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Supporting information

Controlling the nucleophilic properties of cobalt salen complexes for carbon dioxide capture

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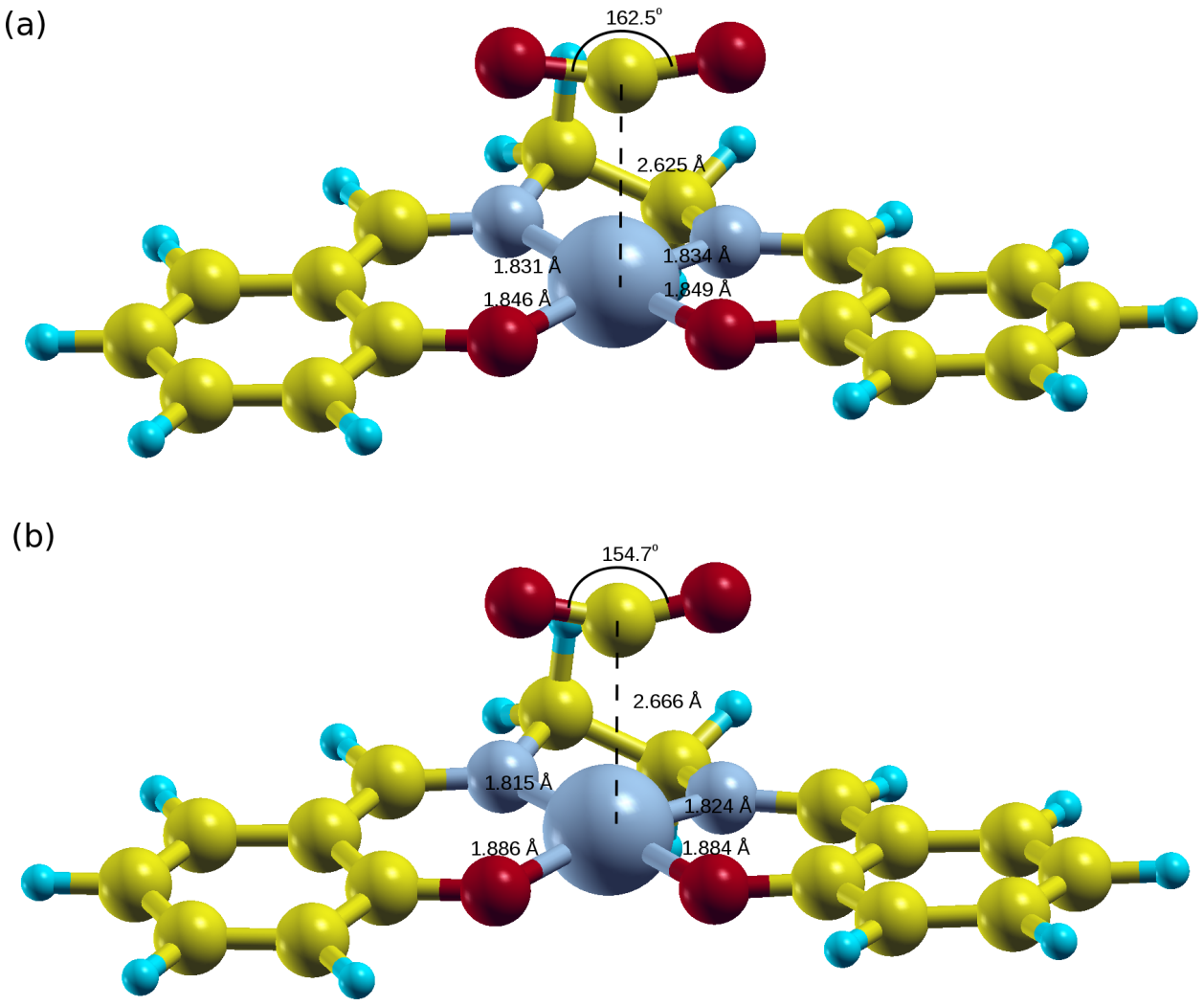

Figure S1. Transition state structure for the formation of (a) Co(salen)-CO_2 and (b) [Co(salen)-CO_2]$^-$, as calculated by nudged elastic band. Refer to Fig. 4 of the original text.

Table S1. Cartesian coordinates (in Angstrom) of each atom of $[Co(salen)]^-$

Atom	*x*	*y*	*z*
C	0.93282221	-2.942902077	-0.252106019
C	2.090597924	-2.249363388	0.439924628
N	1.916237076	-0.808130406	0.210535656
C	3.003159291	-0.055530054	0.255612844
C	3.00262026	1.365750327	0.137017984
C	4.222418815	2.078701283	0.138103114
C	4.268179181	3.462417099	0.041470187
C	3.059617385	4.174758395	-0.056386094
C	1.843220225	3.508607399	-0.062887796
C	1.759342473	2.090726351	0.030803144
O	0.587100992	1.523509781	0.028797894
Co	0.195949541	-0.326398087	0.027884828
O	-1.603495659	0.248437377	-0.029402919
C	-2.674865166	-0.491326797	0.010058198
C	-3.947381857	0.13794199	0.105566625
C	-5.127915122	-0.589334428	0.125225186
C	-5.107866846	-1.993139601	0.047868353
C	-3.883361723	-2.640413951	-0.032460053
C	-2.660487003	-1.933272758	-0.044686592
C	-1.425691687	-2.640527392	-0.124822703
N	-0.235308774	-2.066770194	-0.086329151
H	1.146241659	-3.051353634	-1.328788923
H	0.746327047	-3.946609583	0.167391114
H	2.047383836	-2.446668209	1.523965774
H	3.067681975	-2.599157645	0.066990857
H	3.969590285	-0.555050043	0.405333146
H	5.152775348	1.509525017	0.221568059
H	5.223917025	3.986977191	0.046933607
H	3.075967496	5.264947849	-0.124691435
H	0.901327437	4.054260534	-0.134755778
H	-3.954771571	1.226779517	0.164623236
H	-6.082128329	-0.063928502	0.200342953
H	-6.037114891	-2.562863262	0.05306209
H	-3.847702075	-3.7324535	-0.086943302
H	-1.464610299	-3.733976027	-0.218126943

Table S2. Cartesian coordinates (in Angstrom) of each atom of $[Co(salen)\text{-}CO_2]^-$

Atom	*x*	*y*	*z*
C	0.9411330798	-2.9517346327	-0.2688203698
C	2.0888828195	-2.2524822562	0.4372025555
N	1.9301678541	-0.8152571794	0.179892449
C	2.9939556028	-0.05257355	0.2590126993
C	2.9874659368	1.3670994486	0.1296317633
C	4.2117660366	2.0708410945	0.1393192553

C	4.2648874194	3.451153987	0.0471116046
C	3.0574179422	4.1698173638	-0.0468210772
C	1.8389718091	3.5153879714	-0.0497641558
C	1.7484392233	2.0957747852	0.0298268288
O	0.5735984485	1.5411820942	0.0313929027
Co	0.1939763105	-0.3065807567	-0.0989852662
O	-1.6056972659	0.2667742479	0.0127248133
C	-2.6675790859	-0.4785090739	0.0219129785
C	-3.9458491353	0.1456326417	0.1189410423
C	-5.1176410947	-0.5884665771	0.1293859214
C	-5.0922473764	-1.9944136601	0.0485203565
C	-3.8674259416	-2.6337608451	-0.0328195593
C	-2.6490023105	-1.9185810181	-0.0448717175
C	-1.4183558202	-2.6352213842	-0.1076936219
N	-0.229873257	-2.0827592761	-0.1196794864
H	1.166976802	-3.0566487309	-1.3421947422
H	0.7532649675	-3.955606965	0.1472276111
H	2.0237281191	-2.4330010476	1.5240177572
H	3.0687628649	-2.6148620788	0.0877861391
H	3.9623090234	-0.5354464457	0.4493658419
H	5.1370796514	1.4934434425	0.2163029394
H	5.2229997856	3.9706858043	0.0458513626
H	3.0814129944	5.259328252	-0.1222187103
H	0.9004074024	4.0652698492	-0.1271817181
H	-3.9595622311	1.2343537527	0.1756650782
H	-6.0756416882	-0.0686312473	0.1969703535
H	-6.0198144891	-2.5669274475	0.0484148927
H	-3.823747426	-3.7247623385	-0.0939474686
H	-1.4755586495	-3.7317769518	-0.1509495686
C	0.352201113	-0.2662569547	-2.282229994
O	1.4396396231	0.1822767637	-2.5940895869
O	-0.6906900561	-0.7042291641	-2.7315429913

Table S3. Cartesian coordinates (in Angstrom) of each atom of the transition state in the reaction $[Co(salen)]^- + CO_2 \rightarrow [Co(salen)\text{-}CO_2]^-$.

Atom	*x*	*y*	*z*
C	0.9445610376	-2.9509131571	-0.2292212602
C	2.0934908301	-2.258911981	0.4793190238
N	1.9391107662	-0.8113517203	0.2306459531
C	2.9915442863	-0.0639089766	0.2957151334
C	2.9939039234	1.3601991607	0.1707214711
C	4.2122531376	2.0808125095	0.1570190182
C	4.2533019812	3.4459696915	0.0459131065
C	3.0471675917	4.1688306565	-0.0464413587
C	1.8254324061	3.4979064123	-0.0236588131
C	1.7490810435	2.0863944272	0.0759445387
O	0.5778726948	1.5221869348	0.0896632831
Co	0.1979887987	-0.320084755	-0.0060826509

O	-1.5959843689	0.2549202456	0.0820162275
C	-2.6652916823	-0.4846563596	0.0806835614
C	-3.934274588	0.1479143982	0.1596368953
C	-5.1200413683	-0.5809351613	0.1312465361
C	-5.0912809706	-1.9848380741	0.0368942822
C	-3.8764594404	-2.6293249119	-0.019799172
C	-2.6486633145	-1.9246433564	0.0006915705
C	-1.4143056721	-2.638409648	-0.0714539699
N	-0.2329612225	-2.0821678726	-0.0691927982
H	1.1695234508	-3.0390791418	-1.3043023849
H	0.7576978527	-3.9585355398	0.1735475745
H	2.0327723829	-2.44701821	1.5649096748
H	3.0741807541	-2.6152651051	0.1246814298
H	3.9741798091	-0.5493918988	0.460366063
H	5.1439862621	1.5017823033	0.2307252507
H	5.2121175518	3.9794975251	0.024307055
H	3.0594187861	5.2509097732	-0.1411049986
H	0.8859322429	4.0434617274	-0.097117675
H	-3.9457234037	1.2340590799	0.2266175074
H	-6.0710982699	-0.0537389265	0.1736273525
H	-6.0274246	-2.5517268529	0.0036727159
H	-3.8345937863	-3.7226567373	-0.0939070524
H	-1.4715110297	-3.7354043432	-0.1482856893
C	0.3627103682	-0.2376099798	-2.6656073924
O	1.4192784682	0.1671047109	-2.8502970953
O	-0.6871337079	-0.6408449287	-2.9894258032