Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Interactions of Water and Short-Chain Alcohols with $CoFe_2O_4$ (001) Surfaces at Low Coverages

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1. Adsorption on the Fe^{II} active site

Methanol

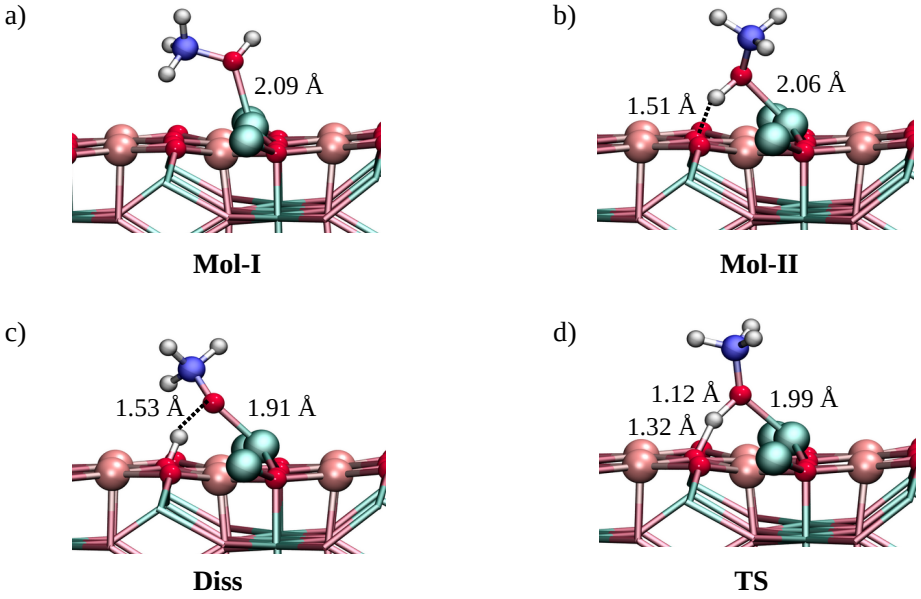

Fig. S1 Optimized geometries for the interactions of methanol on the Fe^{II} active site at the (001)-A CFO surface: (a, b) molecular (Mol-I and Mol-II, depending on the presence of a H-bond with the lattice oxygen), c) dissociated (Diss) adsorption conformations, and d) transition state (TS) for the H-transfer to the surface (i.e., the Mol-II → Diss process).

Ethanol

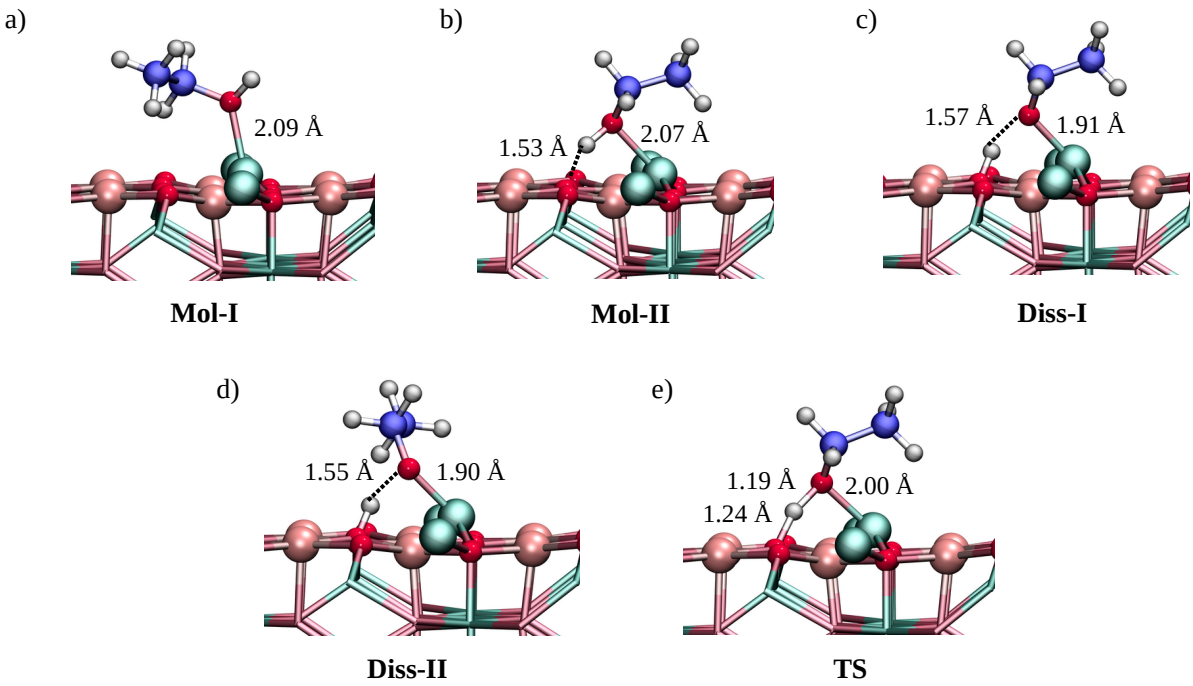

Fig. S2 Optimized geometries for the interactions of ethanol on the Fe^{II} active site at the (001)-A CFO surface: (a, b) molecular (Mol-I and Mol-II, depending on the presence of a H-bond with the lattice oxygen), (c, d) dissociated (Diss-I and Diss-II, according to the orientation of the ethyl group) adsorption conformations, and d) transition state (TS) for the H-transfer to the surface (i.e., the Mol-II → Diss-I process).

Transition states (H-transfer): water and 2-propanol

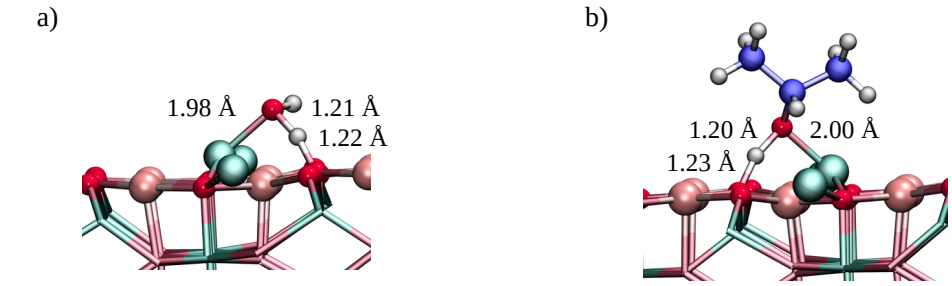

Fig. S3 Transition state structures for the H-abstraction from a) water and b) 2-propanol on the Fe^{II} site to O2 at the (001)-A CFO surface.

2. Adsorption on the 'free' Co^{II} active site

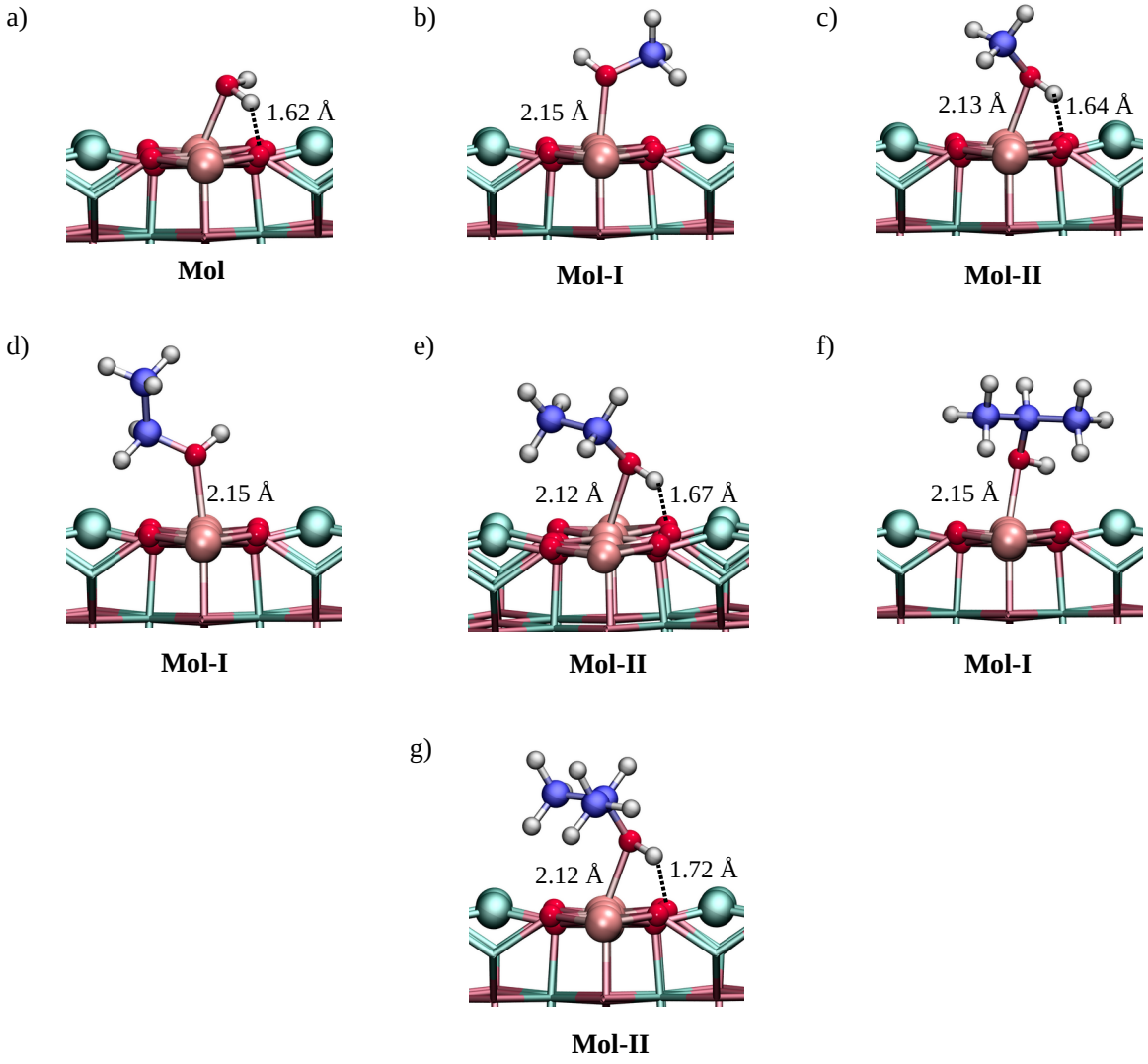

Fig. S4 Optimized geometries for the adsorption of: a) water, (b, c) methanol, (d, e) ethanol, and (f, g) 2-propanol on top of the 'free' Co^{II} active site at the (001)-A CFO surface. Non-H-bonded molecular adsorption conformations are denoted as Mol-I, whereas the H-bonded ones are denotes as Mol-II.

3. Adsorption on the 'hindered' Co^{II} active site

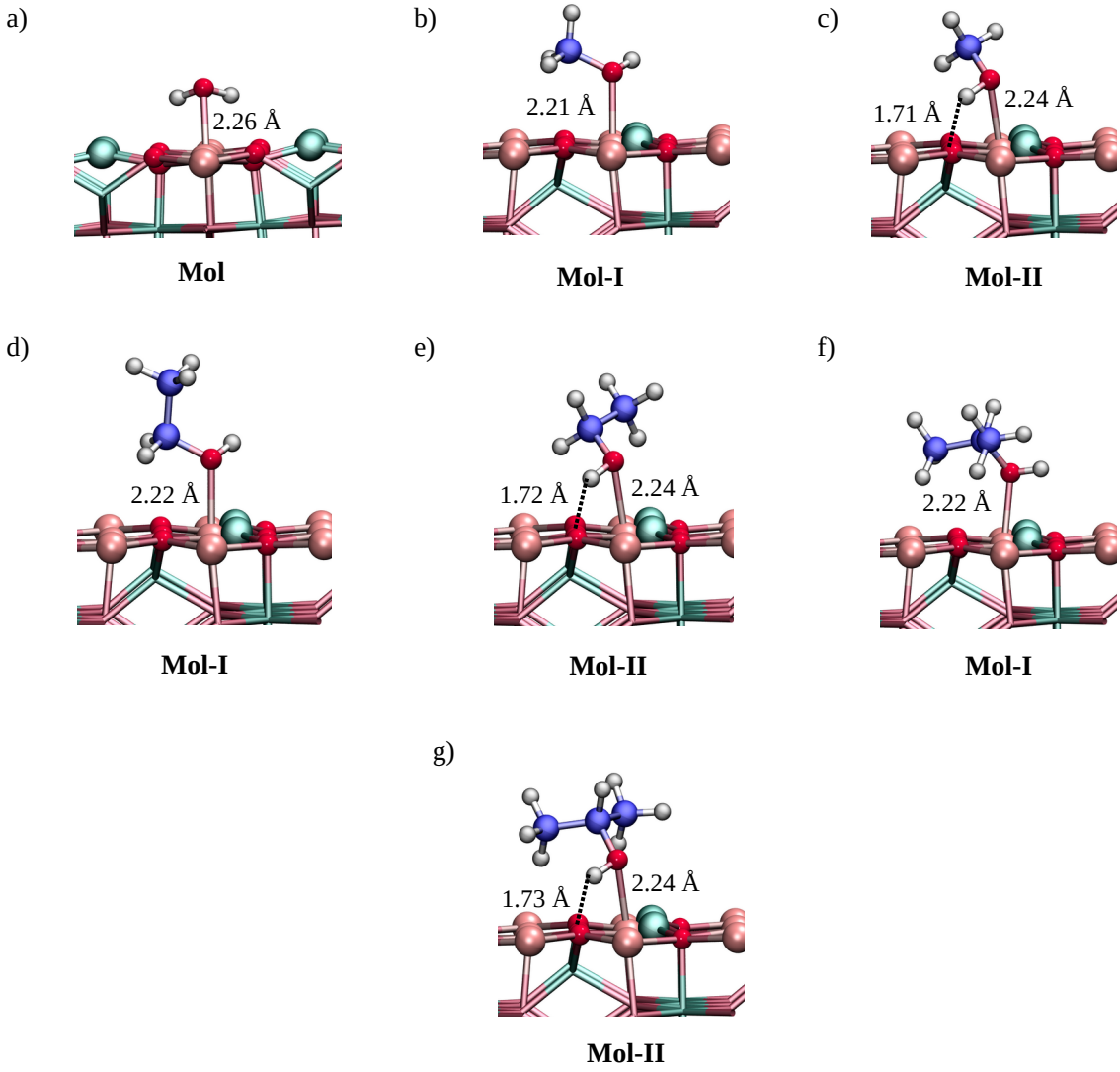

Fig. S5 Optimized geometries for the adsorption of: a) water, (b, c) methanol, (d, e) ethanol, and (f, g) 2-propanol on top of the 'hindered' Co^{II} active site at the (001)-A CFO surface. Non-H-bonded molecular adsorption conformations are denoted as Mol-I, whereas the H-bonded ones are denotes as Mol-II.

4. Adsorption on the Co^{III} active site

Water

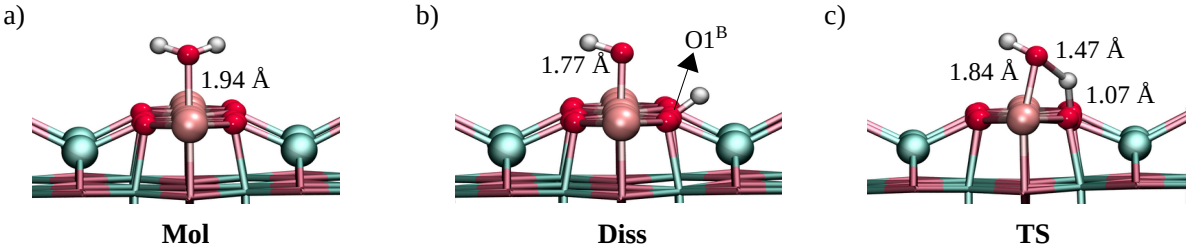

Fig. S6 a) Molecular (Mol) and b) dissociative (Diss) adsorption geometries of water on the Co^{III} site at the (001)-B CFO surface. c) Transition state structure for the Mol → Diss process.

Methanol

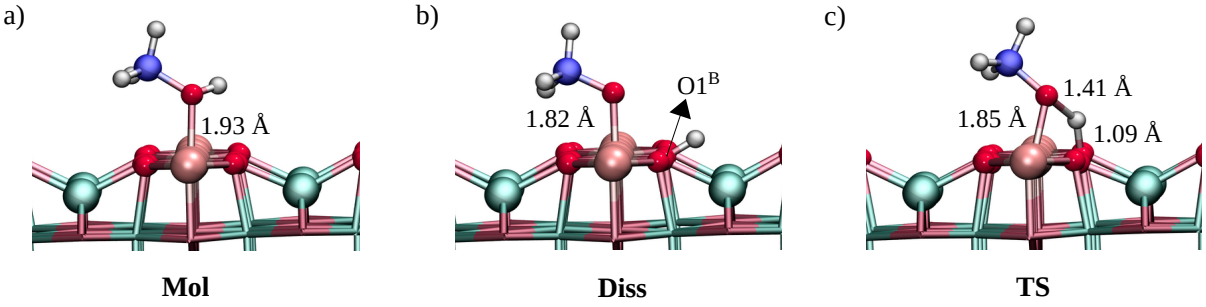

Fig. S7 a) Molecular (Mol) and b) dissociative (Diss) adsorption geometries of methanol on the Co^{III} site at the (001)-B CFO surface. c) Transition state structure for the Mol → Diss process.

Ethanol

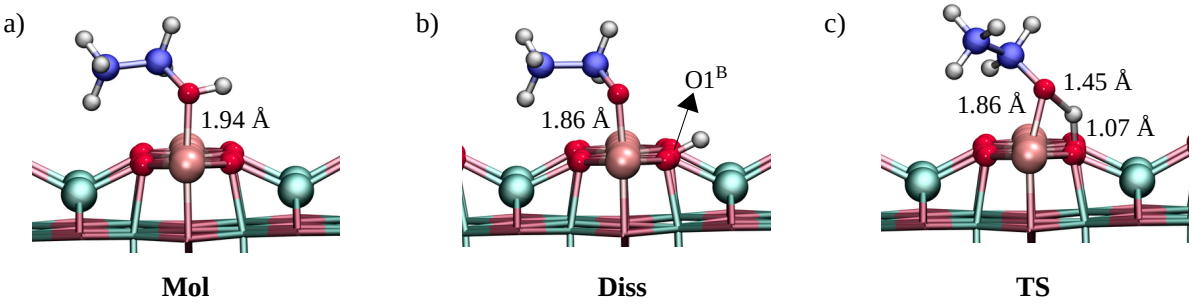

Fig. S8 a) Molecular (Mol) and b) dissociative (Diss) adsorption geometries of ethanol on the Co^{III} site at the (001)-B CFO surface. c) Transition state structure for the Mol → Diss process.

2-propanol

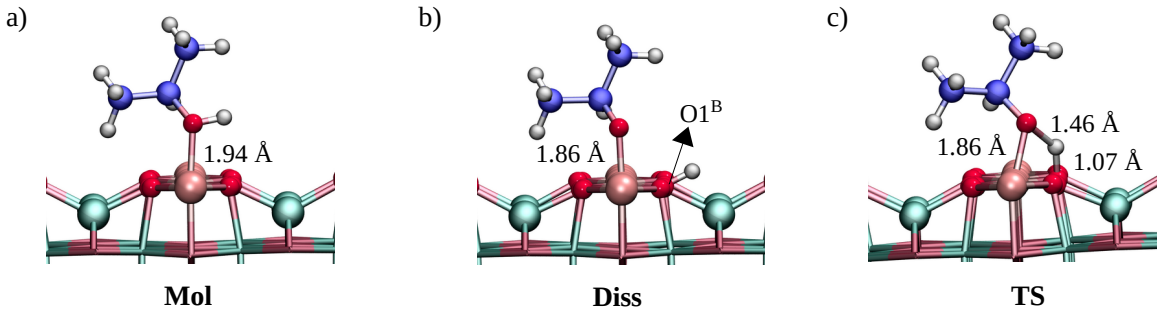

Fig. S9 a) Molecular (Mol) and b) dissociative (Diss) adsorption geometries of 2-propanol on the Co^{III} site at the (001)-B CFO surface. c) Transition state structure for the Mol → Diss process.

Structures with perpendicular orientation of the C─O bond

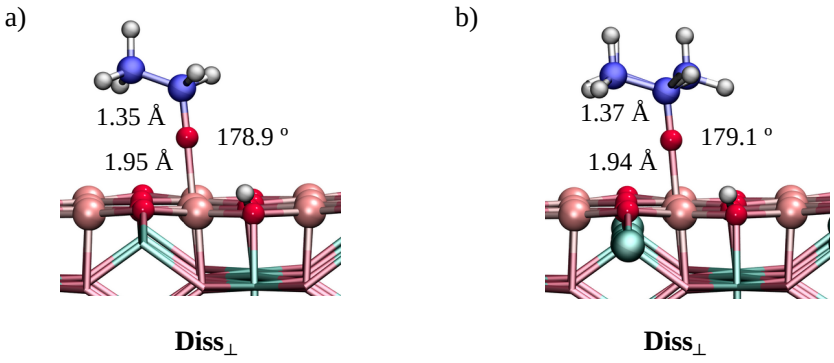

Fig. S10 Optimized geometries for the Diss state of: a) ethanol and b) 2-propanol on the Co^{III} site at the B-termination, with the C─O bond oriented perpendicular to the surface.

Spin density

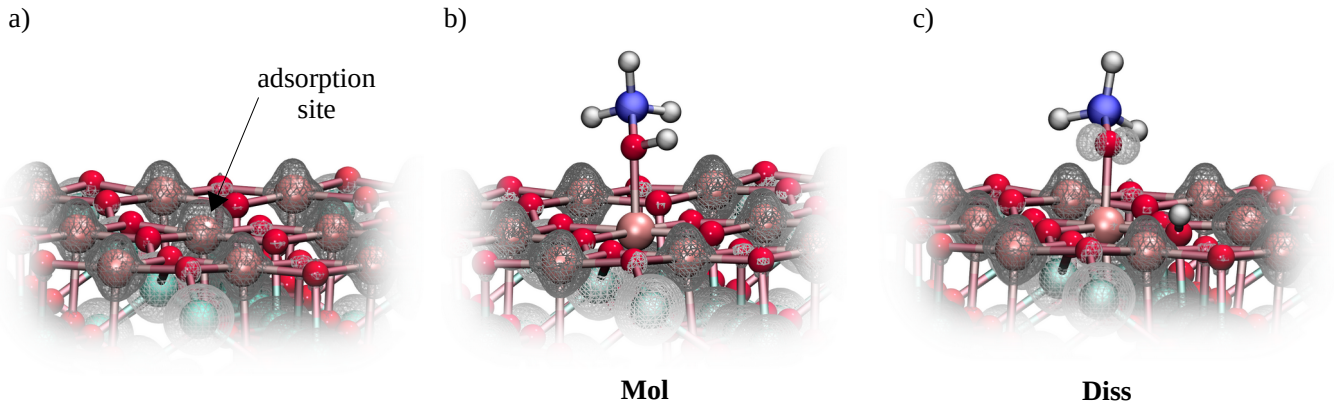

Fig. S11 Spin density analysis for the $Co_{22}Fe_{33}O_{80}$ quantum cluster: a) without adsorbate, b) with methanol adsorbed in a molecular fashion, and c) with methanol adsorbed in a dissociative fashion on top of the Co^{III} site at the B-layer indicates that upon adsorption Co adopts low-spin state with all electrons paired.

5. Adsorption at the $O1^B$ vacancy

Water

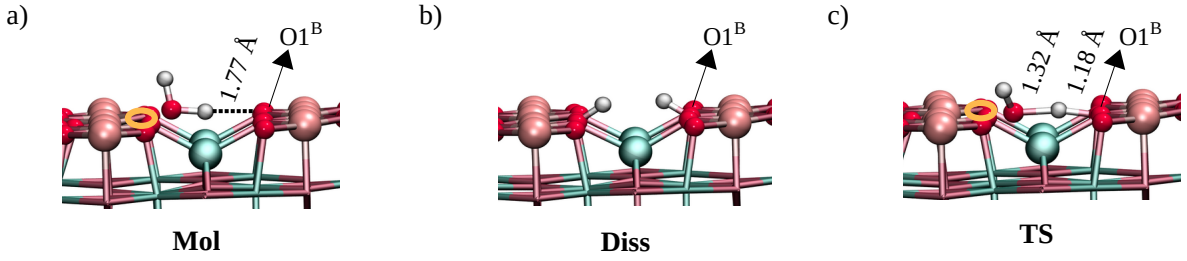

Fig. S12 a) Molecular (Mol) and b) dissociative (Diss) adsorption geometries of water at the $O1^B$ vacancy. c) Transition state structure for the Mol → Diss process.

Methanol

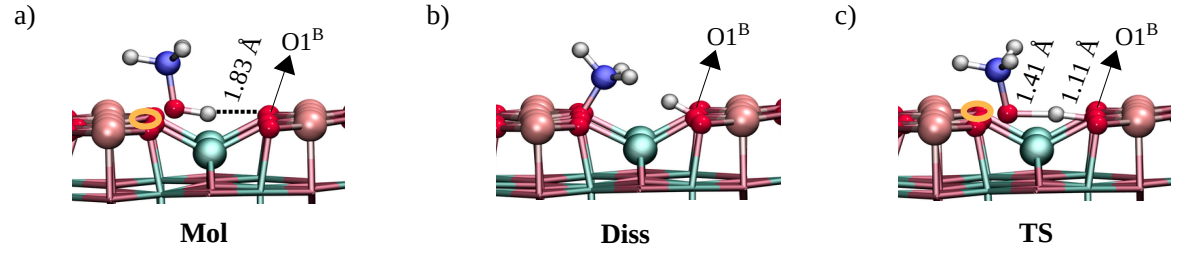

Fig. S13 a) Molecular (Mol) and b) dissociative (Diss) adsorption geometries of methanol at the $O1^B$ vacancy. c) Transition state structure for the Mol → Diss process.

Ethanol

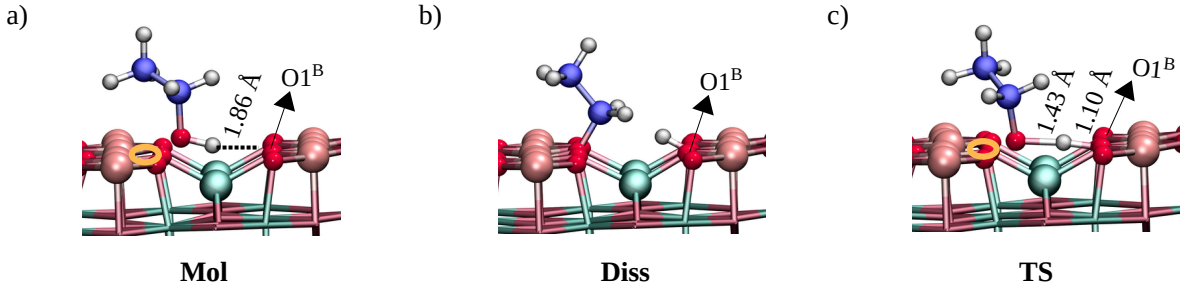

Fig. S14 a) Molecular (Mol) and b) dissociative (Diss) adsorption geometries of ethanol at the $O1^B$ vacancy. c) Transition state structure for the Mol → Diss process.

6. Infrared (IR) spectroscopy

Scaling Factors

The harmonic frequencies for isolated methanol, ethanol, and 2-propanol in the gas phase, computed at the DFT(PBE0)/def2-SVP level of theory, and their comparison with available experimental data from the literature are presented in Table S1, Table S2, and Table S3, respectively.

The individual scaling factors based on the kind of mode, have been determined as follows.

For stretching vibrations involving CH, we averaged all asymmetric and symmetric modes over all three alcohols and obtained a value of 0.956 . In a similar manner, the average correction factor for the OH stretching modes is 0.943.

A factor of 0.976 is obtained for stretching vibrations involving the CC bond, by averaging the corresponding modes in ethanol and 2-propanol. We note, however, that in some cases these modes are coupled with other vibrations, especially in 2-propanol; the strongly coupled vibrations have been considered alongside the deformations involving C, H, and O atoms to calculate a single average scaling factor of 0.984.

To determine a correction factor for the CO stretching, we considered the analogous modes in methanol and ethanol only, where the vibrations associated with CO are almost completely decoupled from other motions. As a result, we obtained a value of 0.920.

The computed scaling factors are summarized in Table S4.

Table S2 A comparison of the experimentally observed and calculated frequencies [cm^{-1}] for gas phase methanol

Mode	Exp.[a]	Theory	Scaling factor
υ(OH)	3681	3897	0.945
$\upsilon_{as}(CH_3)$	3000	3143	0.955
	2960	3054	0.969
$\upsilon_{s}(CH_3)$	2844	2992	0.950
$\delta_{as}(CH_3)$	1477	1496	0.987
	1430[b]	1470	0.973
$\delta_{s}(CH_3)$	1455	1475	0.986
δ_{bend}(OH)	1345	1368	0.983
$\tau(CH_2)$	1165	1177	0.989
$\omega(CH_2)$	1060	1076	0.985
ν(CO)	1033	1146	0.902

[a] from: T. Shimanouchi, *Tables of Molecular Vibrational Frequencies Part 1.*, National Bureau of Standards, Washington, DC, 1967.

[b] from: H. D. Noether, *J. Chem. Phys.*, 1942, **10**, 693–699.

Table S2 A comparison of the experimentally observed and calculated frequencies [cm^{-1}] for gas phase ethanol

Mode	Exp.[a]	Theory	Scaling factor
υ(OH)	3676	3899	0.943
$\upsilon_{as}(CH_3)$	2992	3166	0.945
	2987	3163	0.944
$\upsilon_{as}(CH_2)$	2901	3019	0.961
$\upsilon_{s}(CH_3)$	2943	3063	0.961
$\upsilon_{s}(CH_2)$	2888	2983	0.968
$\delta_{as}(CH_2)$	1500	1514	0.991
$\delta_{as}(CH_3)$	1480	1478	1.001
	1455	1451	1.002
$\delta_{s}(CH_3)$	1367	1379	0.991
δ_{bend}(OH)	1241	1272	0.976
υ_{as}(CCO)	1090	1161	0.939
υ(CC)	1027	1054	0.974
υ_{s}(CCO)	885[b]	926	0.955
$\rho(CH_2)$ and $\rho(CH_3)$	801	819	0.979
δ_{bend}(CCO)	418	421	0.994

[a] from: Durig J. R., Deeb H., Darkhalil I. D., Klaassen J. J., Gounev T. K., Ganguly A., *J. Mol. Struc*, 2011, **985**, 202-210.

[b] from: Barnes A. J., Hallam H. E., *Transactions of the Faraday Society*, 1970, **66**, 1932-1940.

Table S3 A comparison of the experimentally observed and calculated frequencies [cm^{-1}] for gas phase 2-propanol

Mode	Exp.[a]	Theory	Scaling factor
υ(OH)	3653	3886	0.940
$\upsilon_{as}(CH_3)$	2979	3162	0.942
	2971	3138	0.947
$\upsilon_{s}(CH_3)$	2930	3047	0.962
υ(CH)	2884	2978	0.968
$\delta_{as}(CH_3)$	1472	1475	0.998
	1461	1460	1.001
$\delta_{s}(CH_3)$	1391	1399	0.994
		1381	1.000
ω(CH)	1340	1361	0.985
δ(OH), δ(CH)	1251	1280	0.977
υ(CO), $\rho(CH_3)$, υ(CC)	1153	1206	0.956
	1130	1173	0.963
δ(OH), $\rho(CH_3)$, υ(CC)	1074	1104	0.973
υ(CC)	830[b]	849	0.978

[a] from: T. Fuente S. A., Ferretti C. A., Domancich N. F., Díez V. K., Apesteguía C. R., Di Cosimo J. I., Ferullo, R. M., Castellani N. J., *Appl. Surf. Sci*., 2015, **327**, 268-276.

[b] from: Green, J. H. S., *Transactions of the Faraday Society*, 1963, **59**, 1559-1563.

Table S4 Average scaling factors determined for specific type of vibrational modes

Mode	Average scaling factor
υ(OH)	0.943
υ(CH)	0.956
υ(CC)	0.976
υ(CO)	0.920
δ(C,O,H) + strongly coupled vibrations	0.984

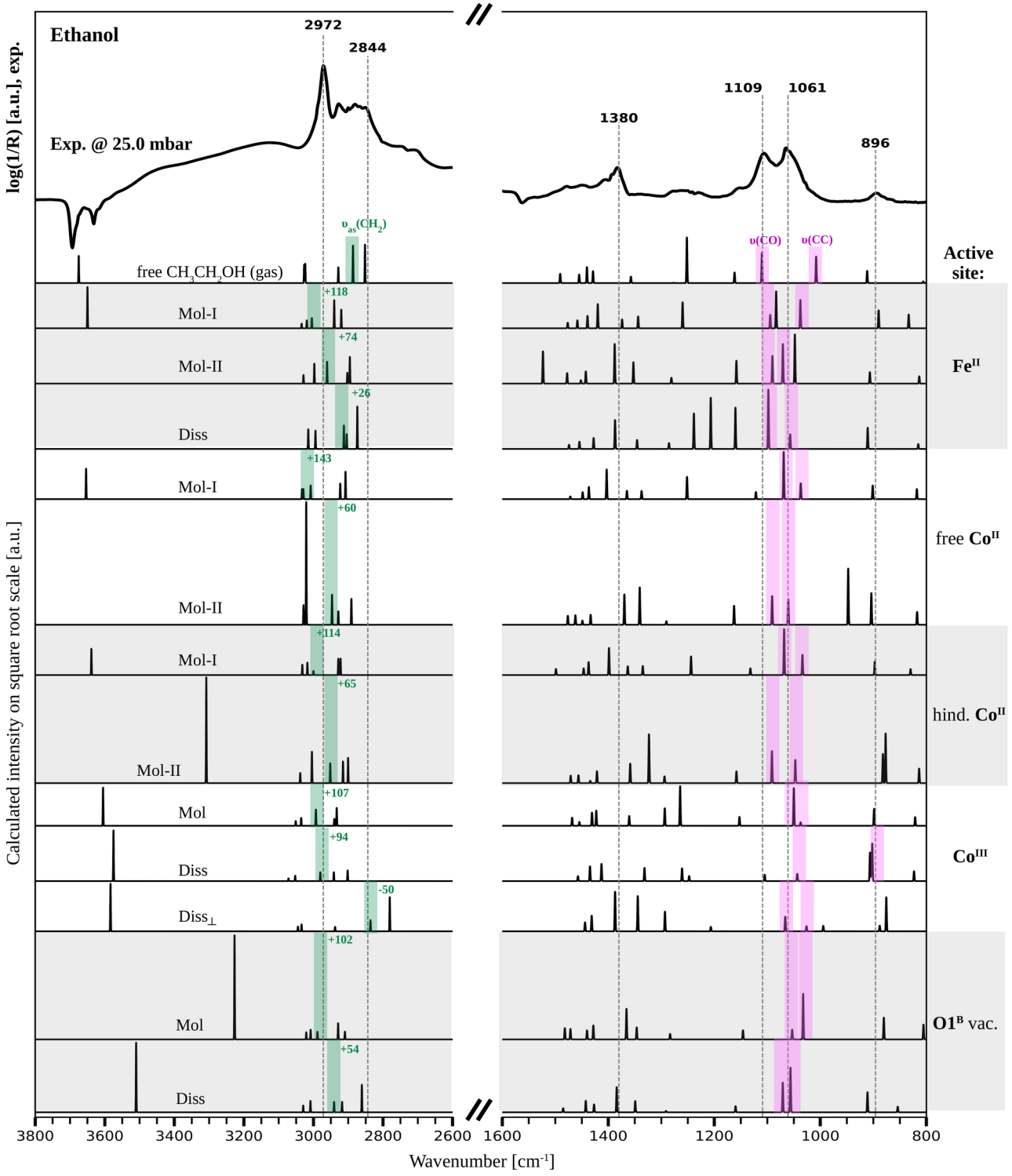

Fig. S15 A comparison of the experimental DRIFT spectrum at 25.0 mbar with simulated IR spectra for the molecular and dissociative adsorptions of ethanol on the different active sites at the CFO (001) surfaces.

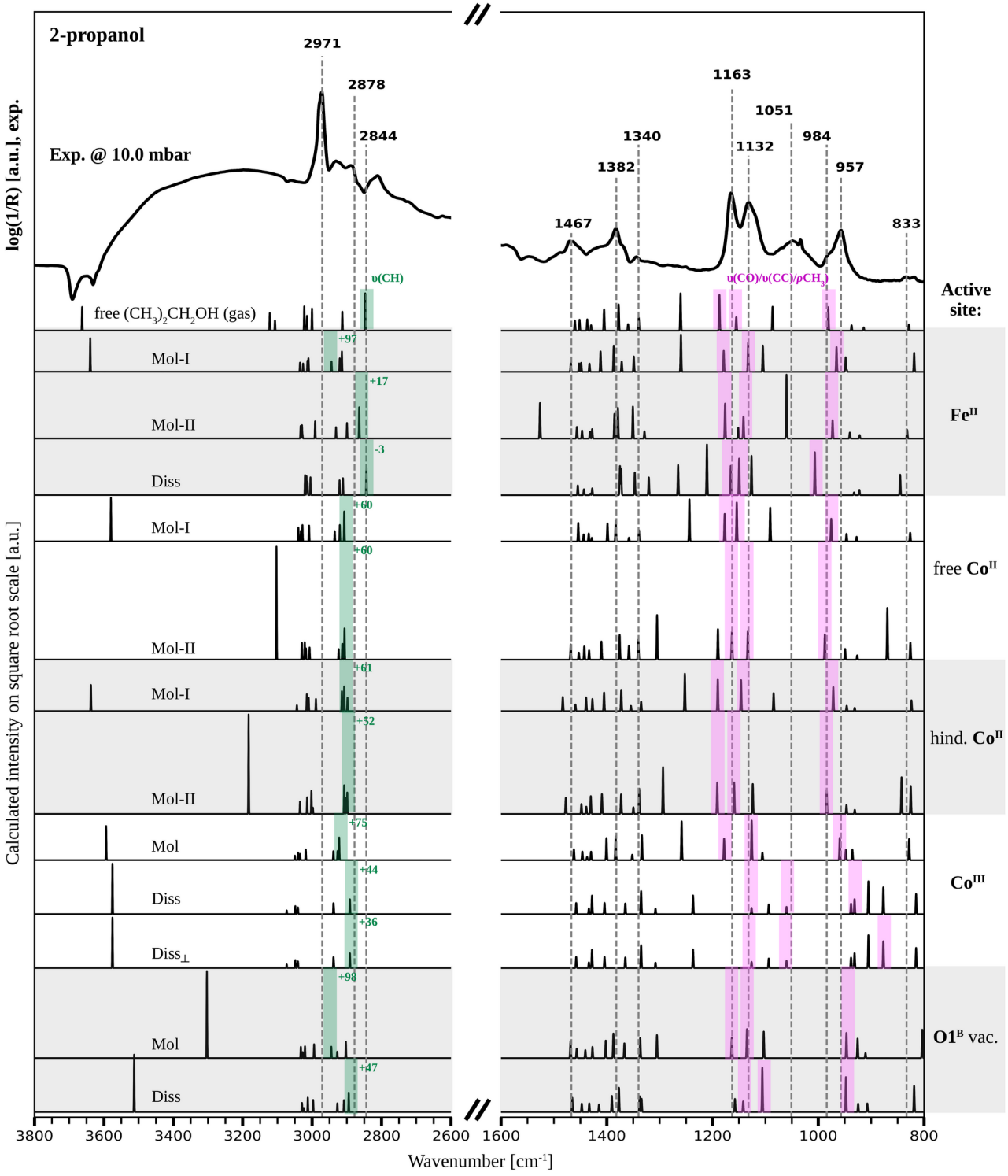

Fig. S16 A comparison of the experimental DRIFT spectrum at 10.0 mbar with simulated IR spectra for the molecular and dissociative adsorptions of 2-propanol on the different active sites at the CFO (001) surfaces.

7. Cluster Coordinates

In the following, we present optimized Cartesian coordinates for the quantum mechanically treated clusters. The letter **f** marks the atoms which are kept fixed during the optimization.

$Co_{10}Fe_{23}O_{42}$

Fe	-0.5699367	0.5700174	20.4591326	f
Fe	3.7224463	4.7549768	20.3069690	
Fe	-0.5699367	9.0474006	20.4591326	f
Fe	7.9074465	0.5700174	20.4591326	f
Fe	7.9074465	9.0474006	20.4591326	f
Fe	-2.2184335	2.2185483	19.2029602	f
Fe	-1.0741790	7.3963361	18.0058464	f
Fe	2.0202520	-2.0201605	19.2029462	f
Fe	7.4032042	-1.0810470	18.0058464	f
Fe	-0.0026180	4.2412724	16.8964711	f
Fe	4.2360690	0.0025826	16.8964424	f
Fe	6.2524722	2.2249544	19.1595282	
Fe	2.0188386	6.4585928	19.1831278	
Fe	1.0810278	1.0741710	18.0057995	f
Fe	7.4032042	7.3963361	18.0058464	f
Fe	3.1733797	3.1540661	17.9332453	
Fe	5.3233106	5.3040162	17.9332581	
Fe	4.2360690	8.4799658	16.8964424	f
Fe	6.2589497	10.6959314	19.2029602	f
Fe	1.0810278	9.5515542	18.0057995	f
Fe	8.4747652	4.2412724	16.8964711	f
Fe	10.4976351	6.4572227	19.2029462	f
Fe	9.5584109	1.0741710	18.0057995	f
Co	-1.0670241	5.2211937	20.1575401	
Co	5.2765398	-1.0858192	20.0590934	
Co	3.1754447	5.3019187	15.9264365	f
Co	5.2929743	3.1843989	15.8889117	f
Co	5.2436769	7.4560769	19.9474807	
Co	7.5386082	5.1959418	20.0377825	
Co	3.2814905	0.9388284	20.0377701	
Co	1.0213842	3.2337584	19.9474848	
Co	3.2562666	9.5444678	20.1575232	
Co	9.5632732	3.2009184	20.0591209	
O	-0.9980033	0.9980221	18.1551197	f
O	-1.1098114	5.3485199	18.0023122	f
O	-3.0555955	5.4153648	20.0824946	f
O	-1.1765765	7.2943693	20.0824715	f
O	-0.9611219	3.0657329	20.1995430	
O	0.9613802	-0.9613703	18.0076104	f
O	5.3605158	-1.1218171	17.9528168	f
O	5.4217877	-3.0620184	20.0824946	f
O	7.3008066	-1.1830138	20.0824715	f
O	3.2712805	-1.2009420	20.1889027	
O	7.3753184	3.1348160	15.8104581	f
O	3.1366160	7.3734952	15.8104591	f
O	1.1038332	5.3407090	15.8104474	f
O	5.3425324	1.1020415	15.8104513	f
O	5.2550615	5.2680265	15.9716443	f

O	3.2093352	3.2223125	15.9716273	f
O	3.2568340	5.2205576	18.1425765	
O	5.1901496	3.2872412	17.9869322	
O	7.4793798	0.9980221	18.1551197	f
O	0.9613802	7.5160129	18.0076104	f
O	1.1270889	3.0889323	17.8626037	
O	3.1178289	1.1029674	17.9338600	
O	5.3884519	7.3503014	17.8625965	
O	7.3744117	5.3595569	17.9338781	
O	5.4556603	5.4075124	19.9506115	
O	3.0699267	3.0217558	19.9506053	
O	7.3264573	7.2794719	19.9719249	
O	1.1979671	1.1509739	19.9718962	
O	3.2777058	7.4113737	20.1560772	
O	5.3184377	0.9586634	20.1586796	
O	1.0660775	5.1997309	20.1561039	
O	7.5187676	3.1589995	20.1586716	
O	7.4793798	9.4754052	18.1551197	f
O	3.1288726	9.5872040	18.0022945	f
O	3.0621269	11.5330613	20.0824610	f
O	1.1830983	9.6540560	20.0825085	f
O	5.4117532	9.4385919	20.1995294	
O	9.4387634	7.5160129	18.0076104	f
O	9.5992108	3.1168782	17.9528470	f
O	11.5395101	3.0556781	20.0824610	f
O	9.6604814	1.1766729	20.0825085	f
O	9.6784025	5.2061837	20.1889014	

$Co_{18}Fe_{23}O_{52}$

Fe	3.6420530	-3.6502481	20.3739565	
Fe	-0.6021112	0.5887422	20.3867742	
Fe	3.6480254	4.8422708	20.3827765	
Fe	7.8911008	0.5935837	20.3697998	
Fe	-1.0741790	-1.0810470	18.0058464	f
Fe	-2.2184335	2.2185483	19.2029602	f
Fe	6.3547261	-2.1160464	14.8667921	f
Fe	-0.0026180	-4.2361107	16.8964711	f
Fe	6.2589497	-6.2588348	19.2029602	f
Fe	1.9691637	-2.0356953	19.1766846	
Fe	7.4032042	-1.0810470	18.0058464	f
Fe	3.1645136	-5.3197379	18.0058424	f
Fe	5.3197223	-3.1645289	18.0058077	f
Fe	2.1160036	2.1226572	14.8667788	f
Fe	4.2374701	0.0022275	16.8734190	
Fe	6.2733058	2.2705962	19.1740435	
Fe	2.0202520	6.4572227	19.2029462	f
Fe	1.0810278	1.0741710	18.0057995	f
Fe	3.1645136	3.1576452	18.0058424	f
Fe	5.3197223	5.3128542	18.0058077	f
Fe	10.4976351	-2.0201605	19.2029462	f
Fe	8.4747652	4.2412724	16.8964711	f
Fe	9.5584109	1.0741710	18.0057995	f
Co	-3.2268927	-1.0116793	20.0511016	f
Co	-0.9829023	-3.2556560	20.1414084	f
Co	-0.9829023	5.2217271	20.1414084	f
Co	3.1754447	-3.1754644	15.9264365	f
Co	1.0542874	-1.0543109	15.8888993	f

Co	5.2411279	-1.0041948	19.9596333	
Co	7.4944808	-3.2556560	20.1414084	f
Co	3.2557849	-7.4943571	20.1413798	f
Co	1.0117978	-5.2503895	20.0511531	f
Co	5.2929743	3.1843989	15.8889117	f
Co	7.4141295	1.0632300	15.9264443	f
Co	5.2504904	7.4657038	20.0511016	f
Co	7.4944808	5.2217271	20.1414084	f
Co	3.2593903	0.9729374	20.0621431	
Co	1.0117978	3.2269936	20.0511531	f
Co	9.4891809	-5.2503895	20.0511531	f
Co	11.7331680	0.9830260	20.1413798	f
Co	9.4891809	3.2269936	20.0511531	f
O	-1.0293355	-1.0163765	15.9716343	f
O	-3.1168673	-1.1218171	17.9528168	f
O	-1.1098114	-3.1288632	18.0023122	f
O	-1.1765765	-1.1830138	20.0824715	f
O	-0.9980033	0.9980221	18.1551197	f
O	-3.1792345	0.9811002	20.2552619	f
O	-0.9810067	3.1793394	20.2552799	f
O	3.1366160	-1.1038879	15.8104591	f
O	1.1038332	-3.1366741	15.8104474	f
O	7.4480476	-1.0163765	15.9716343	f
O	5.2550615	-3.2093566	15.9716443	f
O	3.2093352	-5.2550706	15.9716273	f
O	3.2386224	-3.2722699	18.1466828	
O	5.2000741	-5.2000654	18.0076077	f
O	0.9289920	-0.9467111	17.9891594	
O	1.1218276	-5.3605049	17.9528470	f
O	3.1288726	-7.3675622	18.0022945	f
O	5.3768293	-1.1356903	17.8898629	
O	7.3675717	-3.1288632	18.0023122	f
O	5.4113313	-3.0593966	20.0024577	
O	3.0621269	-5.4217050	20.0824610	f
O	7.3043885	-1.1746071	19.9970263	
O	3.2507629	-1.1159198	20.1596652	
O	5.2981487	-7.4962829	20.2552619	f
O	1.0594679	-3.2576016	20.2552815	f
O	7.4963764	-5.2980437	20.2552799	f
O	7.3753184	3.1348160	15.8104581	f
O	5.3425324	1.1020415	15.8104513	f
O	1.0163556	1.0293354	15.9716438	f
O	5.2550615	5.2680265	15.9716443	f
O	3.2093352	3.2223125	15.9716273	f
O	3.2406886	5.2367111	18.1551042	f
O	5.1881872	3.3110584	17.9871239	
O	7.5112435	1.0020809	18.1463421	
O	1.1218276	3.1168782	17.9528470	f
O	3.1277008	1.1156897	17.9621630	
O	5.3605158	7.3555661	17.9528168	f
O	7.3675717	5.3485199	18.0023122	f
O	5.4217877	5.4153648	20.0824946	f
O	3.0812277	3.0598629	19.9948358	
O	1.1846241	1.1554238	20.0060401	
O	3.2576859	7.4180146	20.2552607	f
O	5.3445354	0.9837041	20.1471383	
O	1.0594679	5.2197816	20.2552815	f
O	7.4963764	3.1793394	20.2552799	f

O	9.4387634	-0.9613703	18.0076104	f
O	11.7350691	-1.0593685	20.2552607	f
O	9.5368510	-3.2576016	20.2552815	f
O	9.4937387	1.0293354	15.9716438	f
O	9.5992108	3.1168782	17.9528470	f
O	11.6062557	1.1098209	18.0022945	f
O	9.6604814	1.1766729	20.0825085	f

$Co_{22}Fe_{33}O_{80}$

Co	6.2901155	-0.0328481	18.9123157	
Co	2.1112770	4.1720010	18.9200480	f
Co	4.1556407	2.1018650	18.9123360	
Co	6.3136327	8.3504321	18.8988198	
Co	4.1720010	10.4889820	18.9200480	f
Co	8.3608540	-2.0775750	18.9200480	f
Co	14.6778340	-0.0168510	18.9200480	f
Co	10.4996146	4.1626460	18.8343703	
Co	8.3639856	6.2982588	18.8393260	
Co	12.5408365	2.1231970	18.9035378	
Co	14.6939125	8.3710176	18.9123570	
Co	10.4889820	12.5497060	18.9200480	f
Co	12.5592634	10.5054230	18.9123753	
Co	16.7385580	6.3001290	18.9200480	f
Fe	5.2360650	-3.1416390	18.1352390	f
Fe	7.3304920	-1.0472130	15.7671390	f
Fe	3.1416390	3.1416390	15.7671390	f
Fe	1.0472130	1.0472130	18.1352390	f
Fe	5.2208545	5.2448810	18.0581073	
Fe	7.3169316	7.3446040	15.7252706	
Fe	4.1722970	-0.0165550	16.9236580	f
Fe	2.1109810	6.2998330	16.9236580	f
Fe	6.2897927	2.1018906	16.8571577	
Fe	6.2811880	6.2811880	12.6403750	f
Fe	4.1722970	8.3611500	16.9236580	f
Fe	6.2998330	10.4886860	16.9236580	f
Fe	10.4886860	-2.0778710	16.9236580	f
Fe	9.4247161	5.2362547	13.7516389	
Fe	11.5342342	3.1272941	15.7221545	
Fe	9.4325833	1.0294346	18.0582314	
Fe	13.6333516	5.2291681	18.0562973	
Fe	15.7081960	7.3304920	15.7671390	f
Fe	12.5500020	-0.0165550	16.9236580	f
Fe	12.5686480	4.1909430	12.6403750	f
Fe	10.4700400	2.0923350	12.6403750	f
Fe	10.4902291	6.2960350	16.8439912	
Fe	8.3657356	4.1715387	16.8445891	
Fe	14.6775380	2.1109810	16.9236580	f
Fe	11.5193440	11.5193440	15.7671390	f
Fe	9.4168291	9.4419047	18.0562392	
Fe	13.6137700	13.6137700	18.1352390	f
Fe	8.3797950	8.3797950	12.6403750	f
Fe	12.5594722	8.3715813	16.8571382	
Fe	8.3611500	12.5500020	16.9236580	f
Fe	14.6775380	10.4886860	16.9236580	f
Fe	16.7388540	4.1722970	16.9236580	f
Fe	17.8026220	9.4249180	18.1352390	f

Co	6.2877923	4.1949627	14.7803576	
Co	4.1897240	6.2824070	14.7977260	f
Co	8.3831315	2.0990764	14.7797551	
Co	10.4712590	0.0008710	14.7977260	f
Co	14.6601120	4.1897240	14.7977260	f
Co	12.5620879	6.2780818	14.7794756	
Co	8.3785760	10.4712590	14.7977260	f
Co	10.4662488	8.3733780	14.7800816	
O	6.4345140	-1.9431900	19.0486120	f
O	2.1430080	-0.0485820	16.9784680	f
O	8.2355610	-0.1813363	18.9473685	
O	4.1402700	-2.0458440	16.9784680	f
O	6.2456289	6.2713961	14.6049173	
O	6.3398184	4.1322284	16.9337243	
O	6.2079412	0.0471899	16.8158611	
O	8.3226632	2.1476465	16.9338406	
O	6.4330084	6.4367380	18.9270716	
O	6.0418893	1.8530942	18.8291018	
O	4.0077270	4.0462823	18.9469440	
O	4.3921200	0.2032680	18.8983060	f
O	2.1430080	8.3291230	16.9784680	f
O	2.2456620	2.2456620	19.0486120	f
O	6.2282340	4.2438970	12.6501320	f
O	1.8911580	6.0800110	18.8983060	f
O	2.0453810	4.2378970	16.8497680	f
O	8.2263286	8.2287266	18.9245519	
O	4.2361854	2.0188603	16.8156879	
O	4.2323050	4.2323050	14.6732600	f
O	4.1029511	6.3332777	16.9310768	
O	6.3381220	8.3228610	12.6499500	f
O	8.3515420	4.1631065	14.8481450	
O	4.1510300	8.3398820	14.8846740	f
O	6.3211010	2.1322490	14.8846740	f
O	8.3228610	6.3381220	12.6499500	f
O	6.3318600	12.5179750	16.9784680	f
O	6.2309375	8.4306612	16.8408102	
O	8.3285905	10.5582451	16.9288410	
O	6.0800110	10.2688630	18.8983060	f
O	4.3921200	8.5809730	18.8983060	f
O	4.2378970	10.4230860	16.8497680	f
O	6.3211010	10.5099530	14.8846740	f
O	8.4267490	-2.1434710	16.8497680	f
O	10.5220766	-0.0859098	16.9313169	
O	10.2688630	-2.2976940	18.8983060	f
O	12.5179750	-2.0458440	16.9784680	f
O	12.5287350	-0.0378220	14.8846740	f
O	8.6049179	4.4096410	18.8109389	
O	8.4211570	0.0434530	14.6732600	f
O	12.5117130	2.1492700	12.6499500	f
O	10.5269750	4.1340090	12.6499500	f
O	8.4327490	2.0393820	12.6501320	f
O	10.4977904	6.3093659	14.8477350	
O	14.6175300	6.2398260	14.6732600	f
O	8.4320589	6.2289491	16.7767124	
O	14.7471096	4.1397681	16.9290610	
O	10.4595891	2.0559318	14.6041638	
O	14.6119380	0.0490450	16.8497680	f

O	16.7068270	2.1430080	16.9784680	f
O	14.8425038	6.4258551	18.9471630	
O	12.6216010	6.2282340	12.6501320	f
O	14.4577150	1.8911580	18.8983060	f
O	12.4203289	4.0345757	18.9276372	
O	12.7698250	0.2032680	18.8983060	f
O	10.5292006	8.3214242	16.9327628	
O	10.6284629	2.2413766	18.9305465	
O	10.2524357	6.0571863	18.8101645	
O	10.4192989	4.2417712	16.7711814	
O	16.6041730	8.2264690	19.0486120	f
O	12.6186282	2.0428405	16.8416176	
O	12.6045415	4.2016550	14.6038133	
O	12.5136113	6.3388013	16.9328564	
O	12.5287350	8.3398820	14.8846740	f
O	14.6988050	2.1322490	14.8846740	f
O	8.5809730	12.7698250	18.8983060	f
O	8.3898524	8.4148383	14.6045611	
O	14.7095650	12.5179750	16.9784680	f
O	10.4286780	10.4286780	14.6732600	f
O	14.6138937	8.4531467	16.8158250	
O	16.7068270	10.5207130	16.9784680	f
O	10.4170860	8.4327490	12.6501320	f
O	14.4577150	10.2688630	18.8983060	f
O	12.4153210	12.4153210	19.0486120	f
O	12.8079151	8.6191179	18.8290406	
O	10.6151306	10.6534318	18.9467318	
O	10.4230860	12.6156020	16.8497680	f
O	12.6422292	10.4248966	16.8156511	
O	16.9586770	4.3921200	18.8983060	f
O	16.8044540	6.2342340	16.8497680	f