(7.0), H ₃₀ (S)(6.0), H ₄₆ (S)(6.0),
40	-3.874	0.0	H ₄₃ (S)(12.0), H ₄₃ (S)(9.0), H ₂₈ (S)(8.0), H ₂₈ (S)(7.0), H ₄₆ (S)(6.0),

Orb.	Energy(eV)	Occ.	Primary Contributors SFO (percent)
41	-3.682	0.0	C ₁₄ (P:Y)(10.0), C ₂₀ (P:Y)(8.0), C ₁₄ (P:Z)(7.0), H ₂₆ (S)(6.0), H ₂₈ (S)(6.0),
42	-3.512	0.0	H ₄₃ (S)(9.0), H ₄₈ (S)(9.0), C ₂₀ (P:Z)(8.0), H ₄₁ (S)(7.0), H ₃₃ (S)(6.0), C ₂₀ (P:Y)(6.0),
43	-3.226	0.0	H ₄₄ (S)(9.0), H ₂₉ (S)(8.0), C ₂₁ (S)(6.0),
44	-2.890	0.0	H ₂₈ (S)(16.0), H ₃₀ (S)(10.0), H ₃₀ (S)(9.0), H ₄₅ (S)(9.0), H ₄₃ (S)(8.0), H ₃₃ (S)(8.0), H ₄₅ (S)(8.0), H ₄₄ (S)(6.0), H ₄₈ (S)(6.0),
45	-2.853	0.0	H ₂₆ (S)(11.0), H ₂₉ (S)(11.0), H ₄₃ (S)(10.0), H ₄₁ (S)(8.0),
46	-2.594	0.0	H ₄₈ (S)(11.0), H ₃₃ (S)(10.0), H ₃₁ (S)(6.0), H ₄₅ (S)(6.0), H ₄₅ (S)(6.0), H ₄₆ (S)(6.0), H ₄₇ (S)(6.0), H ₃₂ (S)(6.0),
47	-2.346	0.0	H ₃₁ (S)(9.0), H ₄₆ (S)(9.0), H ₄₃ (S)(8.0), H ₂₈ (S)(8.0), C ₁₃ (P:X)(7.0), C ₂₀ (P:Z)(6.0), H ₃₂ (S)(6.0), C ₁₉ (P:X)(6.0), H ₃₀ (S)(6.0), H ₄₇ (S)(6.0),
48	-2.075	0.0	H ₄₅ (S)(21.0), H ₃₀ (S)(20.0), H ₄₃ (S)(11.0), H ₂₈ (S)(10.0), H ₃₂ (S)(8.0), H ₄₇ (S)(8.0),
49	-1.770	0.0	C ₁₅ (P:Z)(30.0), C ₂₁ (P:Z)(20.0), H ₃₂ (S)(10.0), C ₁₃ (P:X)(8.0), H ₄₇ (S)(8.0), Mn ₂ (P:Z)(6.0),
50	-1.373	0.0	C ₂₁ (P:Z)(30.0), C ₁₅ (P:Z)(19.0), C ₁₉ (P:X)(9.0), H ₄₇ (S)(8.0), C ₁₃ (P:Z)(7.0), C ₁₄ (P:Y)(7.0),
51	-1.180	0.0	C ₁₄ (P:Y)(17.0), C ₁₃ (P:Z)(16.0), H ₃₃ (S)(12.0), C ₂₀ (P:Y)(10.0), C ₁₉ (P:Z)(10.0), C ₁₅ (P:Y)(9.0), H ₃₁ (S)(7.0), H ₄₈ (S)(7.0), H ₃₂ (S)(6.0), N ₇ (P:Z)(6.0), C ₁₄ (P:Z)(6.0),
			Symmetry Representation for Spin-2-AA
1	-32.574	1.0	O ₄ (S)(46.0), O ₃ (S)(45.0),
2	-30.191	1.0	N ₇ (S)(30.0), N ₈ (S)(29.0), C ₁₃ (S)(13.0), C ₁₄ (S)(9.0), C ₁₅ (S)(6.0),
3	-30.158	1.0	N ₁₀ (S)(33.0), N ₁₁ (S)(26.0), C ₁₉ (S)(14.0), C ₂₀ (S)(8.0),
4	-29.353	1.0	N ₇ (S)(31.0), N ₈ (S)(30.0), C ₁₅ (S)(10.0), C ₁₃ (S)(7.0), H ₂₅ (S)(7.0),
5	-29.299	1.0	N ₁₁ (S)(33.0), N ₁₀ (S)(28.0), C ₂₁ (S)(11.0), C ₁₉ (S)(6.0), H ₄₀ (S)(6.0),
6	-28.662	1.0	O ₅ (S)(90.0),
7	-26.264	1.0	O ₃ (S)(42.0), O ₄ (S)(42.0),
8	-25.216	1.0	C ₂₁ (S)(19.0), C ₁₅ (S)(15.0), C ₂₀ (S)(11.0), C ₁₄ (S)(9.0),
9	-25.179	1.0	C ₁₅ (S)(20.0), C ₂₁ (S)(16.0), C ₁₄ (S)(11.0), C ₂₀ (S)(8.0),
10	-23.551	1.0	C ₁₅ (S)(14.0), C ₁₃ (S)(12.0), C ₁₄ (S)(9.0), N ₈ (S)(8.0),
11	-23.508	1.0	C ₁₉ (S)(13.0), C ₂₁ (S)(13.0), C ₂₀ (S)(9.0), N ₁₁ (S)(8.0),
12	-21.170	1.0	N ₇ (P:X)(10.0), H ₂₉ (S)(10.0), C ₁₃ (S)(9.0), C ₁₄ (S)(8.0),
13	-21.135	1.0	N ₁₀ (P:X)(10.0), H ₄₄ (S)(10.0), C ₂₀ (S)(8.0), C ₁₉ (S)(8.0),

Orb.	Energy(eV)	Occ.	Primary Contributors SFO (percent)
14	-19.913	1.0	N ₇ (P:Y)(9.0), N ₈ (P:X)(8.0), N ₈ (P:Y)(6.0), H ₂₈ (S)(6.0),
15	-19.840	1.0	N ₁₀ (P:Y)(10.0), N ₁₁ (P:X)(8.0), H ₄₃ (S)(7.0), C ₁₉ (P:Y)(6.0), N ₁₁ (P:Y)(6.0),
16	-18.895	1.0	C ₂₁ (P:Y)(12.0), N ₁₁ (P:X)(8.0), N ₁₁ (P:Z)(7.0), C ₁₅ (P:Y)(6.0), N ₁₀ (P:Y)(6.0),
17	-18.880	1.0	C ₁₅ (P:Y)(12.0), N ₈ (P:X)(7.0), N ₈ (P:Z)(7.0), N ₇ (P:Y)(7.0), C ₂₁ (P:Y)(6.0),
18	-18.623	1.0	O ₄ (P:X)(9.0), O ₃ (P:X)(8.0), N ₈ (P:Z)(6.0), N ₁₁ (P:Z)(6.0),
19	-18.399	1.0	N ₁₁ (P:Z)(7.0), N ₈ (P:Z)(6.0), C ₂₀ (P:Y)(6.0),
20	-17.877	1.0	H ₃₁ (S)(10.0), H ₄₆ (S)(8.0), C ₁₄ (P:X)(6.0), O ₃ (P:X)(6.0), O ₄ (P:X)(6.0),
21	-17.689	1.0	C ₂₁ (P:X)(11.0), C ₁₅ (P:X)(10.0), N ₁₁ (P:Y)(7.0), H ₄₆ (S)(7.0), N ₈ (P:Y)(6.0),
22	-17.277	1.0	O ₃ (P:X)(12.0), O ₄ (P:X)(12.0), O ₃ (P:Y)(9.0), C ₂₁ (P:X)(9.0), C ₁₅ (P:X)(8.0), O ₄ (P:Y)(8.0),
23	-16.758	1.0	O ₃ (P:Y)(12.0), O ₄ (P:Y)(12.0), Mn ₁ (D:XY)(9.0), C ₂₁ (P:Z)(9.0),
24	-16.598	1.0	C ₁₅ (P:Z)(13.0), C ₁₄ (P:Z)(11.0), H ₃₀ (S)(8.0), N ₇ (P:X)(7.0), H ₃₃ (S)(7.0), C ₁₅ (P:Y)(6.0),
25	-16.551	1.0	C ₂₀ (P:Z)(12.0), C ₂₁ (P:Y)(8.0), H ₄₅ (S)(8.0), H ₄₈ (S)(7.0),
26	-16.387	1.0	C ₁₅ (P:Z)(8.0), C ₁₃ (P:X)(7.0), N ₈ (P:Y)(7.0),
27	-16.247	1.0	N ₈ (P:X)(6.0), H ₄₇ (S)(6.0),
28	-16.206	1.0	N ₁₁ (P:X)(7.0), C ₁₅ (P:X)(6.0), C ₁₉ (P:X)(6.0), C ₂₁ (P:Z)(6.0), H ₃₂ (S)(6.0),
29	-15.947	1.0	N ₈ (P:X)(8.0), N ₁₁ (P:X)(7.0),
30	-15.611	1.0	O ₅ (P:Z)(47.0), Mn ₁ (D:Z2)(11.0), Mn ₁ (D:X2-Y2)(7.0), Mn ₁ (D:XY)(6.0),
31	-15.010	1.0	O ₅ (P:X)(41.0), Mn ₁ (D:Z2)(9.0), Mn ₁ (D:XY)(6.0), C ₂₁ (P:Z)(6.0),
32	-14.618	1.0	O ₅ (P:Y)(17.0), C ₂₀ (P:X)(6.0),
33	-14.480	1.0	C ₁₄ (P:X)(9.0), H ₂₉ (S)(8.0), H ₃₀ (S)(8.0), C ₂₀ (P:X)(6.0), H ₃₁ (S)(6.0),
34	-14.240	1.0	O ₅ (P:Y)(25.0), Mn ₁ (D:X2-Y2)(8.0),
35	-14.110	1.0	N ₁₀ (P:Y)(11.0), O ₅ (P:X)(10.0), Mn ₁ (D:XY)(8.0), O ₄ (P:Y)(8.0), C ₁₉ (P:Y)(7.0), N ₁₀ (P:X)(6.0),
36	-13.785	1.0	N ₇ (P:Y)(14.0), N ₇ (P:X)(10.0), O ₃ (P:Y)(10.0), Mn ₂ (D:XY)(6.0), Mn ₁ (D:X2-Y2)(6.0),
37	-13.294	1.0	N ₈ (P:Z)(19.0), C ₁₅ (P:Z)(8.0), N ₈ (P:Y)(7.0), Mn ₁ (D:Z2)(6.0),
38	-13.173	1.0	N ₁₁ (P:Z)(21.0), N ₁₁ (P:Y)(8.0), C ₂₁ (P:Z)(8.0), O ₅ (P:Z)(6.0),
39	-12.918	1.0	O ₄ (P:Y)(30.0), O ₃ (P:Y)(18.0), Mn ₁ (D:X2-Y2)(10.0), Mn ₂ (D:X2-Y2)(8.0), O ₅ (P:Y)(6.0),
40	-11.920	1.0	Mn ₁ (D:Z2)(42.0), O ₅ (P:Z)(14.0), O ₅ (P:X)(10.0), Mn ₁ (D:XY)(10.0),
41	-11.663	1.0	Mn ₁ (D:X2-Y2)(22.0), Mn ₁ (D:XY)(17.0), O ₅ (P:Y)(15.0), O ₃ (P:Y)(6.0), N ₁₀ (P:Y)(6.0),
42	-9.580	0.0	Mn ₂ (D:Z2)(32.0), Mn ₂ (D:X2-Y2)(30.0), O ₃ (P:Y)(8.0), Mn ₁ (D:X2-Y2)(7.0),
43	-9.395	0.0	Mn ₂ (D:XY)(35.0), Mn ₂ (D:Z2)(23.0), O ₅ (P:Y)(17.0), Mn ₂ (D:X2-Y2)(11.0),
44	-8.702	0.0	Mn ₁ (D:XY)(17.0), Mn ₂ (D:X2-Y2)(14.0), Mn ₁ (D:X2-Y2)(12.0), O ₃ (P:Y)(11.0), Mn ₁ (D:Z2)(9.0),

Orb.	Energy(eV)	Occ.	Primary Contributors SFO (percent)
			O ₅ (P:Z)(7.0),
45	-7.709	0.0	Mn ₂ (D:XY)(27.0), Mn ₂ (D:Z2)(17.0), Mn ₂ (D:X2-Y2)(14.0), O ₄ (P:Y)(13.0),
46	-6.501	0.0	O ₃ (P:X)(12.0), O ₄ (P:X)(10.0),
47	-6.485	0.0	O ₄ (P:X)(17.0), O ₃ (P:X)(13.0),
48	-5.959	0.0	O ₃ (P:X)(12.0), O ₄ (P:X)(12.0), H ₂₈ (S)(6.0),
49	-5.635	0.0	H ₄₄ (S)(11.0), H ₂₉ (S)(9.0), H ₄₇ (S)(8.0), H ₃₂ (S)(7.0), H ₄₆ (S)(6.0),
50	-5.473	0.0	H ₄₁ (S)(15.0), H ₂₅ (S)(13.0), H ₄₀ (S)(11.0), H ₄₈ (S)(11.0), H ₂₆ (S)(10.0), H ₃₃ (S)(8.0), H ₄₁ (S)(7.0), H ₂₅ (S)(7.0), H ₄₀ (S)(6.0), H ₂₆ (S)(6.0), H ₄₈ (S)(6.0),
51	-5.423	0.0	H ₂₉ (S)(10.0), H ₄₃ (S)(8.0), H ₄₄ (S)(8.0), H ₄₀ (S)(7.0), H ₂₈ (S)(7.0), H ₂₆ (S)(7.0), H ₃₁ (S)(6.0),
52	-4.936	0.0	H ₃₃ (S)(17.0), H ₄₈ (S)(15.0), H ₂₅ (S)(11.0), H ₄₀ (S)(10.0), H ₂₆ (S)(7.0), H ₄₁ (S)(7.0), H ₃₃ (S)(7.0), H ₄₈ (S)(6.0),
53	-4.706	0.0	H ₄₄ (S)(8.0), H ₂₉ (S)(7.0), H ₄₇ (S)(6.0),
54	-4.572	0.0	H ₂₉ (S)(10.0), H ₄₄ (S)(8.0), H ₃₂ (S)(6.0), H ₂₉ (S)(6.0), H ₄₇ (S)(6.0),
55	-4.231	0.0	H ₃₂ (S)(13.0), H ₄₇ (S)(11.0), H ₃₂ (S)(7.0), H ₄₇ (S)(6.0),
56	-4.145	0.0	H ₃₂ (S)(10.0), H ₄₇ (S)(9.0), H ₃₂ (S)(7.0), C ₂₁ (P:Y)(7.0), H ₄₇ (S)(6.0),
57	-4.124	0.0	H ₃₀ (S)(18.0), H ₄₅ (S)(16.0), H ₃₃ (S)(11.0), H ₃₀ (S)(10.0), H ₄₅ (S)(10.0), H ₄₈ (S)(10.0), H ₃₂ (S)(7.0),
58	-4.035	0.0	C ₁₃ (P:X)(12.0), C ₁₉ (P:X)(10.0), C ₁₅ (P:X)(9.0), C ₂₁ (P:X)(7.0), H ₄₇ (S)(7.0), H ₂₈ (S)(6.0),
59	-3.960	0.0	H ₄₇ (S)(16.0), H ₃₂ (S)(11.0), H ₄₄ (S)(11.0), C ₁₉ (P:X)(11.0), C ₂₁ (P:X)(9.0), C ₁₃ (P:X)(9.0), H ₂₉ (S)(8.0), C ₁₅ (P:X)(7.0),
60	-3.701	0.0	H ₃₀ (S)(13.0), H ₄₅ (S)(13.0), H ₃₀ (S)(8.0), H ₄₅ (S)(7.0), H ₃₃ (S)(6.0), H ₄₈ (S)(6.0),
61	-3.449	0.0	H ₃₁ (S)(18.0), H ₄₆ (S)(15.0), H ₃₁ (S)(7.0), H ₄₆ (S)(6.0), Symmetry Representation for Spin-2-AAA
1	-29.263	1.0	N ₈ (S)(62.0), C ₁₄ (S)(14.0), H ₂₆ (S)(11.0),
2	-29.182	1.0	N ₁₁ (S)(62.0), C ₂₀ (S)(14.0), H ₄₁ (S)(11.0),
3	-28.124	1.0	O ₅ (S)(94.0),
4	-25.187	1.0	C ₁₃ (S)(34.0), C ₁₄ (S)(19.0), N ₇ (P:Z)(8.0), H ₂₈ (S)(8.0),
5	-25.144	1.0	C ₁₉ (S)(34.0), C ₂₀ (S)(18.0), N ₁₀ (P:Z)(8.0), H ₄₃ (S)(8.0),
6	-22.031	1.0	C ₁₃ (S)(13.0), C ₁₅ (S)(13.0), C ₁₄ (S)(12.0), N ₈ (P:Y)(11.0), N ₇ (P:Z)(8.0), H ₂₈ (S)(6.0), H ₃₀ (S)(6.0), H ₃₃ (S)(6.0),

Orb.	Energy(eV)	Occ.	Primary Contributors SFO (percent)
7	-22.029	1.0	C ₂₁ (S)(14.0), C ₁₉ (S)(13.0), C ₂₀ (S)(12.0), N ₁₁ (P:Y)(11.0), N ₁₀ (P:Z)(8.0), H ₄₃ (S)(6.0), H ₄₅ (S)(6.0), H ₄₈ (S)(6.0),
8	-20.928	1.0	N ₈ (P:X)(17.0), C ₁₅ (S)(14.0), H ₃₂ (S)(10.0), H ₃₁ (S)(9.0), C ₁₄ (S)(7.0), H ₂₆ (S)(6.0),
9	-20.904	1.0	N ₁₁ (P:X)(17.0), C ₂₁ (S)(13.0), H ₄₇ (S)(10.0), H ₄₆ (S)(9.0), C ₂₀ (S)(7.0), H ₄₁ (S)(6.0),
10	-18.864	1.0	N ₈ (P:X)(14.0), N ₈ (P:Y)(13.0), C ₁₄ (P:Z)(11.0), H ₂₆ (S)(7.0), H ₃₀ (S)(6.0),
11	-18.805	1.0	N ₁₁ (P:X)(14.0), N ₁₁ (P:Y)(13.0), C ₂₀ (P:Z)(11.0), H ₄₁ (S)(7.0), H ₄₅ (S)(6.0),
12	-17.988	1.0	C ₁₉ (P:X)(15.0), C ₂₀ (P:X)(12.0), N ₁₀ (P:Z)(10.0), H ₄₄ (S)(9.0), H ₄₅ (S)(7.0),
13	-17.973	1.0	C ₁₃ (P:X)(15.0), C ₁₄ (P:X)(12.0), N ₇ (P:Z)(10.0), H ₂₉ (S)(9.0), H ₃₀ (S)(7.0),
14	-16.545	1.0	C ₂₀ (P:Y)(12.0), H ₄₆ (S)(9.0), C ₁₉ (P:Y)(8.0), N ₁₁ (P:Z)(6.0), C ₂₀ (P:Z)(6.0), N ₁₀ (P:Z)(6.0),
15	-16.516	1.0	C ₁₄ (P:Y)(13.0), H ₃₁ (S)(10.0), N ₇ (P:Z)(7.0), C ₁₃ (P:Y)(7.0), N ₈ (P:Z)(6.0), C ₁₄ (P:Z)(6.0), C ₁₃ (P:Z)(6.0),
16	-16.293	1.0	N ₈ (P:Z)(13.0), N ₁₁ (P:Z)(7.0),
17	-16.280	1.0	N ₁₁ (P:Z)(13.0), N ₈ (P:Z)(8.0),
18	-16.121	1.0	O ₃ (P:Z)(10.0), O ₄ (P:Z)(9.0), C ₁₃ (P:Y)(9.0), H ₂₈ (S)(9.0), H ₄₃ (S)(6.0),
19	-15.987	1.0	H ₄₃ (S)(11.0), C ₁₉ (P:Y)(10.0), C ₁₃ (P:Y)(10.0), H ₂₈ (S)(9.0),
20	-15.625	1.0	O ₃ (P:Z)(22.0), O ₄ (P:Z)(17.0), O ₅ (P:Y)(9.0), Mn ₁ (D:YZ)(8.0),
21	-15.389	1.0	O ₅ (P:X)(46.0), Mn ₁ (D:XZ)(18.0), Mn ₂ (D:XZ)(6.0), Mn ₁ (D:YZ)(6.0),
22	-14.656	1.0	O ₅ (P:Z)(21.0), Mn ₂ (D:XZ)(12.0), Mn ₁ (D:XZ)(10.0),
23	-14.250	1.0	C ₁₅ (P:X)(11.0), H ₃₂ (S)(11.0), H ₄₇ (S)(9.0), C ₂₁ (P:X)(8.0), H ₃₃ (S)(7.0), H ₄₈ (S)(6.0),
24	-14.097	1.0	C ₂₁ (P:X)(6.0), H ₄₇ (S)(6.0),
25	-14.026	1.0	H ₄₅ (S)(8.0), H ₃₀ (S)(7.0), H ₄₄ (S)(6.0),
26	-14.004	1.0	H ₃₃ (S)(6.0), H ₄₈ (S)(6.0),
27	-13.335	1.0	N ₈ (P:Z)(15.0), O ₅ (P:X)(14.0), N ₈ (P:Y)(10.0), N ₁₁ (P:Z)(8.0), N ₁₁ (P:Y)(6.0),
28	-13.294	1.0	Mn ₁ (D:YZ)(35.0), O ₄ (P:Z)(23.0), O ₅ (P:Y)(16.0),
29	-12.636	1.0	O ₅ (P:Z)(17.0), O ₅ (P:Y)(12.0), Mn ₁ (D:YZ)(12.0), N ₁₁ (P:Z)(10.0), O ₃ (P:Z)(8.0), N ₁₁ (P:X)(6.0),
30	-12.299	1.0	O ₅ (P:Z)(31.0), O ₅ (P:Y)(24.0), O ₃ (P:Z)(10.0), Mn ₂ (D:YZ)(9.0),
31	-10.888	1.0	O ₃ (P:Z)(30.0), O ₄ (P:Z)(23.0), Mn ₁ (D:YZ)(19.0), O ₅ (P:Y)(17.0),
32	-9.422	0.0	Mn ₂ (D:YZ)(50.0), Mn ₂ (D:XZ)(12.0), O ₄ (P:Z)(11.0), Mn ₁ (D:XZ)(7.0), O ₅ (P:Y)(6.0),
33	-8.466	0.0	Mn ₁ (D:XZ)(34.0), O ₅ (P:X)(15.0), Mn ₂ (D:YZ)(12.0), O ₅ (P:Z)(9.0), Mn ₁ (D:YZ)(7.0),

Orb.	Energy(eV)	Occ.	Primary Contributors SFO (percent)
34	-7.535	0.0	Mn ₂ (D:XZ)(51.0), O ₅ (P:Z)(12.0), Mn ₂ (D:YZ)(10.0), O ₅ (P:X)(7.0),
35	-5.356	0.0	H ₄₁ (S)(19.0), H ₂₆ (S)(16.0), H ₄₅ (S)(14.0), H ₃₀ (S)(13.0), H ₄₁ (S)(11.0), H ₄₅ (S)(11.0), H ₂₆ (S)(10.0), H ₃₀ (S)(10.0),
36	-4.788	0.0	H ₃₀ (S)(14.0), H ₄₅ (S)(12.0), H ₄₁ (S)(10.0), H ₂₆ (S)(10.0), H ₂₈ (S)(8.0), H ₃₀ (S)(8.0), H ₄₃ (S)(7.0), H ₄₅ (S)(7.0),
37	-4.394	0.0	H ₄₆ (S)(12.0), H ₄₁ (S)(9.0), H ₄₄ (S)(9.0), H ₃₁ (S)(9.0), H ₄₆ (S)(8.0), H ₂₉ (S)(7.0), H ₂₆ (S)(7.0), H ₃₁ (S)(6.0),
38	-4.187	0.0	H ₃₁ (S)(16.0), H ₄₆ (S)(13.0), H ₂₉ (S)(10.0), H ₃₁ (S)(9.0), H ₄₄ (S)(8.0), H ₄₆ (S)(8.0), H ₄₁ (S)(7.0), H ₂₆ (S)(7.0),
39	-4.025	0.0	H ₃₁ (S)(12.0), H ₄₆ (S)(12.0), H ₂₈ (S)(9.0), H ₄₃ (S)(8.0), H ₃₀ (S)(6.0), H ₃₁ (S)(6.0),
40	-3.874	0.0	H ₄₃ (S)(11.0), H ₂₈ (S)(9.0), H ₄₃ (S)(8.0), H ₂₈ (S)(7.0), H ₃₁ (S)(6.0), H ₄₆ (S)(6.0),
41	-3.684	0.0	C ₁₄ (P:Y)(10.0), C ₂₀ (P:Y)(8.0), C ₁₄ (P:Z)(7.0), H ₂₆ (S)(6.0), H ₂₈ (S)(6.0),
42	-3.512	0.0	H ₄₈ (S)(9.0), H ₄₃ (S)(8.0), C ₂₀ (P:Z)(8.0), H ₄₁ (S)(7.0), H ₃₃ (S)(6.0), C ₂₀ (P:Y)(6.0),
43	-3.229	0.0	H ₄₄ (S)(10.0), H ₂₉ (S)(8.0), C ₂₁ (S)(6.0),
44	-2.890	0.0	H ₂₈ (S)(14.0), H ₃₀ (S)(10.0), H ₄₅ (S)(10.0), H ₄₃ (S)(9.0), H ₃₀ (S)(9.0), H ₄₅ (S)(9.0), H ₃₃ (S)(8.0), H ₄₈ (S)(7.0),
45	-2.851	0.0	H ₂₆ (S)(12.0), H ₂₉ (S)(11.0), H ₄₁ (S)(8.0), H ₄₃ (S)(8.0), C ₁₅ (P:Y)(6.0),
46	-2.594	0.0	H ₃₃ (S)(11.0), H ₄₈ (S)(11.0), H ₃₁ (S)(6.0), H ₄₅ (S)(6.0), H ₄₆ (S)(6.0), H ₄₇ (S)(6.0), H ₃₂ (S)(6.0),
47	-2.347	0.0	H ₄₆ (S)(9.0), H ₃₁ (S)(8.0), H ₄₃ (S)(8.0), H ₂₈ (S)(8.0), C ₁₉ (P:X)(7.0), H ₄₇ (S)(7.0), H ₃₂ (S)(6.0), C ₁₃ (P:X)(6.0), H ₃₀ (S)(6.0), C ₂₀ (P:Z)(6.0),
48	-2.076	0.0	H ₃₀ (S)(21.0), H ₄₅ (S)(20.0), H ₂₈ (S)(11.0), H ₄₃ (S)(10.0), H ₃₂ (S)(9.0), H ₄₇ (S)(8.0),
49	-1.766	0.0	C ₂₁ (P:Z)(28.0), C ₁₅ (P:Z)(22.0), H ₄₇ (S)(11.0), H ₃₂ (S)(8.0), C ₁₉ (P:X)(7.0), C ₁₃ (P:X)(6.0), Mn ₁ (P:Z)(6.0),
50	-1.375	0.0	C ₁₅ (P:Z)(28.0), C ₂₁ (P:Z)(21.0), C ₁₄ (P:Y)(7.0), C ₁₃ (P:X)(7.0), C ₁₃ (P:Z)(7.0), C ₁₉ (P:X)(6.0), H ₃₂ (S)(6.0),
51	-1.181	0.0	C ₁₃ (P:Z)(17.0), C ₁₄ (P:Y)(17.0), H ₃₃ (S)(13.0), C ₁₉ (P:Z)(9.0), C ₂₀ (P:Y)(9.0), C ₁₅ (P:Y)(9.0), H ₃₁ (S)(7.0), N ₇ (P:Z)(7.0), H ₄₈ (S)(7.0), C ₁₄ (P:Z)(6.0),

TABLE S29: Orbital Energies Mn(IV)Mn(IV)(μ -O)₂(μ -O₂) (TACN)₂ HS ACCINT=3.5

Indices	Atoms	Charges	Alpha Spin	Beta Spin	Net Spin
1	Mn _{IV'}	1.1135	4.2768	1.6097	2.6671
2	Mn _{IV}	1.1167	4.2730	1.6103	2.6627
3	O _{p1}	-0.3484	3.2547	3.0937	0.1610
4	O _{p2}	-0.3474	3.2543	3.0931	0.1612
5	O _{μ}	-0.7247	3.4770	3.2477	0.2293
6	O _{μ}	-0.7247	3.4770	3.2477	0.2293
7	N	-0.3939	2.6930	2.7009	-0.0079
8	N	-0.4020	2.6826	2.7194	-0.0368
9	N	-0.4020	2.6826	2.7194	-0.0368
10	N	-0.3940	2.6932	2.7008	-0.0076
11	N	-0.4035	2.6838	2.7197	-0.0359
12	N	-0.4035	2.6838	2.7197	-0.0359
13	C	0.4194	1.7906	1.7900	0.0006
14	C	0.4201	1.7920	1.7879	0.0041
15	C	0.4039	1.7999	1.7962	0.0037
16	C	0.4039	1.7999	1.7962	0.0037
17	C	0.4201	1.7920	1.7879	0.0041
18	C	0.4194	1.7906	1.7900	0.0006
19	C	0.4202	1.7903	1.7895	0.0008
20	C	0.4198	1.7916	1.7886	0.0030
21	C	0.4069	1.7982	1.7950	0.0032
22	C	0.4069	1.7982	1.7950	0.0032
23	C	0.4198	1.7916	1.7886	0.0030
24	C	0.4202	1.7903	1.7895	0.0008
25	H	0.1216	0.4428	0.4357	0.0071
26	H	0.1789	0.4128	0.4082	0.0046
27	H	0.1789	0.4128	0.4082	0.0046
28	H	-0.0608	0.5306	0.5302	0.0004
29	H	-0.0684	0.5341	0.5343	-0.0002
30	H	-0.0727	0.5362	0.5366	-0.0004
31	H	-0.0762	0.5372	0.5389	-0.0017

Indices	Atoms	Charges	Alpha Spin	Beta Spin	Net Spin
32	H	-0.0788	0.5390	0.5398	-0.0008
33	H	-0.0483	0.5238	0.5245	-0.0007
34	H	-0.0483	0.5238	0.5245	-0.0007
35	H	-0.0788	0.5390	0.5398	-0.0008
36	H	-0.0727	0.5362	0.5366	-0.0004
37	H	-0.0762	0.5372	0.5389	-0.0017
38	H	-0.0608	0.5306	0.5302	0.0004
39	H	-0.0684	0.5341	0.5343	-0.0002
40	H	0.1214	0.4428	0.4359	0.0069
41	H	0.1803	0.4121	0.4076	0.0045
42	H	0.1803	0.4121	0.4076	0.0045
43	H	-0.0616	0.5310	0.5306	0.0004
44	H	-0.0689	0.5343	0.5346	-0.0003
45	H	-0.0738	0.5368	0.5370	-0.0002
46	H	-0.0746	0.5369	0.5377	-0.0008
47	H	-0.0795	0.5393	0.5401	-0.0008
48	H	-0.0503	0.5248	0.5255	-0.0007
49	H	-0.0503	0.5248	0.5255	-0.0007
50	H	-0.0795	0.5393	0.5401	-0.0008
51	H	-0.0738	0.5368	0.5370	-0.0002
52	H	-0.0746	0.5369	0.5377	-0.0008
53	H	-0.0616	0.5310	0.5306	0.0004
54	H	-0.0689	0.5343	0.5346	-0.0003

TABLE S29: Orbital Energies Mn(IV)Mn(IV)(μ -O)₂(μ -O₂) (TACN)₂ HS ACCINT=3.5

Orbital Energies and SFO Contributions

Orb.	Energy(eV)	Occ.	Primary Contributors SFO (percent)
Symmetry Representation for Spin-1-AA			
1	-32.722	1.0	O ₃ (S)(46.0), O ₄ (S)(46.0),
2	-30.204	1.0	N ₇ (S)(31.0), N ₈ (S)(28.0), C ₁₃ (S)(14.0), C ₁₄ (S)(8.0), C ₁₅ (S)(6.0),
3	-30.167	1.0	N ₁₀ (S)(33.0), N ₁₁ (S)(26.0), C ₁₉ (S)(15.0), C ₂₀ (S)(8.0),
4	-29.362	1.0	N ₈ (S)(31.0), N ₇ (S)(30.0), C ₁₅ (S)(10.0), C ₁₃ (S)(6.0), H ₂₅ (S)(6.0),
5	-29.309	1.0	N ₁₁ (S)(33.0), N ₁₀ (S)(28.0), C ₂₁ (S)(11.0), C ₁₉ (S)(6.0), H ₄₀ (S)(6.0),
6	-28.773	1.0	O ₅ (S)(89.0),
7	-26.422	1.0	O ₃ (S)(43.0), O ₄ (S)(43.0),
8	-25.221	1.0	C ₂₁ (S)(18.0), C ₁₅ (S)(16.0), C ₂₀ (S)(10.0), C ₁₄ (S)(10.0),
9	-25.188	1.0	C ₁₅ (S)(18.0), C ₂₁ (S)(17.0), C ₁₄ (S)(10.0), C ₂₀ (S)(9.0),
10	-23.558	1.0	C ₁₅ (S)(14.0), C ₁₃ (S)(13.0), C ₁₄ (S)(9.0), N ₈ (S)(8.0),
11	-23.513	1.0	C ₁₉ (S)(13.0), C ₂₁ (S)(13.0), C ₂₀ (S)(9.0), N ₁₁ (S)(8.0),
12	-21.188	1.0	N ₇ (P:X)(11.0), H ₂₉ (S)(11.0), C ₁₃ (S)(10.0), C ₁₄ (S)(9.0),
13	-21.145	1.0	N ₁₀ (P:X)(11.0), H ₄₄ (S)(11.0), C ₂₀ (S)(9.0), C ₁₉ (S)(9.0),
14	-19.943	1.0	N ₇ (P:Y)(10.0), N ₈ (P:X)(9.0), H ₂₈ (S)(7.0), C ₁₃ (P:Y)(6.0), N ₈ (P:Y)(6.0),
15	-19.850	1.0	N ₁₀ (P:Y)(11.0), N ₁₁ (P:X)(9.0), N ₁₁ (P:Y)(7.0), C ₁₉ (P:Y)(7.0), H ₄₃ (S)(7.0),
16	-18.918	1.0	C ₁₅ (P:Y)(14.0), N ₈ (P:Z)(10.0), N ₇ (P:Y)(8.0), N ₈ (P:X)(8.0), H ₃₃ (S)(6.0),
17	-18.893	1.0	C ₂₁ (P:Y)(15.0), N ₁₁ (P:X)(10.0), N ₁₁ (P:Z)(8.0), N ₁₀ (P:Y)(8.0), H ₄₈ (S)(6.0),
18	-18.676	1.0	O ₃ (P:X)(10.0), O ₄ (P:X)(10.0),
19	-18.419	1.0	N ₁₁ (P:Z)(8.0), N ₈ (P:Z)(6.0), C ₂₀ (P:Y)(6.0),
20	-17.918	1.0	H ₃₁ (S)(10.0), O ₄ (P:X)(7.0), O ₃ (P:X)(7.0), H ₄₆ (S)(7.0), C ₁₄ (P:X)(6.0),
21	-17.699	1.0	C ₂₁ (P:X)(11.0), C ₁₅ (P:X)(10.0), N ₁₁ (P:Y)(7.0), H ₄₆ (S)(7.0), N ₈ (P:Y)(6.0),
22	-17.355	1.0	O ₃ (P:X)(10.0), O ₄ (P:X)(10.0), C ₁₅ (P:X)(9.0), C ₂₁ (P:X)(9.0), O ₃ (P:Y)(7.0), O ₄ (P:Y)(7.0),
23	-16.921	1.0	O ₃ (P:Y)(16.0), O ₄ (P:Y)(16.0), Mn ₁ (D:XY)(8.0), Mn ₂ (D:XY)(8.0),
24	-16.633	1.0	C ₁₅ (P:Z)(11.0), C ₁₄ (P:Z)(8.0), C ₂₁ (P:Z)(8.0), H ₃₀ (S)(6.0),
25	-16.576	1.0	C ₂₀ (P:Z)(10.0), C ₁₄ (P:Z)(7.0), C ₂₁ (P:Y)(7.0), H ₄₅ (S)(7.0), H ₄₈ (S)(7.0),
26	-16.417	1.0	C ₁₃ (P:X)(6.0),
27	-16.300	1.0	O ₅ (P:Z)(9.0), C ₂₁ (P:Z)(8.0), C ₁₅ (P:Z)(6.0),
28	-16.256	1.0	C ₁₅ (P:X)(7.0), N ₈ (P:X)(6.0), C ₂₁ (P:X)(6.0),

Orb.	Energy(eV)	Occ.	Primary Contributors SFO (percent)
29	-15.987	1.0	O ₅ (P:Z)(13.0), N ₁₁ (P:X)(6.0),
30	-15.909	1.0	O ₅ (P:Z)(26.0),
31	-15.245	1.0	O ₅ (P:X)(37.0), Mn ₂ (D:Z2)(10.0), Mn ₁ (D:Z2)(10.0), C ₁₅ (P:Z)(6.0),
32	-14.848	1.0	O ₅ (P:Y)(30.0), Mn ₂ (D:X2-Y2)(7.0), Mn ₁ (D:X2-Y2)(7.0),
33	-14.495	1.0	C ₁₄ (P:X)(7.0), C ₂₀ (P:X)(7.0), H ₂₉ (S)(7.0), H ₃₀ (S)(7.0), H ₄₅ (S)(7.0), H ₄₄ (S)(6.0),
34	-14.367	1.0	O ₅ (P:Y)(9.0),
35	-14.255	1.0	O ₅ (P:X)(10.0), Mn ₂ (D:XY)(8.0), Mn ₁ (D:XY)(8.0), N ₇ (P:Y)(6.0),
36	-13.992	1.0	N ₇ (P:Y)(8.0), N ₁₀ (P:Y)(8.0), Mn ₁ (D:XY)(7.0), Mn ₂ (D:XY)(7.0), O ₄ (P:Y)(6.0), N ₁₀ (P:X)(6.0), N ₇ (P:X)(6.0),
37	-13.529	1.0	Mn ₁ (D:Z2)(8.0), Mn ₁ (D:X2-Y2)(7.0), Mn ₂ (D:Z2)(7.0), N ₈ (P:Z)(7.0), Mn ₂ (D:X2-Y2)(6.0),
38	-13.451	1.0	Mn ₁ (D:X2-Y2)(18.0), Mn ₂ (D:X2-Y2)(18.0), O ₃ (P:Y)(13.0), O ₄ (P:Y)(13.0), Mn ₁ (D:XY)(7.0), Mn ₂ (D:XY)(7.0),
39	-13.259	1.0	N ₁₁ (P:Z)(12.0), N ₈ (P:Z)(10.0),
40	-12.440	1.0	Mn ₁ (D:XY)(13.0), Mn ₂ (D:XY)(13.0), O ₃ (P:Y)(8.0), O ₄ (P:Y)(8.0), Mn ₂ (D:Z2)(7.0), Mn ₁ (D:Z2)(6.0),
41	-12.132	1.0	O ₅ (P:Z)(30.0), Mn ₂ (D:Z2)(20.0), Mn ₁ (D:Z2)(20.0), Mn ₂ (D:X2-Y2)(6.0), Mn ₁ (D:X2-Y2)(6.0),
42	-11.486	1.0	O ₅ (P:X)(18.0), Mn ₂ (D:X2-Y2)(13.0), Mn ₁ (D:X2-Y2)(13.0), Mn ₁ (D:Z2)(11.0), Mn ₂ (D:Z2)(10.0), O ₄ (P:Y)(8.0), O ₃ (P:Y)(8.0),
43	-11.056	1.0	O ₅ (P:Y)(41.0), Mn ₂ (D:XY)(11.0), Mn ₁ (D:XY)(11.0), Mn ₁ (D:X2-Y2)(6.0), Mn ₂ (D:X2-Y2)(6.0),
44	-9.119	0.0	Mn ₁ (D:XY)(13.0), Mn ₁ (D:X2-Y2)(12.0), Mn ₂ (D:X2-Y2)(12.0), Mn ₂ (D:XY)(12.0), O ₅ (P:Z)(7.0), O ₃ (P:Y)(6.0),
45	-8.569	0.0	O ₄ (P:Y)(13.0), O ₃ (P:Y)(12.0), Mn ₁ (D:XY)(11.0), Mn ₂ (D:XY)(11.0), O ₅ (P:X)(9.0), Mn ₁ (D:Z2)(7.0), Mn ₂ (D:Z2)(7.0), Mn ₂ (D:X2-Y2)(6.0),
46	-6.656	0.0	O ₃ (P:X)(33.0), O ₄ (P:X)(32.0),
47	-6.512	0.0	Mn ₁ (S)(7.0), Mn ₂ (S)(7.0), H ₂₅ (S)(6.0), H ₄₀ (S)(6.0),
48	-6.015	0.0	O ₃ (P:X)(8.0), O ₄ (P:X)(8.0), H ₂₈ (S)(6.0),
49	-5.652	0.0	H ₂₉ (S)(10.0), H ₄₄ (S)(10.0), H ₃₂ (S)(7.0), H ₄₇ (S)(7.0), H ₂₅ (S)(6.0),
50	-5.492	0.0	H ₄₁ (S)(15.0), H ₂₅ (S)(13.0), H ₂₆ (S)(11.0), H ₄₈ (S)(11.0), H ₄₀ (S)(10.0), H ₃₃ (S)(9.0), H ₄₁ (S)(8.0), H ₂₆ (S)(7.0), H ₂₅ (S)(7.0), H ₄₀ (S)(6.0), H ₄₈ (S)(6.0),
51	-5.443	0.0	H ₂₉ (S)(9.0), H ₄₃ (S)(9.0), H ₄₄ (S)(9.0), H ₄₀ (S)(8.0), H ₂₈ (S)(7.0), H ₂₆ (S)(6.0),
52	-4.953	0.0	H ₃₃ (S)(17.0), H ₄₈ (S)(15.0), H ₄₀ (S)(11.0), H ₂₅ (S)(11.0), H ₄₁ (S)(8.0),

Orb.	Energy(eV)	Occ.	Primary Contributors SFO (percent)
53	-4.730	0.0	H ₃₃ (S)(7.0), H ₂₆ (S)(7.0), H ₄₈ (S)(6.0), H ₂₉ (S)(8.0), H ₄₄ (S)(7.0), H ₃₂ (S)(6.0),
54	-4.582	0.0	H ₂₉ (S)(9.0), H ₄₄ (S)(9.0), H ₄₄ (S)(6.0), H ₂₉ (S)(6.0), H ₄₇ (S)(6.0),
55	-4.248	0.0	H ₃₂ (S)(15.0), H ₄₇ (S)(10.0), H ₃₂ (S)(8.0),
56	-4.156	0.0	H ₃₂ (S)(10.0), H ₄₇ (S)(9.0), H ₄₇ (S)(7.0), H ₃₂ (S)(6.0),
57	-4.135	0.0	H ₃₀ (S)(18.0), H ₄₅ (S)(17.0), H ₃₃ (S)(11.0), H ₃₀ (S)(11.0), H ₄₅ (S)(10.0), H ₄₈ (S)(9.0),
58	-4.043	0.0	C ₁₃ (P:X)(12.0), C ₁₅ (P:X)(10.0), C ₁₉ (P:X)(9.0), C ₂₁ (P:X)(7.0), H ₂₈ (S)(6.0), H ₂₉ (S)(6.0), H ₃₂ (S)(6.0), H ₄₇ (S)(6.0),
59	-3.969	0.0	H ₄₇ (S)(17.0), H ₄₄ (S)(12.0), C ₁₉ (P:X)(12.0), H ₃₂ (S)(11.0), C ₂₁ (P:X)(9.0), H ₂₉ (S)(8.0), C ₁₃ (P:X)(8.0), C ₁₅ (P:X)(6.0),
60	-3.714	0.0	H ₄₅ (S)(14.0), H ₃₀ (S)(13.0), H ₃₀ (S)(8.0), H ₄₅ (S)(7.0), H ₄₈ (S)(7.0), H ₃₃ (S)(6.0),
61	-3.468	0.0	H ₃₁ (S)(18.0), H ₄₆ (S)(14.0), H ₃₁ (S)(7.0), H ₄₆ (S)(6.0),
62	-3.233	0.0	H ₄₆ (S)(18.0), H ₃₁ (S)(14.0), H ₂₅ (S)(8.0), H ₃₁ (S)(6.0), H ₄₀ (S)(6.0), H ₃₀ (S)(6.0), H ₄₆ (S)(6.0),
63	-3.186	0.0	C ₁₉ (P:Y)(9.0), C ₁₉ (P:Y)(8.0), H ₄₁ (S)(8.0), C ₁₃ (P:Y)(7.0), C ₁₃ (P:Y)(6.0), H ₂₆ (S)(6.0), H ₄₁ (S)(6.0), Mn ₂ (S)(6.0), Symmetry Representation for Spin-1-AAA
1	-29.250	1.0	N ₈ (S)(62.0), C ₁₄ (S)(14.0), H ₂₆ (S)(11.0),
2	-29.186	1.0	N ₁₁ (S)(62.0), C ₂₀ (S)(14.0), H ₄₁ (S)(11.0),
3	-28.240	1.0	O ₅ (S)(94.0),
4	-25.194	1.0	C ₁₃ (S)(34.0), C ₁₄ (S)(19.0), N ₇ (P:Z)(8.0), H ₂₈ (S)(8.0),
5	-25.148	1.0	C ₁₉ (S)(34.0), C ₂₀ (S)(18.0), N ₁₀ (P:Z)(8.0), H ₄₃ (S)(8.0),
6	-22.037	1.0	C ₁₃ (S)(13.0), C ₁₅ (S)(13.0), C ₁₄ (S)(12.0), N ₈ (P:Y)(11.0), N ₇ (P:Z)(8.0), H ₂₈ (S)(6.0), H ₃₀ (S)(6.0), H ₃₃ (S)(6.0),
7	-22.032	1.0	C ₂₁ (S)(14.0), C ₁₉ (S)(13.0), C ₂₀ (S)(12.0), N ₁₁ (P:Y)(11.0), N ₁₀ (P:Z)(8.0), H ₄₃ (S)(6.0), H ₄₅ (S)(6.0), H ₄₈ (S)(6.0),
8	-20.940	1.0	N ₈ (P:X)(18.0), C ₁₅ (S)(14.0), H ₃₂ (S)(10.0), H ₃₁ (S)(9.0), C ₁₄ (S)(7.0), H ₂₆ (S)(6.0),
9	-20.908	1.0	N ₁₁ (P:X)(17.0), C ₂₁ (S)(13.0), H ₄₆ (S)(10.0), H ₄₇ (S)(10.0), C ₂₀ (S)(8.0), H ₄₁ (S)(6.0),
10	-18.887	1.0	N ₈ (P:X)(14.0), N ₈ (P:Y)(13.0), C ₁₄ (P:Z)(11.0), H ₂₆ (S)(7.0),
11	-18.810	1.0	N ₁₁ (P:X)(15.0), N ₁₁ (P:Y)(13.0), C ₂₀ (P:Z)(11.0), H ₄₁ (S)(7.0), H ₄₅ (S)(6.0),

Orb.	Energy(eV)	Occ.	Primary Contributors SFO (percent)
12	-17.999	1.0	C ₁₃ (P:X)(13.0), C ₁₄ (P:X)(9.0), N ₇ (P:Z)(8.0), H ₂₉ (S)(7.0), C ₁₉ (P:X)(6.0), H ₃₀ (S)(6.0),
13	-17.986	1.0	C ₁₉ (P:X)(13.0), C ₂₀ (P:X)(10.0), N ₁₀ (P:Z)(8.0), H ₄₄ (S)(7.0), C ₁₃ (P:X)(6.0), H ₄₅ (S)(6.0),
14	-16.579	1.0	C ₁₄ (P:Y)(12.0), C ₁₃ (P:Y)(8.0), N ₈ (P:Z)(7.0), H ₃₁ (S)(7.0),
15	-16.550	1.0	C ₂₀ (P:Y)(12.0), C ₁₉ (P:Y)(8.0), H ₄₆ (S)(8.0), N ₁₁ (P:Z)(6.0),
16	-16.305	1.0	N ₈ (P:Z)(11.0), N ₁₁ (P:Z)(7.0),
17	-16.287	1.0	N ₁₁ (P:Z)(12.0), N ₈ (P:Z)(8.0),
18	-16.243	1.0	O ₃ (P:Z)(16.0), O ₄ (P:Z)(16.0),
19	-16.003	1.0	C ₁₃ (P:Y)(10.0), H ₂₈ (S)(10.0), H ₄₃ (S)(9.0), C ₁₉ (P:Y)(8.0),
20	-15.826	1.0	O ₃ (P:Z)(9.0), O ₄ (P:Z)(9.0), C ₁₉ (P:Y)(7.0), H ₄₃ (S)(7.0), O ₅ (P:Y)(6.0),
21	-15.614	1.0	O ₅ (P:X)(41.0), Mn ₂ (D:XZ)(11.0), Mn ₁ (D:XZ)(11.0), Mn ₂ (D:YZ)(6.0), Mn ₁ (D:YZ)(6.0),
22	-14.911	1.0	O ₅ (P:Z)(21.0), Mn ₂ (D:XZ)(13.0), Mn ₁ (D:XZ)(13.0),
23	-14.273	1.0	C ₁₅ (P:X)(10.0), H ₃₂ (S)(10.0), C ₂₁ (P:X)(9.0), H ₄₇ (S)(9.0), H ₃₃ (S)(6.0), H ₄₈ (S)(6.0),
24	-14.124	1.0	C ₂₁ (P:X)(7.0), H ₄₇ (S)(7.0),
25	-14.030	1.0	H ₃₀ (S)(8.0), H ₄₅ (S)(7.0), H ₂₉ (S)(6.0),
26	-14.020	1.0	H ₄₅ (S)(7.0),
27	-13.478	1.0	O ₅ (P:Y)(25.0), Mn ₂ (D:YZ)(21.0), O ₃ (P:Z)(19.0), O ₄ (P:Z)(7.0), Mn ₁ (D:YZ)(6.0),
28	-13.450	1.0	Mn ₁ (D:YZ)(32.0), O ₄ (P:Z)(16.0), Mn ₂ (D:YZ)(13.0), Mn ₁ (D:XZ)(8.0), Mn ₂ (D:XZ)(7.0),
29	-13.329	1.0	O ₅ (P:X)(13.0), N ₁₁ (P:Z)(11.0), N ₈ (P:Z)(9.0), N ₁₁ (P:Y)(7.0), N ₈ (P:Y)(6.0),
30	-12.542	1.0	O ₅ (P:Z)(41.0), N ₁₁ (P:Z)(11.0), N ₈ (P:Z)(8.0),
31	-11.387	1.0	O ₅ (P:Y)(48.0), Mn ₂ (D:YZ)(20.0), Mn ₁ (D:YZ)(20.0),
32	-10.935	1.0	O ₃ (P:Z)(37.0), O ₄ (P:Z)(37.0), Mn ₁ (D:YZ)(7.0), Mn ₂ (D:YZ)(7.0),
33	-8.726	0.0	O ₅ (P:X)(26.0), Mn ₁ (D:XZ)(21.0), Mn ₂ (D:XZ)(14.0), Mn ₁ (D:YZ)(7.0), Mn ₂ (D:YZ)(6.0),
34	-8.489	0.0	Mn ₂ (D:XZ)(27.0), O ₅ (P:Z)(26.0), Mn ₁ (D:XZ)(21.0),
35	-5.372	0.0	H ₄₁ (S)(18.0), H ₂₆ (S)(16.0), H ₄₅ (S)(14.0), H ₃₀ (S)(13.0), H ₄₁ (S)(11.0), H ₃₀ (S)(11.0), H ₄₅ (S)(11.0), H ₂₆ (S)(10.0),
36	-4.798	0.0	H ₃₀ (S)(14.0), H ₄₅ (S)(12.0), H ₄₁ (S)(10.0), H ₂₆ (S)(9.0), H ₂₈ (S)(8.0), H ₃₀ (S)(8.0), H ₄₃ (S)(7.0), H ₄₅ (S)(7.0),
37	-4.412	0.0	H ₃₁ (S)(10.0), H ₄₆ (S)(10.0), H ₂₆ (S)(8.0), H ₄₁ (S)(8.0), H ₄₄ (S)(8.0), H ₂₉ (S)(8.0), H ₃₁ (S)(7.0), H ₄₆ (S)(7.0),
38	-4.208	0.0	H ₃₁ (S)(14.0), H ₄₆ (S)(14.0), H ₄₄ (S)(9.0), H ₂₉ (S)(9.0), H ₃₁ (S)(8.0), H ₄₁ (S)(8.0), H ₄₆ (S)(8.0), H ₂₆ (S)(6.0),

Orb.	Energy(eV)	Occ.	Primary Contributors SFO (percent)
39	-4.035	0.0	H ₃₁ (S)(13.0), H ₄₆ (S)(12.0), H ₂₈ (S)(10.0), H ₄₃ (S)(7.0), H ₃₀ (S)(6.0), H ₃₁ (S)(6.0),
40	-3.881	0.0	H ₄₃ (S)(12.0), H ₂₈ (S)(8.0), H ₄₃ (S)(8.0), H ₂₈ (S)(7.0), H ₄₆ (S)(7.0),
41	-3.692	0.0	C ₁₄ (P:Y)(10.0), C ₂₀ (P:Y)(8.0), C ₁₄ (P:Z)(7.0), H ₂₆ (S)(6.0), H ₂₈ (S)(6.0),
42	-3.516	0.0	H ₄₃ (S)(9.0), H ₄₈ (S)(9.0), C ₂₀ (P:Z)(8.0), H ₄₁ (S)(7.0), H ₃₃ (S)(6.0), C ₂₀ (P:Y)(6.0),
43	-3.255	0.0	H ₄₄ (S)(9.0), H ₂₉ (S)(8.0), C ₂₁ (S)(6.0),
44	-2.898	0.0	H ₂₈ (S)(15.0), H ₃₀ (S)(10.0), H ₃₀ (S)(9.0), H ₄₅ (S)(9.0), H ₄₅ (S)(9.0), H ₃₃ (S)(8.0), H ₄₃ (S)(8.0), H ₄₄ (S)(6.0), H ₄₈ (S)(6.0),
45	-2.865	0.0	H ₂₆ (S)(11.0), H ₂₉ (S)(11.0), H ₄₃ (S)(10.0), H ₄₁ (S)(8.0), C ₁₅ (P:Y)(6.0),
46	-2.603	0.0	H ₄₈ (S)(11.0), H ₃₃ (S)(10.0), H ₃₁ (S)(6.0), H ₄₆ (S)(6.0), H ₄₇ (S)(6.0), H ₃₂ (S)(6.0),
47	-2.362	0.0	H ₃₁ (S)(9.0), H ₄₆ (S)(9.0), H ₄₃ (S)(8.0), H ₂₈ (S)(8.0), C ₁₃ (P:X)(7.0), C ₁₉ (P:X)(7.0), H ₃₂ (S)(6.0), H ₃₀ (S)(6.0), C ₂₀ (P:Z)(6.0), H ₄₇ (S)(6.0),
48	-2.080	0.0	H ₃₀ (S)(21.0), H ₄₅ (S)(20.0), H ₂₈ (S)(11.0), H ₄₃ (S)(10.0), H ₃₂ (S)(8.0), H ₄₇ (S)(8.0),
49	-1.807	0.0	C ₁₅ (P:Z)(26.0), C ₂₁ (P:Z)(24.0), H ₃₂ (S)(10.0), H ₄₇ (S)(10.0), C ₁₃ (P:X)(6.0),
50	-1.419	0.0	C ₂₁ (P:Z)(26.0), C ₁₅ (P:Z)(24.0), C ₁₉ (P:X)(8.0), C ₁₃ (P:X)(6.0), C ₁₃ (P:Z)(6.0), C ₁₄ (P:Y)(6.0), H ₄₇ (S)(6.0),
51	-1.187	0.0	C ₁₃ (P:Z)(17.0), C ₁₄ (P:Y)(17.0), H ₃₃ (S)(12.0), C ₁₉ (P:Z)(9.0), C ₂₀ (P:Y)(9.0), C ₁₅ (P:Y)(9.0), H ₃₁ (S)(7.0), N ₇ (P:Z)(7.0), H ₄₈ (S)(7.0), C ₁₄ (P:Z)(6.0), H ₃₂ (S)(6.0),
52	-1.107	0.0	C ₂₀ (P:Y)(19.0), C ₁₉ (P:Z)(17.0), C ₁₄ (P:Y)(9.0), C ₁₃ (P:Z)(8.0), H ₄₈ (S)(8.0), C ₂₁ (P:Y)(7.0), C ₂₀ (P:Z)(7.0), C ₁₉ (P:Y)(6.0), H ₄₆ (S)(6.0), H ₄₇ (S)(6.0), N ₁₀ (P:Z)(6.0), Symmetry Representation for Spin-2-AA
1	-32.470	1.0	O ₃ (S)(46.0), O ₄ (S)(46.0),
2	-30.196	1.0	N ₇ (S)(30.0), N ₈ (S)(28.0), C ₁₃ (S)(14.0), C ₁₄ (S)(8.0), C ₁₅ (S)(6.0),
3	-30.159	1.0	N ₁₀ (S)(32.0), N ₁₁ (S)(26.0), C ₁₉ (S)(14.0), C ₂₀ (S)(8.0), C ₂₁ (S)(6.0),
4	-29.358	1.0	N ₈ (S)(31.0), N ₇ (S)(30.0), C ₁₅ (S)(10.0), C ₁₃ (S)(6.0), H ₂₅ (S)(6.0),
5	-29.305	1.0	N ₁₁ (S)(33.0), N ₁₀ (S)(28.0), C ₂₁ (S)(11.0), C ₁₉ (S)(6.0), H ₄₀ (S)(6.0),
6	-28.420	1.0	O ₅ (S)(91.0),
7	-26.141	1.0	O ₃ (S)(42.0), O ₄ (S)(42.0),
8	-25.217	1.0	C ₂₁ (S)(18.0), C ₁₅ (S)(16.0), C ₂₀ (S)(11.0), C ₁₄ (S)(10.0),

Orb.	Energy(eV)	Occ.	Primary Contributors SFO (percent)
9	-25.176	1.0	C ₁₅ (S)(18.0), C ₂₁ (S)(17.0), C ₁₄ (S)(10.0), C ₂₀ (S)(9.0),
10	-23.553	1.0	C ₁₅ (S)(14.0), C ₁₃ (S)(12.0), C ₁₄ (S)(9.0), N ₈ (S)(8.0),
11	-23.508	1.0	C ₁₉ (S)(13.0), C ₂₁ (S)(13.0), C ₂₀ (S)(9.0), N ₁₁ (S)(8.0),
12	-21.175	1.0	N ₇ (P:X)(11.0), H ₂₉ (S)(11.0), C ₁₃ (S)(10.0), C ₁₄ (S)(9.0),
13	-21.133	1.0	N ₁₀ (P:X)(11.0), H ₄₄ (S)(11.0), C ₂₀ (S)(9.0), C ₁₉ (S)(9.0),
14	-19.907	1.0	N ₇ (P:Y)(11.0), N ₈ (P:X)(10.0), N ₈ (P:Y)(7.0), C ₁₃ (P:Y)(7.0), H ₂₈ (S)(7.0),
15	-19.826	1.0	N ₁₀ (P:Y)(11.0), N ₁₁ (P:X)(10.0), H ₄₃ (S)(8.0), C ₁₉ (P:Y)(7.0), N ₁₁ (P:Y)(7.0),
16	-18.890	1.0	C ₁₅ (P:Y)(16.0), N ₈ (P:Z)(11.0), N ₇ (P:Y)(9.0), N ₈ (P:X)(9.0), H ₃₃ (S)(7.0),
17	-18.873	1.0	C ₂₁ (P:Y)(16.0), N ₁₁ (P:X)(11.0), N ₁₁ (P:Z)(9.0), N ₁₀ (P:Y)(9.0), H ₄₈ (S)(7.0),
18	-18.593	1.0	O ₄ (P:X)(8.0), O ₃ (P:X)(7.0), N ₈ (P:Z)(7.0), N ₁₁ (P:Z)(6.0),
19	-18.387	1.0	N ₁₁ (P:Z)(8.0), N ₈ (P:Z)(6.0), C ₂₀ (P:Y)(6.0),
20	-17.854	1.0	H ₃₁ (S)(10.0), H ₄₆ (S)(8.0), N ₈ (P:Y)(6.0), C ₁₄ (P:X)(6.0), O ₃ (P:X)(6.0), O ₄ (P:X)(6.0),
21	-17.684	1.0	C ₂₁ (P:X)(11.0), C ₁₅ (P:X)(9.0), N ₁₁ (P:Y)(8.0), H ₄₆ (S)(7.0),
22	-17.210	1.0	O ₃ (P:X)(14.0), O ₄ (P:X)(14.0), O ₃ (P:Y)(9.0), O ₄ (P:Y)(9.0), C ₁₅ (P:X)(8.0), C ₂₁ (P:X)(8.0),
23	-16.630	1.0	C ₁₅ (P:Z)(13.0), C ₁₄ (P:Z)(6.0), N ₇ (P:X)(6.0),
24	-16.586	1.0	C ₂₁ (P:Z)(11.0), C ₂₀ (P:Z)(10.0), H ₄₅ (S)(7.0), H ₄₈ (S)(7.0), C ₂₁ (P:Y)(6.0), N ₁₀ (P:X)(6.0),
25	-16.508	1.0	O ₃ (P:Y)(7.0), O ₄ (P:Y)(7.0), C ₁₄ (P:Z)(6.0), C ₁₅ (P:Y)(6.0),
26	-16.370	1.0	C ₂₁ (P:Z)(9.0), C ₁₅ (P:Z)(7.0), N ₁₁ (P:Y)(6.0), C ₁₉ (P:X)(6.0), C ₁₃ (P:X)(6.0),
27	-16.198	1.0	N ₈ (P:X)(9.0), C ₁₅ (P:X)(6.0), C ₂₁ (P:X)(6.0),
28	-16.143	1.0	O ₃ (P:Y)(10.0), O ₄ (P:Y)(9.0), C ₂₁ (P:Z)(8.0), O ₃ (P:X)(6.0), C ₁₅ (P:Z)(6.0), O ₄ (P:X)(6.0),
29	-15.925	1.0	N ₁₁ (P:X)(8.0), O ₄ (P:Y)(6.0), N ₈ (P:X)(6.0), O ₃ (P:Y)(6.0),
30	-15.100	1.0	O ₅ (P:Z)(60.0),
31	-14.710	1.0	O ₅ (P:X)(52.0),
32	-14.505	1.0	C ₁₄ (P:X)(10.0), H ₃₀ (S)(10.0), H ₂₉ (S)(9.0), C ₁₃ (P:X)(6.0), H ₃₁ (S)(6.0),
33	-14.476	1.0	C ₂₀ (P:X)(10.0), H ₄₅ (S)(10.0), H ₄₄ (S)(9.0), H ₄₆ (S)(7.0), C ₁₉ (P:X)(6.0),
34	-13.954	1.0	N ₇ (P:Y)(10.0), N ₁₀ (P:Y)(8.0), O ₅ (P:X)(6.0), N ₇ (P:X)(6.0),
35	-13.876	1.0	O ₅ (P:Y)(24.0), N ₁₀ (P:Y)(9.0), N ₇ (P:Y)(8.0),
36	-13.449	1.0	O ₅ (P:Y)(22.0),
37	-13.122	1.0	N ₈ (P:Z)(20.0), O ₅ (P:Y)(12.0), N ₈ (P:Y)(7.0), C ₁₅ (P:Z)(7.0), N ₈ (P:X)(6.0),
38	-13.077	1.0	N ₁₁ (P:Z)(22.0), O ₅ (P:X)(11.0), N ₁₁ (P:Y)(7.0), C ₂₁ (P:Z)(7.0), N ₁₁ (P:X)(6.0),

Orb.	Energy(eV)	Occ.	Primary Contributors SFO (percent)
39	-12.671	1.0	O ₃ (P:Y)(31.0), O ₄ (P:Y)(31.0), Mn ₁ (D:X2-Y2)(6.0), Mn ₂ (D:X2-Y2)(6.0),
40	-9.984	0.0	Mn ₁ (D:XY)(24.0), Mn ₂ (D:XY)(24.0), Mn ₂ (D:Z2)(11.0), Mn ₁ (D:Z2)(10.0), Mn ₂ (D:X2-Y2)(8.0), Mn ₁ (D:X2-Y2)(8.0),
41	-9.799	0.0	Mn ₁ (D:Z2)(25.0), Mn ₂ (D:Z2)(25.0), Mn ₂ (D:X2-Y2)(13.0), O ₅ (P:Z)(12.0), Mn ₁ (D:X2-Y2)(11.0),
42	-9.069	0.0	Mn ₁ (D:X2-Y2)(25.0), Mn ₂ (D:X2-Y2)(24.0), Mn ₁ (D:Z2)(17.0), Mn ₂ (D:Z2)(16.0),
43	-8.719	0.0	O ₅ (P:Y)(21.0), Mn ₁ (D:XY)(19.0), Mn ₂ (D:XY)(18.0), Mn ₁ (D:Z2)(11.0), Mn ₂ (D:Z2)(10.0), Mn ₁ (D:X2-Y2)(6.0), Mn ₂ (D:X2-Y2)(6.0),
44	-7.885	0.0	Mn ₁ (D:X2-Y2)(16.0), Mn ₂ (D:X2-Y2)(15.0), Mn ₁ (D:XY)(13.0), Mn ₂ (D:XY)(13.0), O ₅ (P:Z)(6.0),
45	-7.407	0.0	Mn ₁ (D:Z2)(13.0), Mn ₁ (D:XY)(13.0), Mn ₂ (D:Z2)(13.0), Mn ₂ (D:XY)(13.0), O ₅ (P:X)(9.0), O ₄ (P:Y)(8.0), O ₃ (P:Y)(8.0),
46	-6.484	0.0	Mn ₂ (S)(7.0), Mn ₁ (S)(6.0), H ₂₅ (S)(6.0),
47	-6.383	0.0	O ₃ (P:X)(19.0), O ₄ (P:X)(19.0),
48	-5.893	0.0	O ₃ (P:X)(17.0); O ₄ (P:X)(17.0), H ₂₈ (S)(6.0),
49	-5.629	0.0	H ₂₉ (S)(10.0), H ₄₄ (S)(10.0), H ₃₂ (S)(8.0), H ₄₇ (S)(8.0),
50	-5.456	0.0	H ₄₁ (S)(14.0), H ₂₅ (S)(13.0), H ₄₈ (S)(11.0), H ₂₆ (S)(10.0), H ₄₀ (S)(10.0), H ₃₃ (S)(8.0), H ₄₁ (S)(7.0), H ₂₅ (S)(7.0), H ₄₀ (S)(6.0), H ₂₆ (S)(6.0), H ₄₈ (S)(6.0),
51	-5.412	0.0	H ₂₉ (S)(10.0), H ₄₃ (S)(9.0), H ₄₄ (S)(9.0), H ₂₆ (S)(7.0), H ₄₀ (S)(7.0), H ₂₈ (S)(6.0),
52	-4.932	0.0	H ₃₃ (S)(17.0), H ₄₈ (S)(15.0), H ₄₀ (S)(11.0), H ₂₅ (S)(11.0), H ₂₆ (S)(7.0), H ₄₁ (S)(7.0), H ₃₃ (S)(7.0), H ₄₈ (S)(6.0),
53	-4.693	0.0	H ₂₉ (S)(9.0), H ₄₄ (S)(7.0),
54	-4.570	0.0	H ₄₄ (S)(10.0), H ₂₉ (S)(9.0), H ₄₄ (S)(6.0), H ₄₇ (S)(6.0),
55	-4.226	0.0	H ₃₂ (S)(15.0), H ₄₇ (S)(10.0), H ₃₂ (S)(8.0), H ₄₇ (S)(6.0),
56	-4.140	0.0	H ₃₂ (S)(12.0), H ₄₇ (S)(8.0), H ₃₂ (S)(7.0), C ₁₅ (P:Y)(6.0), H ₄₇ (S)(6.0),
57	-4.121	0.0	H ₃₀ (S)(17.0), H ₄₅ (S)(17.0), H ₃₀ (S)(11.0), H ₃₃ (S)(10.0), H ₄₅ (S)(9.0), H ₄₈ (S)(9.0), H ₄₇ (S)(6.0), C ₂₁ (P:Y)(6.0),
58	-4.035	0.0	C ₁₃ (P:X)(12.0), C ₁₅ (P:X)(9.0), C ₁₉ (P:X)(9.0), C ₂₁ (P:X)(7.0), H ₄₇ (S)(7.0), H ₃₂ (S)(6.0), H ₂₈ (S)(6.0),
59	-3.959	0.0	H ₄₇ (S)(16.0), H ₄₄ (S)(11.0), C ₁₉ (P:X)(11.0), H ₃₂ (S)(10.0), C ₂₁ (P:X)(9.0), H ₂₉ (S)(8.0), C ₁₃ (P:X)(8.0), C ₁₅ (P:X)(7.0), Symmetry Representation for Spin-2-AAA
1	-29.260	1.0	N ₈ (S)(62.0), C ₁₄ (S)(14.0), H ₂₆ (S)(11.0),
2	-29.197	1.0	N ₁₁ (S)(62.0), C ₂₀ (S)(14.0), H ₄₁ (S)(11.0),