

Principal Components of Mn(salen) Catalysts

Supporting Information for Reviewers

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Relevant coefficients of the DefBas-3 basis set.

BASIS SET INFORMATION

There are 6 groups of distinct atoms

Group	1	Type Mn	: 17s11p6d1f contracted to 6s4p3d1f pattern {842111/6311/411/1}
Group	2	Type N	: 11s6p1d contracted to 5s3p1d pattern {62111/411/1}
Group	3	Type O	: 11s6p1d contracted to 5s3p1d pattern {62111/411/1}
Group	4	Type C	: 11s6p1d contracted to 5s3p1d pattern {62111/411/1}
Group	5	Type H	: 5s contracted to 3s pattern {311}
Group	6	Type Cl	: 14s9p1d contracted to 5s5p1d pattern {73211/51111/1}

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BASIS SET IN INPUT FORMAT

Basis set for element : H
NewGTO H
S 3
1 34.0613410000 0.0254393072
2 5.1235746000 0.1900859489
3 1.1646626000 0.8524411301
S 1
1 0.3272304100 1.0000000000
S 1
1 0.1030724100 1.0000000000
end;

Basis set for element : C
NewGTO C
S 6
1 13575.3496820000 0.0006064549
2 2035.2333680000 0.0046979088
3 463.2256235900 0.0243324776
4 131.2001959800 0.0973999683
5 42.8530158910 0.3019558425
6 15.5841857660 0.6623360915
S 2
1 6.2067138508 0.6559530854
2 2.5764896527 0.3758563329
S 1
1 0.5769633942 1.0000000000
S 1
1 0.2297283136 1.0000000000
S 1
1 0.0951644400 1.0000000000
P 4
1 34.6972322440 0.0113272200
2 7.9582622826 0.0761696592
3 2.3780826883 0.3019225220
4 0.8143320818 0.7278502735
P 1
1 0.2888754725 1.0000000000
P 1
1 0.1005682367 1.0000000000
D 1
1 0.8000000000 1.0000000000

end;

Basis set for element : N

NewGTO N

S 6

1	19730.8006470000	0.0005862639
2	2957.8958745000	0.0045428821
3	673.2213359500	0.0235584136
4	190.6824949400	0.0947091933
5	62.2954418980	0.2971978492
6	22.6541611820	0.6691624689

S 2

1	8.9791477428	0.6459668363
2	3.6863002370	0.3870057440

S 1

1	0.8466007680	1.0000000000
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S 1

1	0.3364713377	1.0000000000
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S 1

1	0.1364765367	1.0000000000
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P 4

1	49.2003805100	0.0114488252
2	11.3467905370	0.0784223379
3	3.4273972411	0.3081809474
4	1.1785525134	0.7202719637

P 1

1	0.4164220497	1.0000000000
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P 1

1	0.1426082601	1.0000000000
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D 1

1	1.0000000000	1.0000000000
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end;

Basis set for element : 0

NewGTO 0

S 6

1	27032.3826310000	0.0005722733
2	4052.3871392000	0.0044353233
3	922.3272271000	0.0230201076
4	261.2407098900	0.0928224906
5	85.3546413510	0.2937850002
6	31.0350352450	0.6740160450

S 2

1	12.2608607280	0.6383993702
2	4.9987076005	0.3953458713

S	1		
	1	1.1703108158	1.0000000000
S	1		
	1	0.4647474099	1.0000000000
S	1		
	1	0.1850453636	1.0000000000
P	4		
	1	63.2749548010	0.0120183321
	2	14.6270493790	0.0830054217
	3	4.4501223456	0.3199174393
	4	1.5275799647	0.7071554292
P	1		
	1	0.5293511794	1.0000000000
P	1		
	1	0.1747842127	1.0000000000
D	1		
	1	1.2000000000	1.0000000000

end;

Basis set for element : Cl

NewGTO Cl

S	7		
	1	69507.9909450000	0.0005145739
	2	10426.1568800000	0.0039781345
	3	2373.2334061000	0.0204561787
	4	671.5642007100	0.0801481029
	5	218.4199979000	0.2345477031
	6	77.5722497140	0.4454336858
	7	28.8888152770	0.3546684250
S	3		
	1	127.1052718500	0.1129368806
	2	39.3395829610	0.4837351424
	3	7.6740679989	-1.2292297390
S	2		
	1	3.8745627630	0.6729682164
	2	1.8385832573	0.3495605141
S	1		
	1	0.5022905754	1.0000000000
S	1		
	1	0.1796272342	1.0000000000
P	5		
	1	666.5042328400	0.0033502508
	2	157.6424169000	0.0267639704
	3	50.2625209780	0.1236268236
	4	18.5360781050	0.3584578792

5	7.2940532777	0.6167729635
P 1		
1	2.9433248995	1.0000000000
P 1		
1	1.0404970818	1.0000000000
P 1		
1	0.3845641508	1.0000000000
P 1		
1	0.1306964273	1.0000000000
D 1		
1	0.6500000000	1.0000000000

end;

Basis set for element : Mn

NewGTO Mn

S 8		
1	277185.0015300000	0.0002418656
2	41550.7698900000	0.0018752946
3	9455.9700152000	0.0097512595
4	2676.5206482000	0.0396246641
5	871.4668753000	0.1288296214
6	312.9830642000	0.3052591758
7	121.4445405100	0.4346431672
8	47.9225988290	0.2263400217
S 4		
1	303.6672316300	-0.0245709140
2	93.8814031870	-0.1159363731
3	14.8794212140	0.5506944896
4	6.2865200745	0.5366603595
S 2		
1	9.4858591337	-0.3767154211
2	1.5698706158	1.1717588005
S 1		
1	0.6590321361	1.0000000000
S 1		
1	0.1068629237	1.0000000000
S 1		
1	0.0392674354	1.0000000000
P 6		
1	1444.7978182000	0.0027745622
2	342.0655119700	0.0223976772
3	109.5840089100	0.1043445351
4	40.7479881730	0.2977077474
5	16.1886265660	0.4772528898
6	6.5484505964	0.2785381470

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P 3
  1 25.3570864370 -0.0199847359
  2  3.4830168782  0.3843357437
  3  1.3858800906  0.6768530881
P 1
  1  0.5255509489  1.0000000000
D 4
  1 56.5631891190  0.1033484355
  2 16.2787347110  0.6294052421
  3  5.6964273914  0.2010051750
  4  2.1411147942  0.3554675997
D 1
  1  0.7829180194  1.0000000000
D 1
  1  0.2595231121  1.0000000000
P 1
  1  0.1276500000  1.0000000000
F 1
  1  2.2500000000  1.0000000000
end;
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