SUPPORTING INFORMATION

Vibrational Solvatochromism in Vaska's Complex Adducts

Christopher J. Huber, Timothy C. Anglin, Brynna H. Jones, Nagilthes Muthu, and Aaron M. Massari

Department of Chemistry, University of Minnesota – Twin Cities

207 Pleasant St SE, Minneapolis, MN 55455

*Corresponding Author. Email: massari@umn.edu

Table S1. Compilation of AN, and measured ν_{CO}, ν_{OO}, $\nu_{Ir\text{-}H}$ values for all 16 solvents.

solvent	acceptor number, AN [a]	ν_{CO} (cm^{-1})						ν_{OO} (cm^{-1})	$\nu_{Ir\text{-}H}$ (cm^{-1})
		VC	VC-H_2	VC-O_2	VC-S_X	VC-I_2	VC-Br_2	VC-O_2	VC-H_2
THF	8	1966.8	1991.4	2006.1	2049.5	2069.2	2075.5	--[c]	2094.9
benzene	8.2	1967.1	1991.8	2003.7	2053.4	2068.8	2075.9	862.5	2091.5
chlorobenzene	9 [b]	1965.1	1990.1	2006.6	2051.4	2068.7	2075.9	861.6	2095.8
toluene	10 [b]	1965.8	1990.4	2004.6	2054.1	2069.1	2075.4	862.6	2092
acetone	12.5	1965.4	1991.9	2004.1	2048.6	2070.5	2074.2	--[c]	2095.7
o-dichlorobenzene	14.1 [b]	1961.1	1991.7	2008.9	2046.2	2068.8	2075.7	861.0	2089.8
pyridine	14.2	1963.1	1989.6	2007.3	2058.1	2067.9	2076.6	--[c]	2090.5
benzonitrile	15.5	1964.6	1990.3	2008.9	2053.8	2068.3	2074.1	--[c]	2095.7
DMF	16	1963.6	1989.9	2006.6	2047.7	2069.4	2076.5	--[c]	2093.8
acetonitrile	18.9	1966.6	1991.6	2009.5	2046.7	2068.6	2075.9	859.2	--[c]
DMSO	19.3	1962.1	1989.6	2007.2	2049.9	2068.2	2067.7	--[c]	2091.1
dichloromethane	20.4	1964.6	1994.2	2012.3	2054.2	2068.6	2073.5	860.1	2096
chloroform	23.1	1965	1996.7	2013.9	2051.7	2070.1	2076	858.5	2097.7
phenylethanol	33.8	1967.6	--[c]	2013.1	2053.1	2069.3	2076.4	--[c]	--[c]
benzyl alcohol	36.8	1968.3	1996.1	2013.3	2053.2	2069.1	2076.4	853.6	2098
m-cresol	50.4	1974.5	2001.4	2022.6	--[c]	2072.2	--[c]	852.2	2099.4
mean ν		1965.7	1992.4	2009.3	2051.4	2069.2	2075.0	859.0	2094.3
standard dev.		3.1	3.3	4.8	3.3	1.0	2.2	3.8	2.9

a. Acceptor numbers obtained from refs 1 and 2 (below) unless otherwise noted.

b. Values obtained from the frequency of acetone carbonyl in this solvent.[3]

c. Peak not observed.

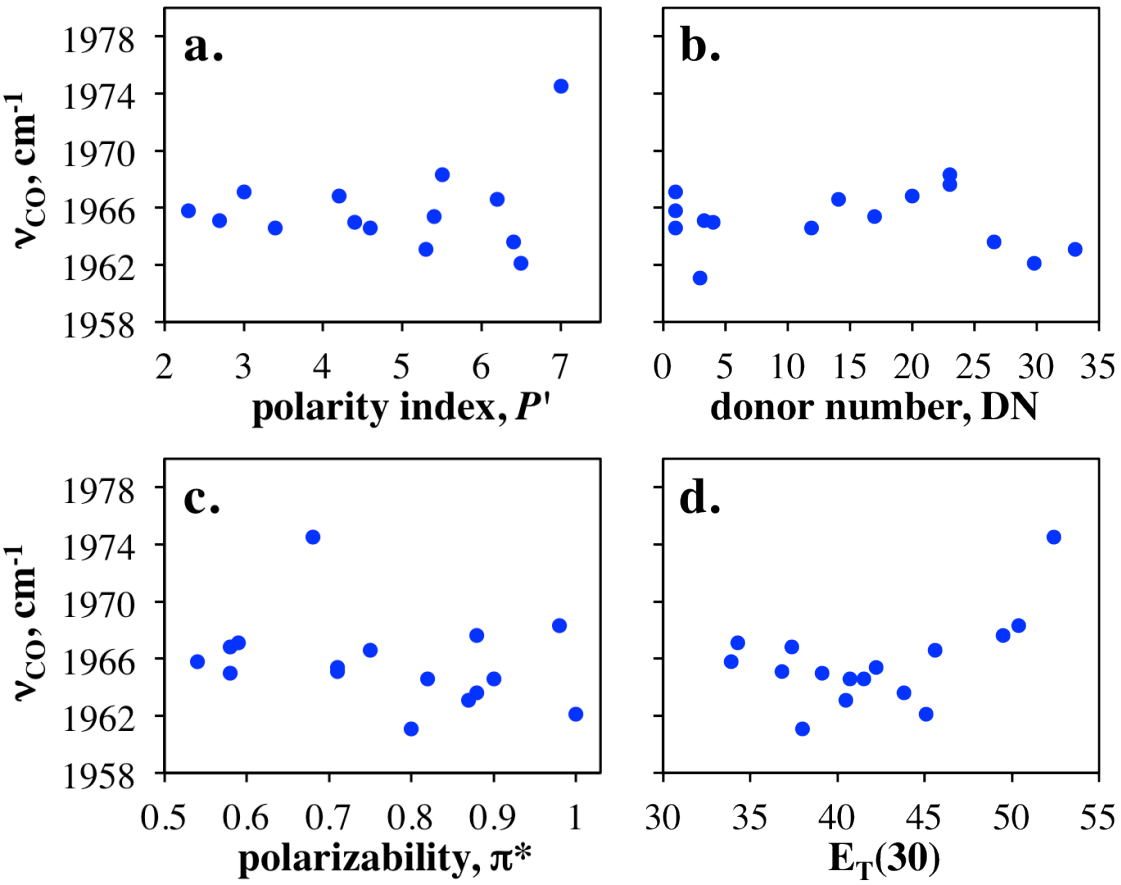

Figure S1. Center frequency of the CO stretch (ν_{CO}) for Vaska's complex (VC) as a function of a) polarity index, b) donor number, c) polarizability, and d) $E_T(30)$.

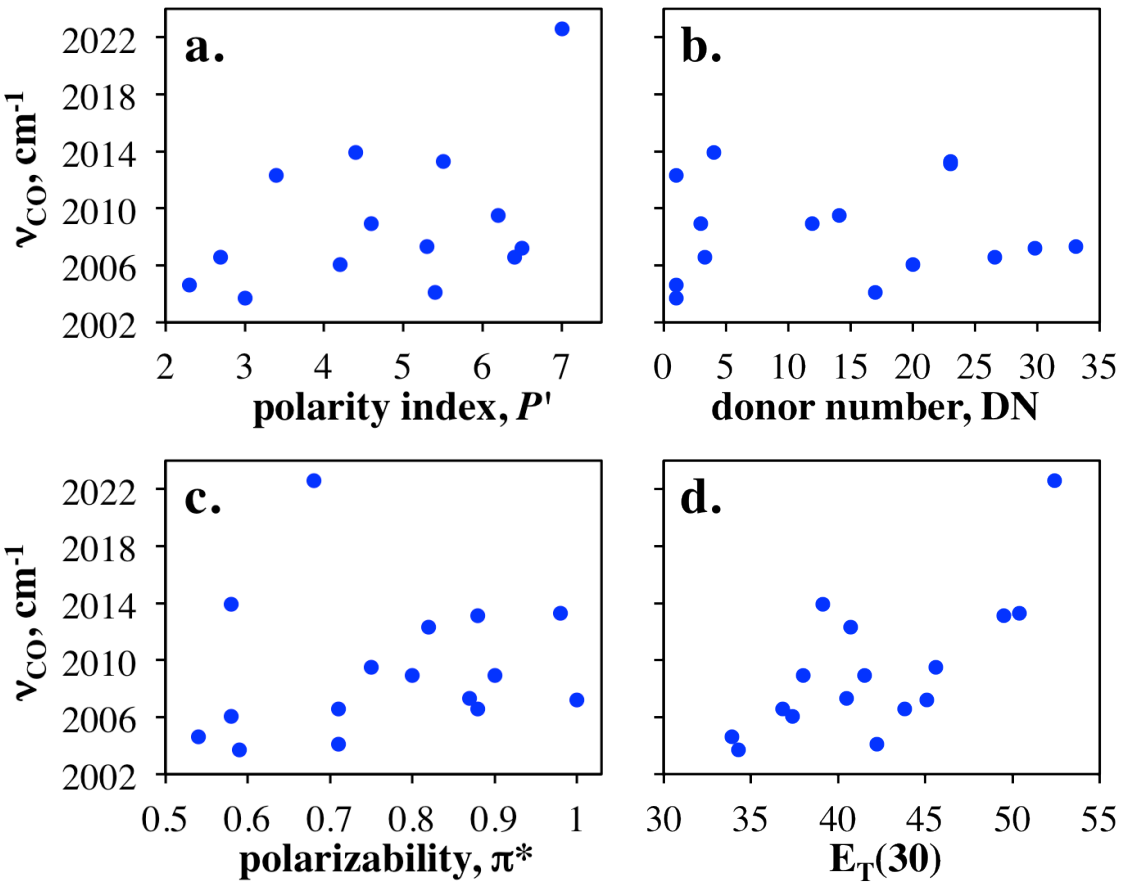

Figure S2. Center frequency of the CO stretch (ν_{CO}) for the O_2 adduct of Vaska's complex (VC-O_2) as a function of a) polarity index, b) donor number, c) polarizability, and d) E_T(30).

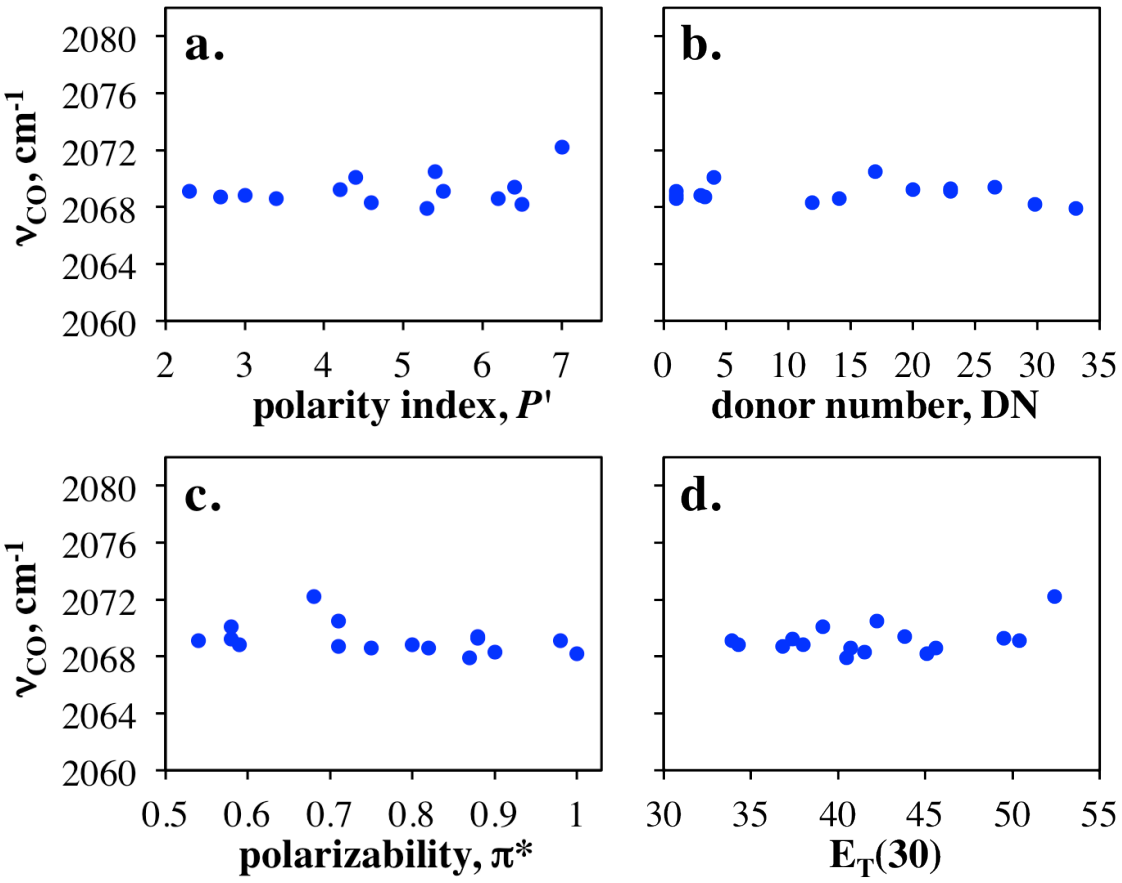

Figure S3. Center frequency of the CO stretch (ν_{CO}) for the I_2 adduct of Vaska's complex (VC-I_2) as a function of a) polarity index, b) donor number, c) polarizability, and d) $E_T(30)$.

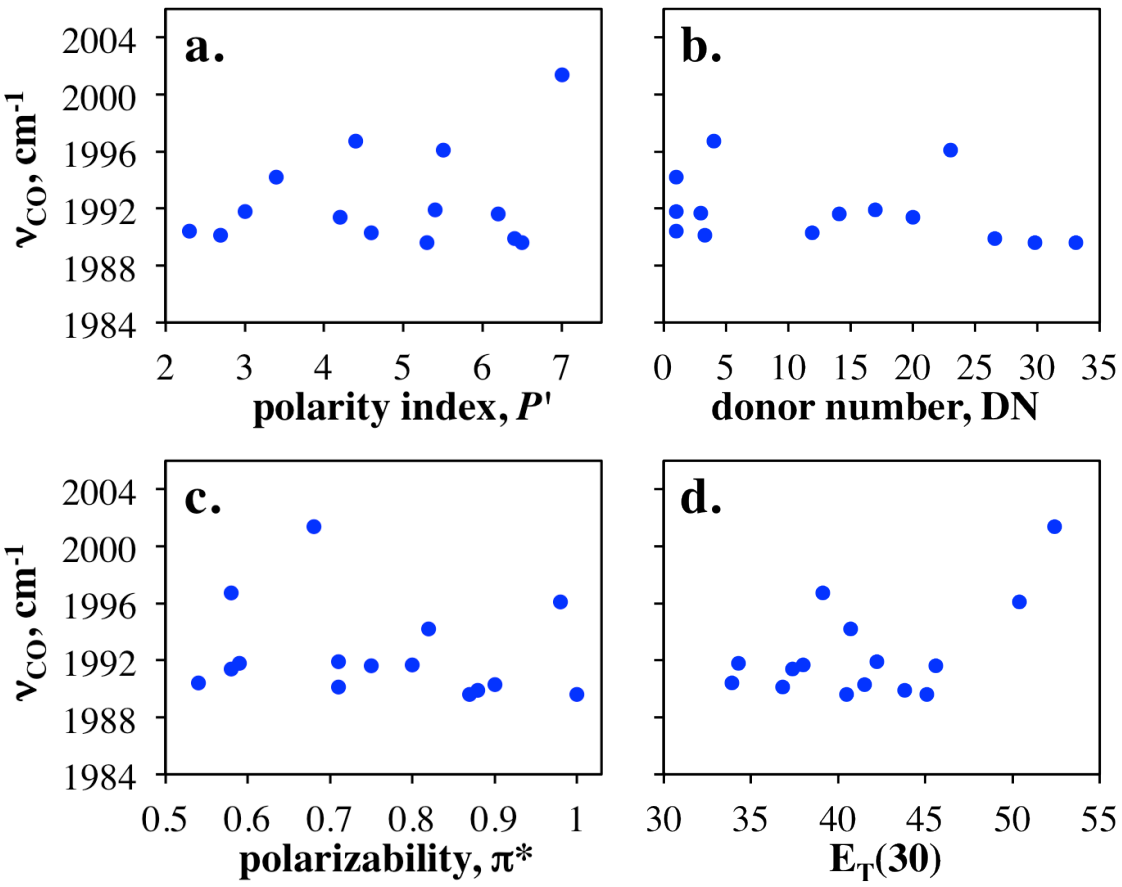

Figure S4. Center frequency of the CO stretch (ν_{CO}) for the H_2 adduct of Vaska's complex (VC-H_2) as a function of a) polarity index, b) donor number, c) polarizability, and d) $E_T(30)$.

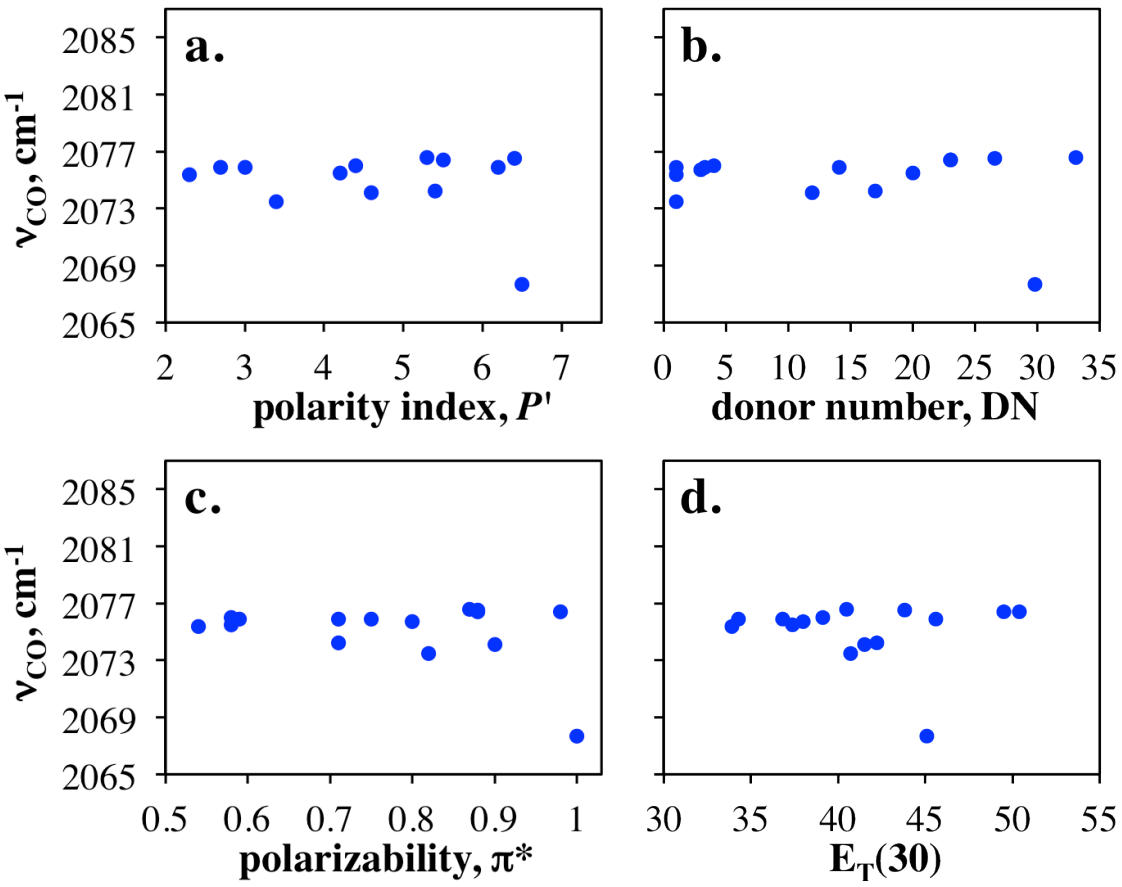

Figure S5. Center frequency of the CO stretch (ν_{CO}) for the Br_2 adduct of Vaska's complex (VC-Br_2) as a function of a) polarity index, b) donor number, c) polarizability, and d) $E_T(30)$.

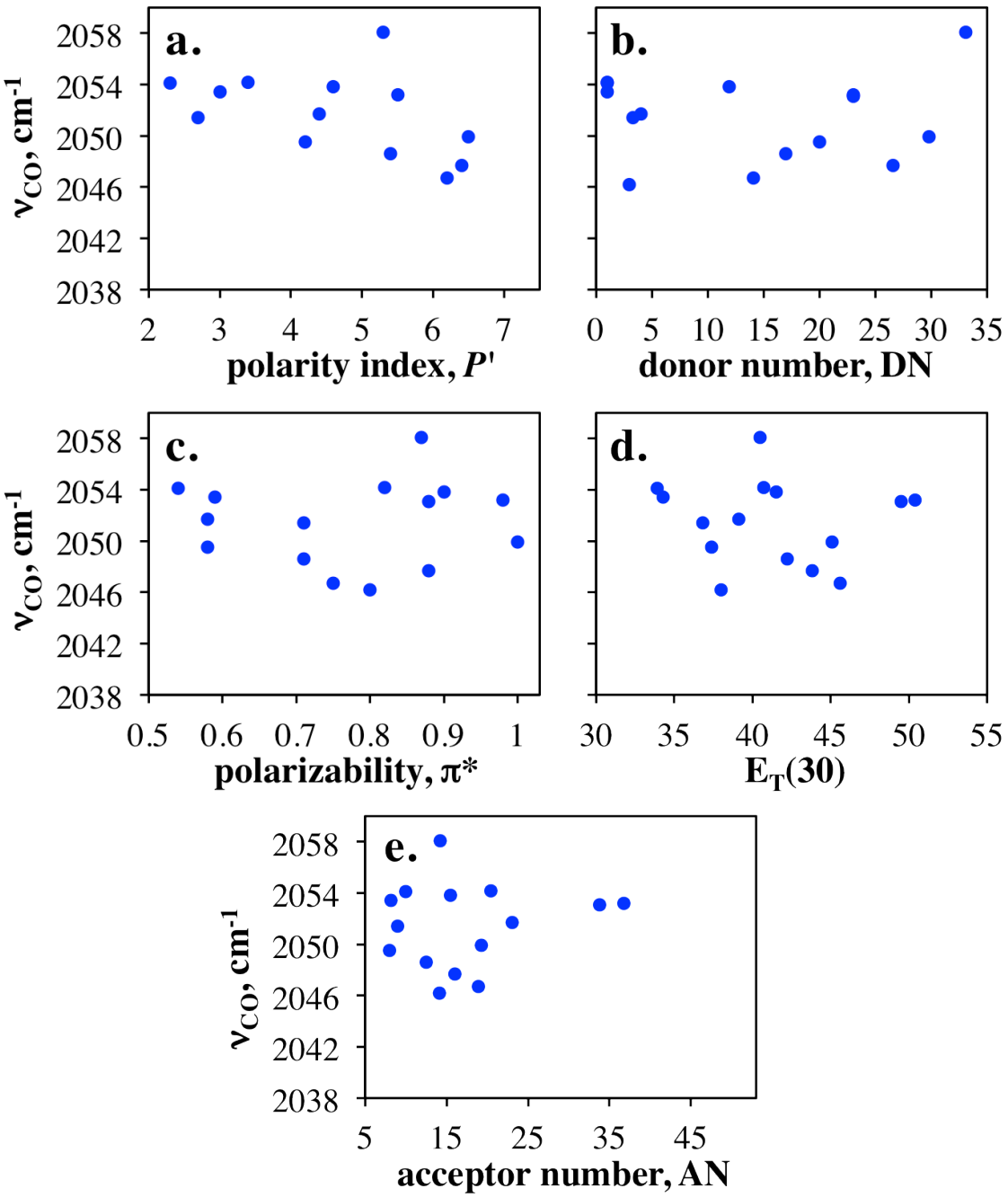

Figure S6. Center frequency of the CO stretch (ν_{CO}) for the sulfur allotrope adduct of Vaska's complex (VC-S_X) as a function of a) polarity index, b) donor number, c) polarizability, d) $E_T(30)$, and e) acceptor number.

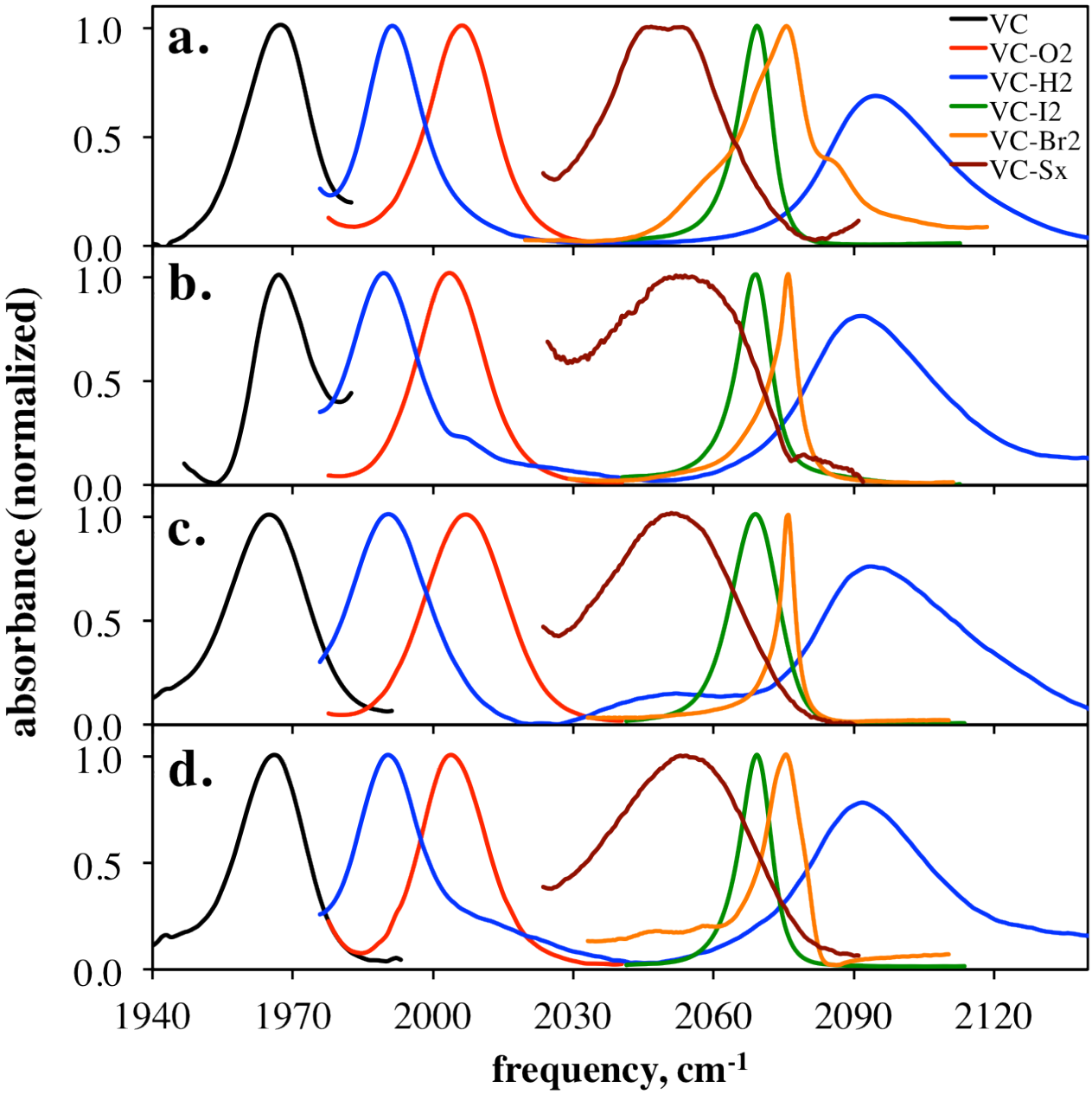

Figure S7. Solvent-subtracted, baseline, and normalized FTIR spectra showing the CO stretch (ν_{CO}) for VC, VC-O_2, VC-H_2, VC-Br_2, VC-I_2, and VC-S_X (colors coded as listed in legend) measured in a) THF (AN = 8), b) benzene (AN = 8.2), c) chlorobenzene (AN = 9), and d) toluene (AN = 10). The peak at ~2095 cm^{-1} is the Ir-H stretching mode ($\nu_{Ir\text{-}H}$) for VC-H_2.

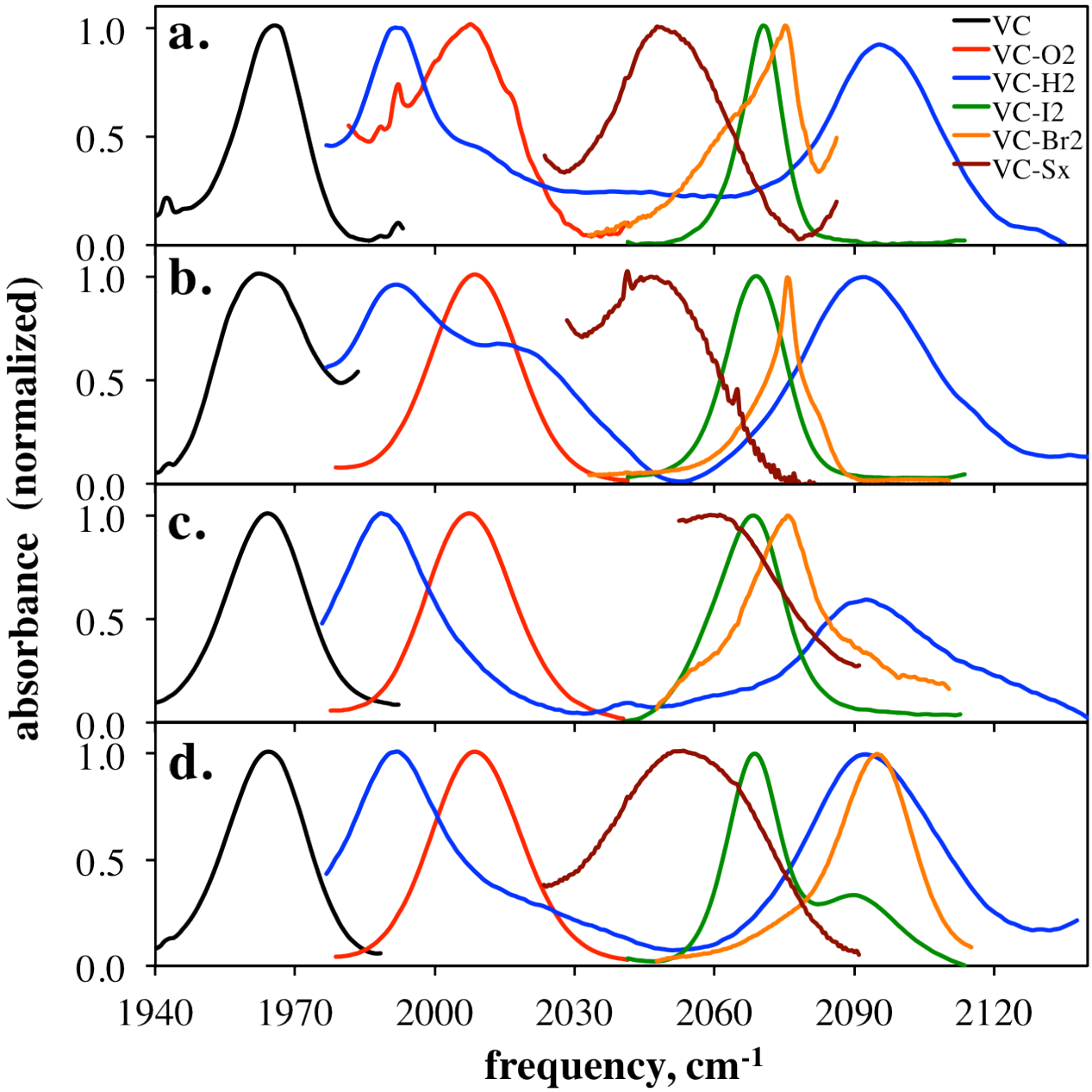

Figure S8. Solvent-subtracted, baseline, and normalized FTIR spectra showing the CO stretch (ν_{CO}) for VC, VC-O_2, VC-H_2, VC-Br_2, VC-I_2, and VC-S_X (colors coded as listed in legend) measured in a) acetone (AN = 12.5), b) *o*-dichlorobenzene (AN = 14.1), c) pyridine (AN = 14.2), and d) benzonitrile (AN = 15.5). The peak at ~2095 cm^{-1} is the Ir-H stretching mode ($\nu_{Ir\text{-}H}$) for VC-H_2. The extra peak at ~2100 cm^{-1} for VC-Br_2 and VC-I_2 in benzonitrile is the CN stretching mode, presumably coordinated to the iridium.

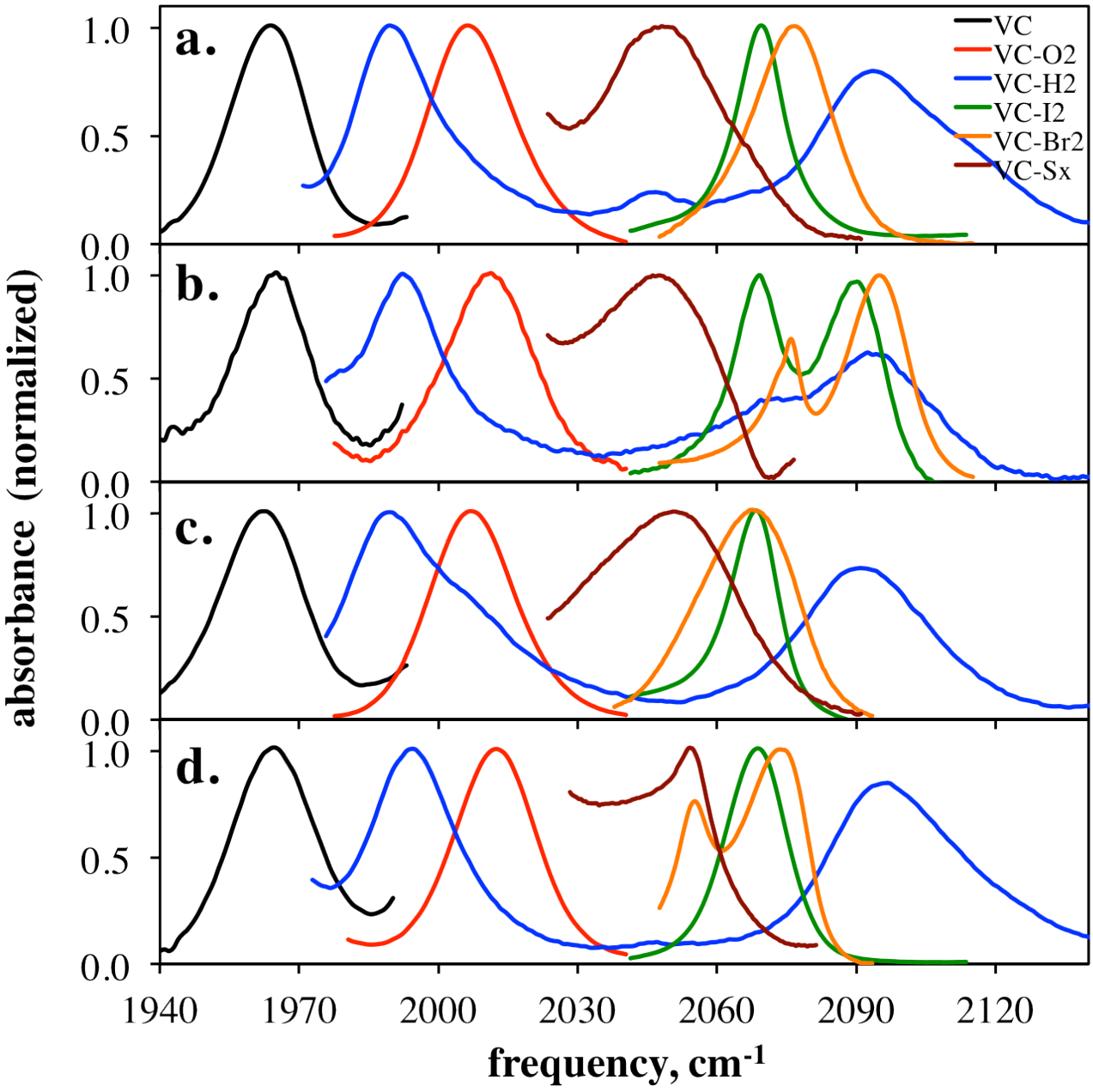

Figure S9. Solvent-subtracted, baseline, and normalized FTIR spectra showing the CO stretch (ν_{CO}) for VC, VC-O_2, VC-H_2, VC-Br_2, VC-I_2, and VC-S_X (colors coded as listed in legend) measured in a) DMF (AN = 16), b) acetonitrile (AN = 18.9), c) DMSO (AN = 19.3), and d) dichloromethane (AN = 20.4). The peak at ~2095 cm^{-1} is the Ir-H stretching mode ($\nu_{Ir\text{-}H}$) for VC-H_2. The extra peak at ~2100 cm^{-1} for VC-Br_2 and VC-I_2 in acetonitrile is the CN stretching mode, presumably coordinated to the iridium.

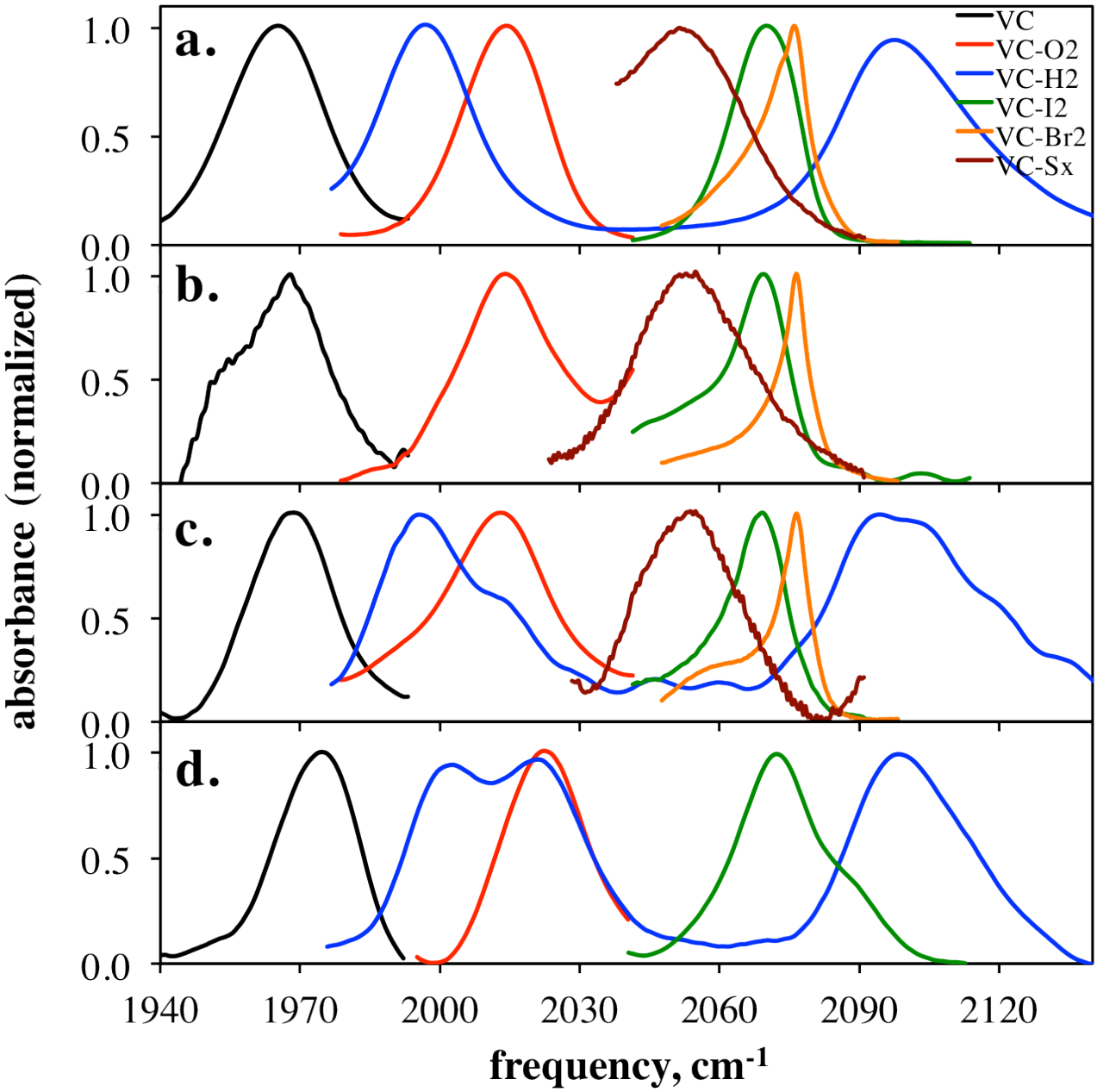

Figure S10. Solvent-subtracted, baseline, and normalized FTIR spectra showing the CO stretch (ν_{CO}) for VC, VC-O_2, VC-H_2, VC-Br_2, VC-I_2, and VC-S_X (colors coded as listed in legend) measured in a) chloroform (AN = 23.1), b) phenylethanol (AN = 33.8), c) benzyl alcohol (AN = 36.8), and d) *m*-cresol (AN = 50.4). The peak at ~2095 cm^{-1} is the Ir-H stretching mode ($\nu_{Ir\text{-}H}$) for VC-H_2.

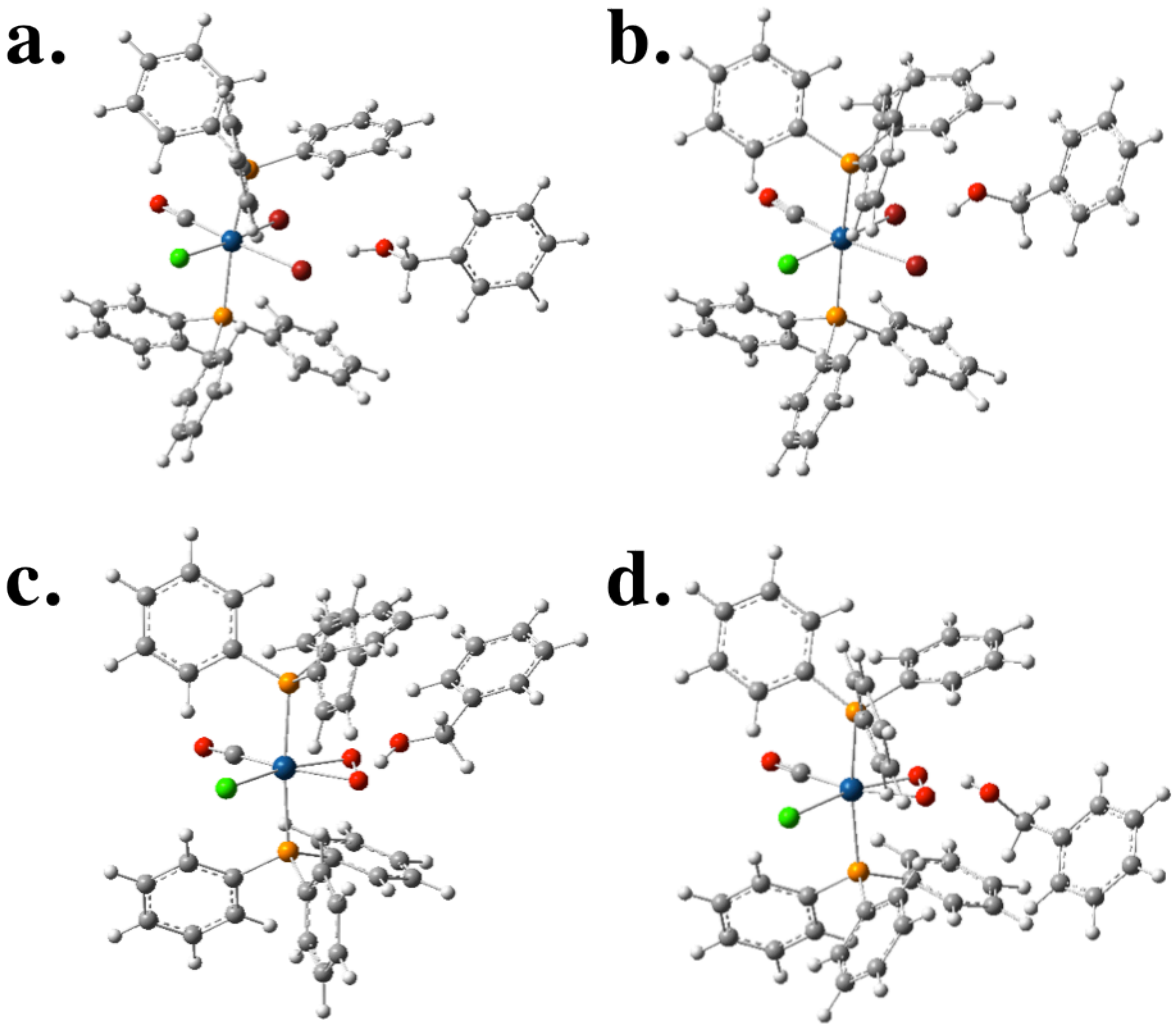

Figure S11. DFT optimized structures of a) and b) VC-Br_2 adducts and c) and d) VC-O_2 adducts microsolvated with one benzyl alcohol (BnOH) molecule. Microsolvation was initiated with BnOH with a hydrogen bonding geometry to the *cis* (a and c) and *trans* (b and d) Br/O atoms. Note that attempts to generate a microsolvate for the Br complex analogous to the *cis* coordinated species of the O_2 complex smoothly optimized to the structure shown at upper left, which has weak interactions with both *cis* and *trans* Br atoms. The tabulated nuclear coordinates of the optimized microsolvated structures are provided in Table S2 below.

Table S2. Cartesian coordinates (Å) for BnOH microsolvates of VC-O_2 and VC-Br_2.

cis VC-O_2•BnOH complex

center number	atomic number	atomic type	coordinates (Å)		
			X	Y	Z
1	77	0	-0.765287	0.528321	-0.117903
2	17	0	-2.528482	2.337663	0.414837
3	6	0	-1.036448	0.790031	-1.931736
4	8	0	-1.146942	0.880908	-3.086569
5	15	0	-2.427506	-1.210703	0.033996
6	15	0	1.021105	2.153843	-0.000286
7	6	0	-1.619892	-2.825133	-0.14669
8	6	0	-1.175549	-3.207901	-1.42155
9	6	0	-1.364119	-3.650366	0.951566
10	6	0	-0.515	-4.418073	-1.594622
11	1	0	-1.351773	-2.556749	-2.279809
12	6	0	-0.688042	-4.856782	0.772753
13	1	0	-1.692075	-3.354595	1.947509
14	6	0	-0.270128	-5.244495	-0.496932
15	1	0	-0.177697	-4.71183	-2.586904
16	1	0	-0.491374	-5.494711	1.632453
17	1	0	0.255367	-6.187818	-0.633714
18	6	0	2.637742	1.331825	-0.07538
19	6	0	2.943287	0.598922	-1.232353
20	6	0	3.569148	1.402371	0.963274
21	6	0	4.177785	-0.023984	-1.358945
22	1	0	2.208469	0.51966	-2.036262
23	6	0	4.803875	0.764001	0.835416
24	1	0	3.338312	1.958101	1.871331
25	6	0	5.113064	0.062137	-0.325774
26	1	0	4.407707	-0.590408	-2.259826
27	1	0	5.525804	0.820984	1.648405
28	1	0	6.077711	-0.433876	-0.424397
29	6	0	-3.282677	-1.232465	1.639603
30	6	0	-4.380253	-2.081141	1.837586
31	6	0	-2.835023	-0.424579	2.690312

32	6	0	-5.014326	-2.12247	3.075099
33	1	0	-4.740599	-2.71219	1.025075
34	6	0	-3.475396	-0.468056	3.925718
35	1	0	-1.985048	0.236573	2.534915
36	6	0	-4.562897	-1.316386	4.119408
37	1	0	-5.865309	-2.784659	3.222783
38	1	0	-3.122433	0.16546	4.737387
39	1	0	-5.063063	-1.34874	5.085694
40	6	0	0.992279	3.127937	1.53305
41	6	0	1.712781	4.325548	1.632134
42	6	0	0.270284	2.66058	2.636393
43	6	0	1.714439	5.038521	2.827208
44	1	0	2.274708	4.700696	0.776721
45	6	0	0.274251	3.378437	3.828596
46	1	0	-0.293762	1.733596	2.549606
47	6	0	0.996563	4.565968	3.924996
48	1	0	2.276264	5.967834	2.899439
49	1	0	-0.29226	3.010023	4.681846
50	1	0	0.997376	5.128064	4.857234
51	6	0	1.058389	3.374092	-1.354497
52	6	0	-0.148769	3.91961	-1.812406
53	6	0	2.26681	3.81003	-1.914335
54	6	0	-0.14445	4.88318	-2.816181
55	1	0	-1.093236	3.590848	-1.376025
56	6	0	2.263068	4.773709	-2.919766
57	1	0	3.213322	3.400014	-1.56482
58	6	0	1.059943	5.309883	-3.372691
59	1	0	-1.087579	5.298378	-3.166524
60	1	0	3.206757	5.105434	-3.348776
61	1	0	1.060678	6.061356	-4.160348
62	6	0	-3.73794	-1.204457	-1.233041
63	6	0	-4.198189	0.013527	-1.749562
64	6	0	-4.325492	-2.401217	-1.668592
65	6	0	-5.225095	0.032168	-2.689223
66	1	0	-3.758645	0.950387	-1.406367
67	6	0	-5.352089	-2.37499	-2.608067
68	1	0	-3.977768	-3.357163	-1.279434

69	6	0	-5.801905	-1.160044	-3.120905
70	1	0	-5.572724	0.984345	-3.085515
71	1	0	-5.798871	-3.30974	-2.941544
72	1	0	-6.601587	-1.143191	-3.859337
73	8	0	0.638305	-0.876815	0.258279
74	8	0	0.156247	-0.459449	1.533452
75	1	0	1.407098	-2.486853	-0.472157
76	8	0	2.267992	-2.893644	-0.68374
77	6	0	3.045984	-2.744162	0.484604
78	1	0	2.611501	-3.323752	1.321452
79	1	0	3.050151	-1.69039	0.819548
80	6	0	4.459011	-3.186433	0.245974
81	6	0	4.900098	-3.607093	-1.009736
82	6	0	5.376465	-3.140036	1.302239
83	6	0	6.232586	-3.970635	-1.206775
84	1	0	4.194094	-3.643051	-1.836449
85	6	0	6.704935	-3.502509	1.107591
86	1	0	5.041494	-2.804845	2.285305
87	6	0	7.139841	-3.918776	-0.151892
88	1	0	6.561679	-4.295461	-2.193195
89	1	0	7.40614	-3.45839	1.939898
90	1	0	8.179953	-4.20125	-0.307171

trans VC-O_2•BnOH complex

center number	atomic number	atomic type	coordinates (Å)		
			X	Y	Z
1	77	0	-0.755752	0.374812	-0.099612
2	17	0	-1.424304	1.588677	2.027969
3	6	0	-1.442391	1.783057	-1.091604
4	8	0	-1.849234	2.640096	-1.763602
5	15	0	-2.839769	-0.83302	0.001056
6	15	0	1.416575	1.453545	-0.058795
7	6	0	-2.83395	-2.270173	-1.104093
8	6	0	-2.663177	-2.046306	-2.478021
9	6	0	-2.978884	-3.576092	-0.629014
10	6	0	-2.661044	-3.116422	-3.364159

11	1	0	-2.536085	-1.028619	-2.850642
12	6	0	-2.965565	-4.647028	-1.521736
13	1	0	-3.105075	-3.762342	0.436673
14	6	0	-2.810649	-4.419103	-2.885911
15	1	0	-2.533517	-2.93561	-4.429824
16	1	0	-3.079856	-5.661805	-1.145264
17	1	0	-2.802851	-5.25693	-3.580863
18	6	0	2.601727	0.781643	-1.260368
19	6	0	2.147153	0.479693	-2.552661
20	6	0	3.953422	0.605959	-0.94633
21	6	0	3.037504	0.012911	-3.514606
22	1	0	1.094208	0.612398	-2.801769
23	6	0	4.839772	0.137146	-1.913344
24	1	0	4.316526	0.817754	0.058252
25	6	0	4.383979	-0.162377	-3.194518
26	1	0	2.677116	-0.221857	-4.514431
27	1	0	5.888215	-0.006679	-1.656018
28	1	0	5.077473	-0.53809	-3.945093
29	6	0	-3.201368	-1.461621	1.667551
30	6	0	-4.524342	-1.647412	2.08623
31	6	0	-2.148739	-1.796952	2.528292
32	6	0	-4.788418	-2.166816	3.350891
33	1	0	-5.35104	-1.387469	1.425508
34	6	0	-2.419355	-2.316654	3.789809
35	1	0	-1.119247	-1.64475	2.207607
36	6	0	-3.73806	-2.500677	4.202914
37	1	0	-5.819433	-2.306507	3.670535
38	1	0	-1.596165	-2.571443	4.454721
39	1	0	-3.9473	-2.901797	5.193027
40	6	0	2.200256	1.419799	1.575714
41	6	0	3.198896	2.345138	1.909142
42	6	0	1.821239	0.445341	2.505292
43	6	0	3.819778	2.280647	3.153033
44	1	0	3.4935	3.114008	1.194782
45	6	0	2.442987	0.386873	3.748479
46	1	0	1.036446	-0.265791	2.24982
47	6	0	3.44308	1.302049	4.071638

48	1	0	4.597475	2.998975	3.405392
49	1	0	2.142026	-0.373261	4.466825
50	1	0	3.92783	1.25643	5.045289
51	6	0	1.260786	3.221164	-0.480525
52	6	0	0.650157	4.077008	0.448433
53	6	0	1.628541	3.718878	-1.735028
54	6	0	0.409686	5.406705	0.119663
55	1	0	0.354928	3.696366	1.42597
56	6	0	1.381927	5.051619	-2.058271
57	1	0	2.111792	3.07129	-2.46478
58	6	0	0.769859	5.895555	-1.135789
59	1	0	-0.062954	6.063247	0.847874
60	1	0	1.675251	5.428892	-3.036306
61	1	0	0.576408	6.935625	-1.392104
62	6	0	-4.303646	0.137878	-0.485394
63	6	0	-4.427559	1.45389	-0.017979
64	6	0	-5.322396	-0.408481	-1.276459
65	6	0	-5.54643	2.21196	-0.347403
66	1	0	-3.645461	1.882898	0.61056
67	6	0	-6.438976	0.357151	-1.604471
68	1	0	-5.249614	-1.433784	-1.635696
69	6	0	-6.55167	1.666694	-1.144237
70	1	0	-5.629671	3.233934	0.017645
71	1	0	-7.223714	-0.075896	-2.221991
72	1	0	-7.424062	2.263055	-1.405425
73	8	0	0.006809	-1.14488	-1.219195
74	8	0	0.092168	-1.575472	0.137613
75	1	0	1.772752	-1.759499	0.55293
76	8	0	2.714895	-1.91759	0.808523
77	6	0	3.320365	-2.621015	-0.247244
78	1	0	2.922612	-3.651401	-0.322248
79	1	0	3.100338	-2.144789	-1.222323
80	6	0	4.809962	-2.67181	-0.062716
81	6	0	5.59578	-3.36466	-0.990659
82	6	0	5.442267	-2.009596	0.991891
83	6	0	6.981198	-3.392917	-0.871053
84	1	0	5.110439	-3.87997	-1.821318

85	6	0	6.831602	-2.038466	1.114245
86	1	0	4.838948	-1.462631	1.714725
87	6	0	7.606416	-2.727131	0.184384
88	1	0	7.577084	-3.935202	-1.604122
89	1	0	7.310276	-1.516655	1.942196
90	1	0	8.690962	-2.747577	0.279902

cis VC-Br_2•BnOH complex

center number	atomic number	atomic type	coordinates (Å)		
			X	Y	Z
1	77	0	-1.067103	0.175907	-0.107421
2	17	0	-2.743847	0.524459	1.663352
3	6	0	-2.392275	0.404745	-1.379153
4	8	0	-3.173592	0.527464	-2.223753
5	35	0	0.946418	-0.215344	1.488156
6	35	0	0.461954	-0.114028	-2.127966
7	15	0	-1.379813	-2.255891	0.054658
8	15	0	-0.444196	2.563681	-0.00657
9	6	0	0.064769	-3.169912	-0.559985
10	6	0	0.268305	-3.376212	-1.931547
11	6	0	1.056972	-3.569136	0.346719
12	6	0	1.429152	-3.995631	-2.382573
13	1	0	-0.476842	-3.044885	-2.651498
14	6	0	2.22679	-4.167161	-0.112518
15	1	0	0.918716	-3.406057	1.414235
16	6	0	2.41246	-4.385412	-1.475899
17	1	0	1.570542	-4.159892	-3.449108
18	1	0	2.993699	-4.465958	0.6002
19	1	0	3.325642	-4.858634	-1.833074
20	6	0	1.327938	2.855741	-0.307682
21	6	0	1.871933	2.812595	-1.600303
22	6	0	2.189652	3.022236	0.785911
23	6	0	3.244905	2.933907	-1.789686
24	1	0	1.226872	2.67306	-2.462923
25	6	0	3.562563	3.137652	0.590272
26	1	0	1.791359	3.056262	1.798085

27	6	0	4.094182	3.086776	-0.696178
28	1	0	3.650759	2.897934	-2.798726
29	1	0	4.217514	3.263878	1.450805
30	1	0	5.169526	3.166724	-0.847353
31	6	0	-1.662933	-2.975281	1.717355
32	6	0	-2.050348	-4.324045	1.759995
33	6	0	-1.468692	-2.282704	2.915033
34	6	0	-2.235749	-4.964591	2.979604
35	1	0	-2.205484	-4.880704	0.835861
36	6	0	-1.661761	-2.929154	4.134675
37	1	0	-1.164831	-1.241668	2.897235
38	6	0	-2.043716	-4.266757	4.171001
39	1	0	-2.533275	-6.011379	2.996832
40	1	0	-1.510293	-2.377486	5.06077
41	1	0	-2.192202	-4.767696	5.126092
42	6	0	-0.774022	3.402989	1.586752
43	6	0	-1.091007	4.769013	1.582228
44	6	0	-0.633774	2.739221	2.811391
45	6	0	-1.264902	5.453336	2.781873
46	1	0	-1.199712	5.307449	0.642144
47	6	0	-0.806921	3.429885	4.007204
48	1	0	-0.383979	1.681453	2.827387
49	6	0	-1.125429	4.785827	3.996103
50	1	0	-1.510965	6.513392	2.763011
51	1	0	-0.696321	2.900239	4.951716
52	1	0	-1.265057	5.322142	4.933105
53	6	0	-1.411787	3.561336	-1.184918
54	6	0	-2.807493	3.438653	-1.106794
55	6	0	-0.856837	4.498137	-2.063178
56	6	0	-3.629563	4.215532	-1.914009
57	1	0	-3.255456	2.743844	-0.393247
58	6	0	-1.68581	5.26952	-2.875866
59	1	0	0.219258	4.649247	-2.104592
60	6	0	-3.068596	5.126479	-2.808233
61	1	0	-4.710245	4.109558	-1.8426
62	1	0	-1.242803	5.992151	-3.558498
63	1	0	-3.711439	5.731879	-3.444466

64	6	0	-2.845495	-2.83224	-0.868949
65	6	0	-4.039125	-2.11845	-0.686925
66	6	0	-2.858411	-3.994898	-1.649545
67	6	0	-5.213846	-2.542079	-1.298678
68	1	0	-4.052488	-1.232415	-0.048931
69	6	0	-4.037126	-4.411305	-2.26444
70	1	0	-1.954505	-4.587608	-1.772723
71	6	0	-5.212841	-3.684705	-2.096528
72	1	0	-6.131844	-1.976969	-1.14948
73	1	0	-4.032726	-5.313523	-2.873149
74	1	0	-6.13073	-4.013237	-2.580438
75	1	0	2.576592	-0.55585	-0.512285
76	8	0	3.519828	-0.673402	-0.732835
77	6	0	4.238852	-0.622822	0.485604
78	1	0	3.884627	-1.412223	1.176146
79	1	0	4.084051	0.33668	1.008481
80	6	0	5.69873	-0.819836	0.202582
81	6	0	6.661175	0.007468	0.785511
82	6	0	6.121443	-1.854916	-0.639177
83	6	0	8.018814	-0.197983	0.544412
84	1	0	6.340367	0.824499	1.433662
85	6	0	7.475404	-2.058578	-0.887405
86	1	0	5.375789	-2.499517	-1.103907
87	6	0	8.429497	-1.231472	-0.294201
88	1	0	8.756391	0.45718	1.005886
89	1	0	7.789586	-2.867395	-1.545882
90	1	0	9.488972	-1.391055	-0.488718

trans VC-Br_2•BnOH complex

center number	atomic number	atomic type	coordinates (Å)		
			X	Y	Z
1	77	0	-0.801919	0.503559	-0.055284
2	17	0	-1.461355	1.546908	2.081987
3	6	0	-1.465827	1.907408	-1.060196
4	8	0	-1.822227	2.748341	-1.771634
5	35	0	0.277172	-1.602281	1.037685

6	35	0	-0.287199	-0.546522	-2.321876
7	15	0	-2.946291	-0.725685	0.004301
8	15	0	1.391276	1.606453	0.05856
9	6	0	-2.917996	-2.381687	-0.749484
10	6	0	-2.931218	-2.549862	-2.14227
11	6	0	-2.819348	-3.512772	0.07182
12	6	0	-2.872852	-3.824715	-2.6952
13	1	0	-2.985743	-1.68508	-2.79815
14	6	0	-2.747187	-4.784906	-0.488041
15	1	0	-2.801449	-3.40564	1.154791
16	6	0	-2.777192	-4.944063	-1.870974
17	1	0	-2.895497	-3.940789	-3.777077
18	1	0	-2.671359	-5.653361	0.163399
19	1	0	-2.725978	-5.939937	-2.307442
20	6	0	2.455548	1.081549	-1.312271
21	6	0	2.313457	1.674412	-2.5732
22	6	0	3.317577	-0.009469	-1.154423
23	6	0	3.054535	1.205016	-3.651804
24	1	0	1.617328	2.502086	-2.713269
25	6	0	4.047627	-0.483765	-2.241091
26	1	0	3.427965	-0.479095	-0.176311
27	6	0	3.920514	0.12504	-3.487662
28	1	0	2.947432	1.678756	-4.6259
29	1	0	4.721897	-1.329309	-2.108832
30	1	0	4.496632	-0.243874	-4.334515
31	6	0	-3.659185	-1.014452	1.667659
32	6	0	-5.053748	-1.03492	1.810109
33	6	0	-2.855975	-1.301916	2.777678
34	6	0	-5.630129	-1.337939	3.040636
35	1	0	-5.698741	-0.817859	0.960292
36	6	0	-3.438572	-1.607054	4.004093
37	1	0	-1.773151	-1.285765	2.681122
38	6	0	-4.824823	-1.623389	4.140039
39	1	0	-6.714296	-1.349082	3.135653
40	1	0	-2.80152	-1.827206	4.858792
41	1	0	-5.277169	-1.857629	5.102108
42	6	0	2.404511	1.350544	1.560836

43	6	0	3.769533	1.672804	1.500124
44	6	0	1.853997	0.933886	2.777075
45	6	0	4.567584	1.560711	2.633555
46	1	0	4.217414	2.000526	0.562669
47	6	0	2.65911	0.827295	3.9091
48	1	0	0.798053	0.687793	2.838908
49	6	0	4.01485	1.134512	3.84
50	1	0	5.626439	1.805595	2.570135
51	1	0	2.21964	0.494886	4.847783
52	1	0	4.641909	1.043349	4.725094
53	6	0	1.314593	3.431887	-0.081028
54	6	0	0.196975	4.143124	0.37083
55	6	0	2.4253	4.142729	-0.561284
56	6	0	0.182222	5.53519	0.326025
57	1	0	-0.663373	3.612844	0.776125
58	6	0	2.404723	5.532689	-0.604848
59	1	0	3.308533	3.610478	-0.910956
60	6	0	1.282667	6.232176	-0.164236
61	1	0	-0.696141	6.072788	0.678122
62	1	0	3.271031	6.069749	-0.986498
63	1	0	1.268747	7.319943	-0.201026
64	6	0	-4.254701	0.246734	-0.816022
65	6	0	-4.402878	1.579475	-0.402389
66	6	0	-5.169492	-0.288456	-1.729279
67	6	0	-5.424952	2.368331	-0.917071
68	1	0	-3.721247	1.999394	0.340823
69	6	0	-6.188	0.509018	-2.248002
70	1	0	-5.107813	-1.332243	-2.02742
71	6	0	-6.314683	1.836445	-1.849214
72	1	0	-5.52593	3.400565	-0.587681
73	1	0	-6.88985	0.082163	-2.961903
74	1	0	-7.112047	2.454945	-2.256894
75	1	0	2.58555	-1.585815	1.847563
76	8	0	3.534577	-1.804761	1.887464
77	6	0	3.759438	-2.834657	0.944025
78	1	0	3.023881	-2.774154	0.121684
79	1	0	3.609449	-3.82671	1.407777

80	6	0	5.147399	-2.744793	0.375839
81	6	0	5.611621	-3.758858	-0.470113
82	6	0	5.977328	-1.652295	0.636144
83	6	0	6.873253	-3.677704	-1.050599
84	1	0	4.971507	-4.617491	-0.678276
85	6	0	7.244212	-1.572497	0.058126
86	1	0	5.620283	-0.861805	1.293902
87	6	0	7.69585	-2.581093	-0.788816
88	1	0	7.217685	-4.473695	-1.709422
89	1	0	7.880044	-0.714017	0.271513
90	1	0	8.684033	-2.517132	-1.241631

Full author list for reference 33.

Frisch, M. J. T., G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J.

REFERENCES

(1) Marcus, Y., *Chem. Soc. Rev.* **1993,** 22, 409-416.

(2) Mayer, U.; Gutmann, V.; Gerger, W., *Monatsh. Chem.* **1975,** 106, 1235-1257.

(3) Symons, M. C. R.; Eaton, G.; Shippey, T. A.; Harvey, J. M., *Chem. Phys. Lett.* **1980,** 69, 344-347.