

Electronic properties of a cytosine decavanadate: toward a better understanding of chemical and biological properties of decavanadates

Nada Bošnjaković-Pavlović,^{a,b} Anne Spasojević-de Biré,^a Isabel Tomaz,^c Nouzha
Bouhmaida,^d Fernando Avecilla,^e Ubavka B. Mioč,^b João Costa Pessoa,^c and Nour Eddine
Ghermani*,^{a,f}*

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Figure S-1. Local coordinate scheme of the cytosine – decavanadate for the definition orientation of multipole in molecules a) decavanadate; b) molecules of cytosine.

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Figure S-6 Dynamic deformation electron density maps: a) DV-horizontal plane; b) DV-vertical plane; c) cytosinium A; d) cytosinium B; e) cytosine C. Contour intervals are $0.05 \text{ e}\text{\AA}^{-3}$.

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Figure S-10. Behavior of $\rho(r_{\text{cp}})$ of the V-O bond as a function of the interatomic distance.

Table S-1

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Table S-5.

bond	angles	bond	angles
O13-V1-O23	103.11(3)	O21-V4-O27	106.63(3)
O13-V1-O20	103.22(3)	O21-V4-O31	96.76(2)
O13-V1-O32	100.82(3)	O21-V4-O32	95.98(2)
O13-V1-O31	100.19(3)	O21-V4-O61	86.12(2)
O23-V1-O20	94.63(3)	O27-V4-O31	99.05(2)
O23-V1-O32	90.72(2)	O27-V4-O32	97.37(3)
O23-V1-O61	80.22(2)	O27-V4-O61	88.94(2)
O20-V1-O31	89.17(2)	O31-V4-O61	81.33(2)
O20-V1-O61	80.31(2)	O31-V4-O61	80.60(2)
O32-V1-O31	75.58(2)	O32-V4-O61	80.74(2)
O32-V1-O61	75.02(2)	O32-V4-O61	79.32(2)
O31-V1-O61	75.92(2)	O61-V4-O61	78.29(2)
O12-V2-O24	104.29(3)	O10-V5-O22	103.90(3)
O12-V2-O25	101.85(3)	O10-V5-O24	101.90(3)
O12-V2-O31	100.23(3)	O10-V5-O23	100.89(3)
O12-V2-O32	98.51(3)	O10-V5-O27	98.74(3)
O24-V2-O25	96.06(3)	O22-V5-O24	91.70(3)
O24-V2-O31	90.57(2)	O22-V5-O23	91.73(3)
O24-V2-O61	80.99(2)	O22-V5-O61	82.74(2)
O25-V2-O32	89.02(2)	O24-V5-O27	83.71(2)
O25-V2-O61	81.21(2)	O24-V5-O61	78.06(2)
O31-V2-O32	75.31(2)	O23-V5-O27	83.80(2)
O31-V2-O61	75.61(2)	O23-V5-O61	78.22(2)
O32-V2-O61	75.64(2)	O27-V5-O61	74.62(2)
O11-V3-O22	103.27(3)		
O11-V3-O20	101.64(3)		
O11-V3-O25	102.46(3)		
O11-V3-O21	100.55(3)		
O22-V3-O20	90.40(3)		
O22-V3-O25	91.39(3)		
O22-V3-O61	81.21(2)		
O20-V3-O21	83.75(3)		
O20-V3-O61	77.56(2)		
O25-V3-O21	84.49(2)		
O25-V3-O61	77.82(2)		
O21-V3-O61	77.56(2)		

Table S-6.

	x	y	z
V1	0.29699(1)	0.180735(9)	0.607957(9)
V2	0.48687(1)	0.204386(9)	0.397722(9)
V3	0.80492(1)	0.03889(1)	0.35350(1)
V4	0.62264(1)	0.012011(9)	0.565293(9)
V5	0.42411(1)	-0.01176(1)	0.765785(9)
O10	0.44477(8)	-0.00891(6)	0.88502(5)
O11	0.96210(7)	0.05674(6)	0.32460(6)
O12	0.41066(7)	0.34373(5)	0.40334(5)
O13	0.21850(7)	0.31956(5)	0.61038(5)
O20	0.14362(6)	0.12371(5)	0.63319(5)
O21	0.78247(6)	0.03258(5)	0.50985(4)
O22	0.75274(7)	0.03330(5)	0.22519(4)
O23	0.34439(7)	0.14708(5)	0.73701(4)
O24	0.47651(6)	0.16877(5)	0.26761(4)
O25	0.67951(6)	0.19092(5)	0.37275(5)
O27	0.61716(6)	0.01206(5)	0.69468(4)
O31	0.31567(6)	0.15222(4)	0.45516(4)
O32	0.50169(6)	0.17158(4)	0.55010(4)
O61	0.41967(6)	-0.01120(4)	0.59106(4)
O2a	0.04277(9)	0.53660(7)	0.79461(5)
O2b	0.3788(1)	0.53156(6)	0.80918(6)
O2c	0.7840(2)	0.41101(9)	0.79150(7)
N1a	-0.0745(1)	0.73016(8)	0.80652(6)
N3a	-0.04486(9)	0.61322(7)	0.95634(5)
N4a	-0.1426(1)	0.68943(8)	1.11838(6)
N1b	0.4815(1)	0.33744(7)	0.81957(6)
N3b	0.3720(1)	0.44574(7)	0.96921(6)
N4b	0.3706(1)	0.35989(8)	1.13155(7)
N1c	0.8695(2)	0.2151(1)	0.8073(1)
N3c	0.7724(1)	0.32949(7)	0.95379(6)
N4c	0.7490(1)	0.24673(7)	0.11644(7)
C2a	-0.0220(1)	0.62228(8)	0.85010(6)
C4a	-0.1209(1)	0.70573(8)	1.01647(7)
C5a	-0.1774(1)	0.81711(8)	0.96981(8)
C6a	-0.1533(1)	0.82454(9)	0.86440(8)
C2b	0.4088(1)	0.44247(8)	0.86373(7)
C4b	0.4067(1)	0.34932(8)	1.02977(7)
C5b	0.4790(1)	0.23954(8)	0.98191(8)
C6b	0.5136(1)	0.23794(8)	0.87683(8)
C2c	0.8097(2)	0.3226(1)	0.84908(8)
C4c	0.7909(1)	0.23413(8)	1.01560(7)
C5c	0.8547(1)	0.12133(9)	0.9724(1)
C6c	0.8968(2)	0.1156(1)	0.8685(1)
O1w	0.58750(8)	0.33784(6)	0.61038(5)
O2w	0.88345(9)	0.19867(7)	0.57141(8)
O3w	-0.13508(8)	0.48724(6)	0.58692(6)
O4w	-0.05148(8)	0.72711(6)	0.59767(6)
O5w	0.28767(8)	0.58816(6)	0.61736(5)

Table S-7

	U₁₁	U₂₂	U₃₃	U₁₂	U₁₃	U₂₃
V1	0.00344(1)	0.001239(5)	0.001335(5)	-0.00045(1)	-0.00024(1)	-0.000033(8)
V2	0.00377(1)	0.001209(5)	0.001415(5)	-0.00094(1)	-0.00030(1)	0.000384(8)
V3	0.00326(1)	0.002325(7)	0.001736(5)	-0.00193(1)	0.00012(1)	0.000269(9)
V4	0.00294(1)	0.001366(5)	0.001263(5)	-0.00111(1)	-0.00103(1)	0.000192(8)
V5	0.00473(1)	0.002033(6)	0.001080(4)	-0.00170(1)	-0.00076(1)	0.000262(8)
O10	0.00827(8)	0.00294(4)	0.00120(2)	-0.00227(8)	-0.00201(7)	0.00036(5)
O11	0.00420(6)	0.00363(4)	0.00330(4)	-0.00352(8)	0.00067(7)	0.00012(6)
O12	0.00530(6)	0.00130(3)	0.00274(3)	-0.00044(6)	-0.00050(7)	0.00051(5)
O13	0.00562(6)	0.00131(3)	0.00255(3)	0.00023(6)	-0.00052(7)	-0.00032(4)
O20	0.00319(5)	0.00208(3)	0.00208(3)	-0.00104(6)	-0.00027(5)	0.00024(4)
O21	0.00334(5)	0.00237(3)	0.00196(2)	-0.00228(6)	-0.00105(5)	0.00022(4)
O22	0.00445(5)	0.00219(3)	0.00147(2)	-0.00168(6)	0.00045(5)	0.00037(4)
O23	0.00497(5)	0.00170(3)	0.00122(2)	-0.00094(6)	-0.00069(5)	-0.00025(4)
O24	0.00480(5)	0.00170(3)	0.00133(2)	-0.00095(6)	-0.00113(5)	0.00055(4)
O25	0.00393(5)	0.00166(3)	0.00210(2)	-0.00189(6)	-0.00029(5)	0.00031(4)
O27	0.00445(5)	0.00233(3)	0.00139(2)	-0.00167(6)	-0.00174(5)	0.00016(4)
O31	0.00312(4)	0.00137(2)	0.00144(2)	-0.00068(5)	-0.00087(5)	0.00028(3)
O32	0.00349(5)	0.00135(2)	0.00142(2)	-0.00124(5)	-0.00100(5)	0.00006(3)
O61	0.00313(4)	0.00142(2)	0.00122(2)	-0.00104(5)	-0.00063(5)	0.00020(3)
O2a	0.00808(8)	0.00403(4)	0.00175(3)	-0.0011(1)	0.00042(8)	-0.00094(6)
O2b	0.0120(1)	0.00289(4)	0.00201(3)	-0.0032(1)	-0.00256(9)	0.00100(6)
O2c	0.0211(2)	0.00634(7)	0.00214(4)	-0.0131(2)	0.0004(1)	0.00127(9)
N1a	0.00761(9)	0.00393(5)	0.00200(3)	-0.0026(1)	-0.00062(9)	0.00051(7)
N3a	0.00566(7)	0.00361(4)	0.00163(3)	-0.00091(9)	-0.00001(7)	-0.00075(6)
N4a	0.00771(9)	0.00369(5)	0.00189(3)	0.0004(1)	0.00034(8)	-0.00106(6)
N1b	0.00795(9)	0.00289(4)	0.00243(4)	-0.0032(1)	-0.00145(9)	-0.00022(6)
N3b	0.00756(9)	0.00279(4)	0.00199(3)	-0.00332(9)	-0.00226(8)	0.00108(6)
N4b	0.0091(1)	0.00355(5)	0.00219(3)	-0.0038(1)	-0.0029(1)	0.00184(7)
N1c	0.0269(3)	0.0063(1)	0.00335(6)	-0.0131(3)	0.0097(2)	-0.0042(1)
N3c	0.00737(9)	0.00349(5)	0.00185(3)	-0.0047(1)	0.00003(8)	0.00025(6)
N4c	0.0095(1)	0.00289(4)	0.00227(3)	-0.0031(1)	-0.0010(1)	0.00128(6)
C2a	0.00516(8)	0.00371(5)	0.00173(3)	-0.0020(1)	0.00013(8)	-0.00072(6)
C4a	0.00533(8)	0.00331(5)	0.00202(3)	-0.0013(1)	-0.00019(8)	-0.00050(7)
C5a	0.0071(1)	0.00306(5)	0.00293(5)	-0.0013(1)	-0.0000(1)	-0.00021(8)
C6a	0.0081(1)	0.00338(5)	0.00298(5)	-0.00240(1)	-0.0007(1)	0.00091(8)
C2b	0.0074(1)	0.00263(4)	0.00213(4)	-0.0034(1)	-0.00236(9)	0.00095(6)
C4b	0.00653(9)	0.00292(4)	0.00231(4)	-0.0036(1)	-0.00268(9)	0.00130(7)
C5b	0.0068(1)	0.00264(4)	0.00336(5)	-0.0030(1)	-0.0031(1)	0.00135(7)
C6b	0.0073(1)	0.00265(4)	0.00336(5)	-0.0028(1)	-0.0023(1)	-0.00014(8)
C2c	0.0144(2)	0.00497(7)	0.00200(4)	-0.0096(2)	0.0013(1)	-0.00003(9)
C4c	0.00522(8)	0.00276(4)	0.00282(4)	-0.0019(1)	-0.00011(9)	-0.00027(7)
C5c	0.0081(1)	0.00290(5)	0.00469(7)	-0.0015(1)	0.0017(1)	-0.0015(1)
C6c	0.0174(2)	0.00462(8)	0.00548(9)	-0.0063(2)	0.0094(2)	-0.0051(1)
O1w	0.00670(7)	0.00301(4)	0.00262(3)	-0.00396(8)	-0.00121(8)	-0.00083(5)
O2w	0.00543(7)	0.00317(4)	0.00571(6)	-0.00255(9)	-0.0034(1)	-0.00048(8)
O3w	0.00529(7)	0.00371(4)	0.00254(3)	-0.00143(8)	-0.00033(7)	0.00055(6)
O4w	0.00495(6)	0.00391(4)	0.00251(3)	-0.00119(8)	-0.00232(7)	0.00136(6)
O5w	0.00602(7)	0.00317(4)	0.00241(3)	-0.00376(8)	-0.00160(7)	0.00051(5)

Table S-8.

Cytosine	O2	N1	N3	N4	C2	C4	C5	C6
A	0.0271(2)	0.0263(2)	0.0222(2)	0.0276(2)	0.0214(2)	0.0219(2)	0.0270(3)	0.0287(3)
B	0.0307(3)	0.0251(2)	0.0223(2)	0.0273(2)	0.0223(3)	0.0216(2)	0.0250(2)	0.0257(3)
C	0.0498(5)	<i>0.0646(2)</i>	0.0233(2)	0.0275(3)	0.0363(4)	0.0222(2)	0.0334(3)	<i>0.0531(6)</i>

Table S-9.

Vanadium atoms	Type of vanadium atoms	Type of oxygen atoms	bond	distance
V1	III	f	V1-O13	1.6189(6)
		c	V1-O23	1.8132(6)
		c	V1-O20	1.8338(6)
		b	V1-O32	1.9981(6)
		b	V1-O31	2.0205(5)
		a	V1-O61	2.2679(6)
V2	III	f	V2-O12	1.6230(6)
		c	V2-O24	1.8141(6)
		c	V2-O25	1.8240(6)
		b	V2-O31	2.0040(5)
		b	V2-O32	2.0268(6)
		a	V2-O61	2.2414(5)
V3	II	g	V3-O11	1.6115(6)
		c	V3-O20	1.8504(6)
		c	V3-O25	1.8716(5)
		d	V3-O22	1.8871(6)
		e	V3-O21	2.0183(6)
		a	V3-O61	2.3324(5)
V4	I	e	V4-O27	1.6848(5)
		e	V4-O21	1.7059(6)
		b	V4-O31	1.9217(5)
		b	V4-O32	1.9427(5)
		a	V4-O61	2.0781(5)
		a	V4-O61	2.1583(5)
V5	II	g	V5-O10	1.6120(6)
		d	V5-O22	1.8795(6)
		c	V5-O23	1.8795(5)
		c	V5-O24	1.8911(5)
		e	V5-O27	2.0697(6)
		a	V5-O61	2.2937(5)

Table S-10.

bond	Cytosinium A	Cytosinium B	Cytosine C
C4-N4	1.325(1)	1.322(1)	1.317(1)
C4-C5	1.430(1)	1.428(1)	1.427(11)
C5-C6	1.360(1)	1.359(1)	1.351(2)
C6-N1	1.357(1)	1.358(1)	1.385(2)
N1-C2	1.372(1)	1.363(1)	1.362(2)
C2-N3	1.372(1)	1.365(1)	1.357(1)
N3-C4	1.351(1)	1.354(1)	1.351(1)
C2-O2	1.242(1)	1.240(1)	1.254(2)

Table S-11.

bond	Experimental data	Literature data, CSD	
		Average data	<min, max>
	Cytosinium B		
C4-N4	1.322(1)	1.312	1.296-1.327
C4-C5	1.428(1)	1.417	1.387-1.430
C5-C6	1.359(1)	1.343	1.329-1.354
C6-N1	1.358(1)	1.357	1.344-1.372
N1-C2	1.363(1)	1.365	1.336-1.381
C2-N3	1.365(1)	1.376	1.360-1.394
N3-C4	1.354(1)	1.354	1.341-1.362
C2-O2	1.240(1)	1.220	1.196-1.246

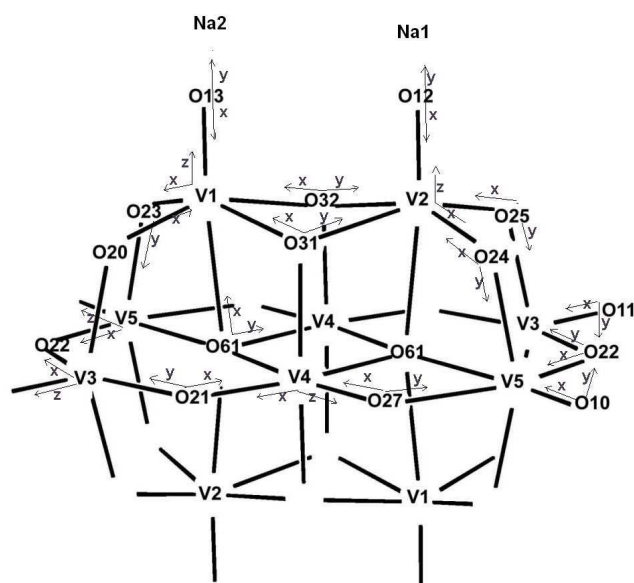
bond	Cytosine C	Average data	<min, max>
C4-N4	1.317(1)	1.329	1.320-1.342
C4-C5	1.427(11)	1.426	1.411-1.440
C5-C6	1.351(2)	1.340	1.332-1.353
C6-N1	1.385(2)	1.356	1.353-1.361
N1-C2	1.362(2)	1.372	1.365-1.382
C2-N3	1.357(1)	1.351	1.332-1.364
N3-C4	1.351(1)	1.345	1.337-1.353
C2-O2	1.254(2)	1.255	1.241-1.274

Table S-13.

angle	Experimental data	Experimental data	Literature data CSD	Literature data, CSD
	Cytosinium B	Cytosine C	cytosinium	cytosine
N1-C2-N3	117.78(8)	117.66(8)	114.95	119.40
C2-N3-C4	122.26(8)	122.01(9)	124.65	119.32
N3-C4-C5	119.16(9)	120.57(9)	117.86	121.80
C4-C5-C6	117.68(8)	116.9(1)	117.98	117.21
C5-C6-N1	121.09(9)	120.7(1)	121.79	120.55
C6-N1-C2	122.01(8)	121.9(1)	122.67	121.68
N1-C2-O2	120.49(8)	120.4(1)	123.42	118.85
N3-C2-O2	121.73(9)	121.8(1)	121.62	121.73
N3-C4-N4	118.71(8)	119.03(8)	118.84	117.76
N4-C4-C5	122.12(8)	120.40(9)	123.28	120.43

Table S-12.

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a)

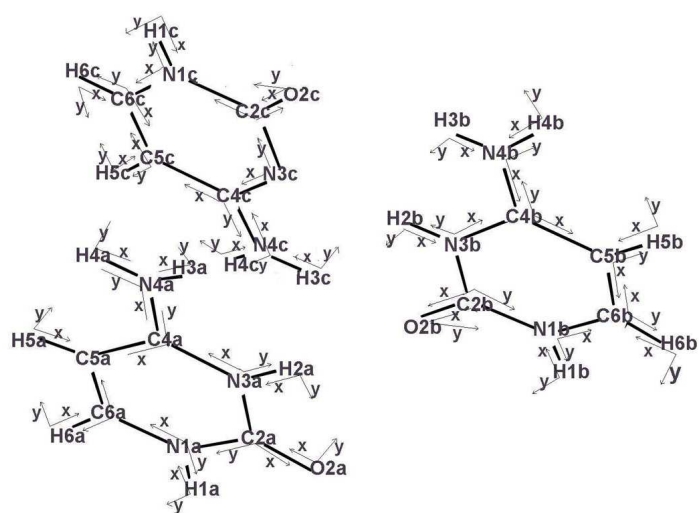
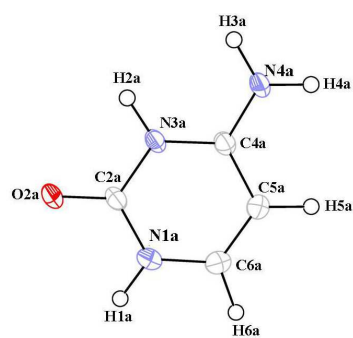
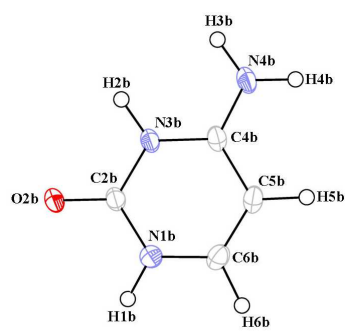


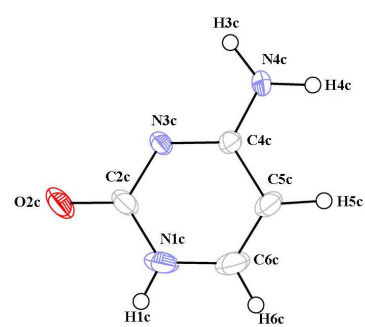
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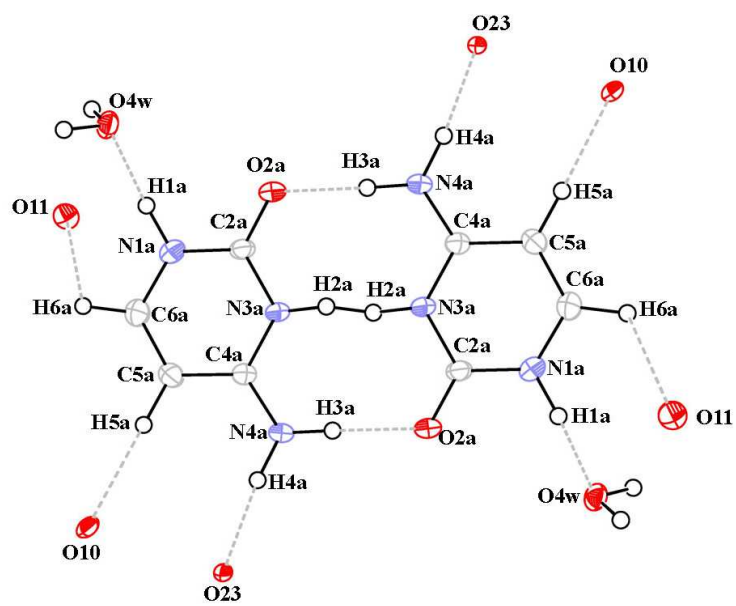


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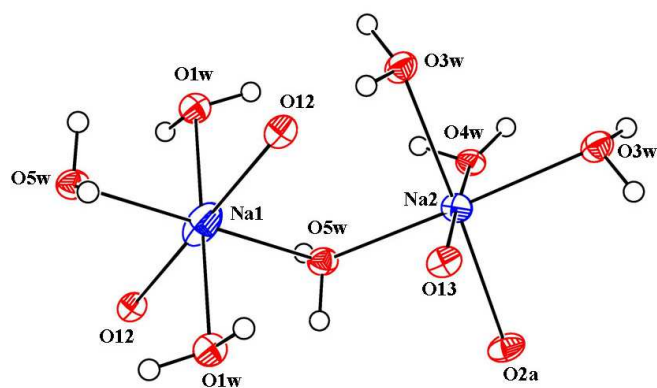


c)

Figure S-2.



a)



b)

Figure S-3.

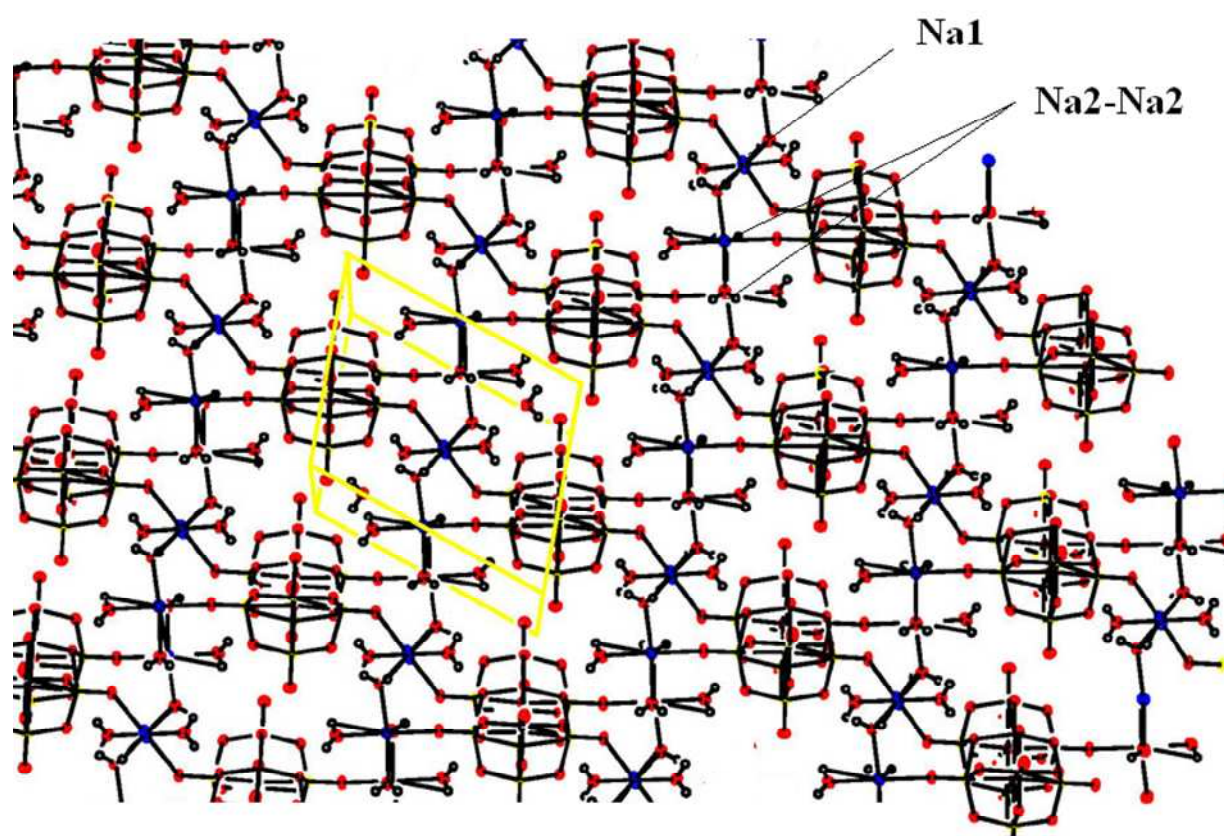


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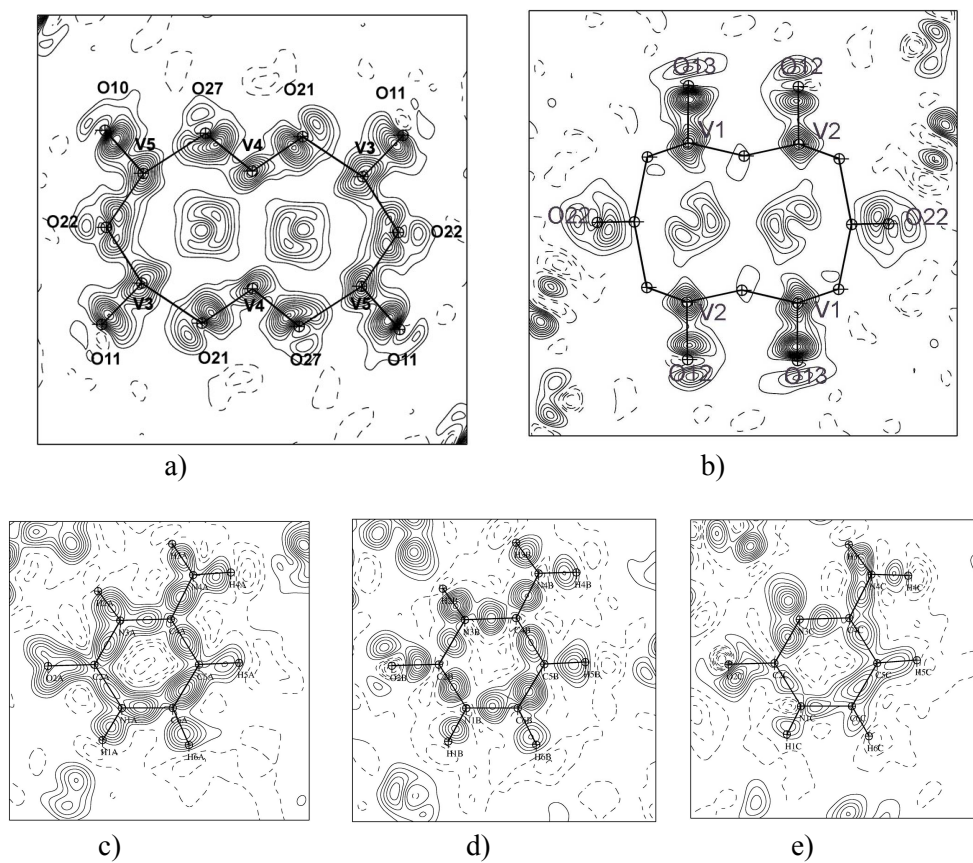


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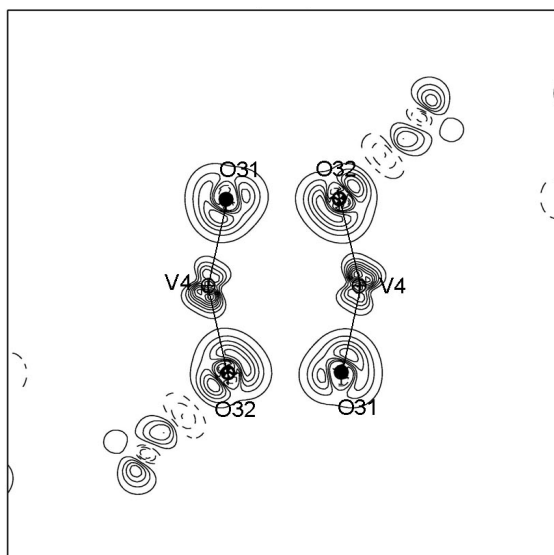


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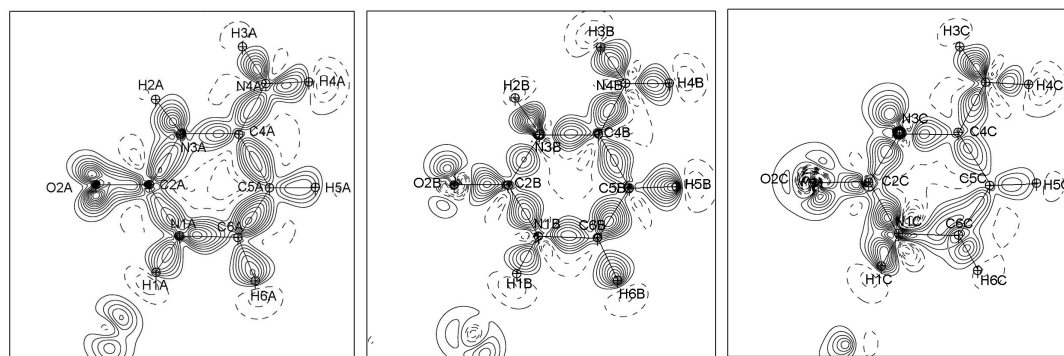
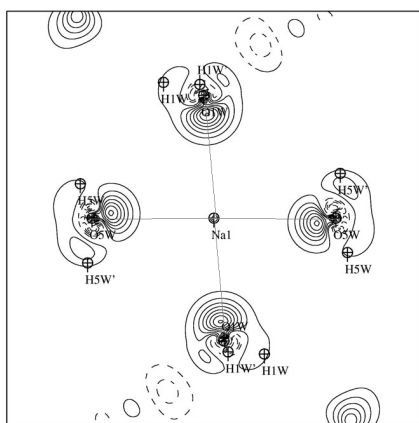
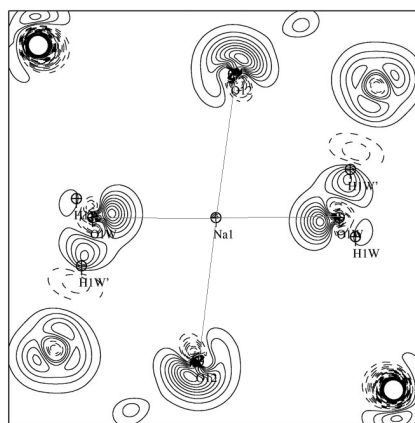


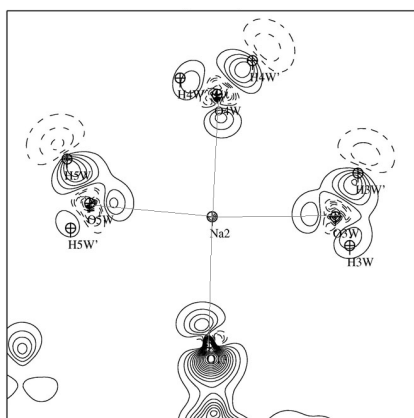
Figure S-8.



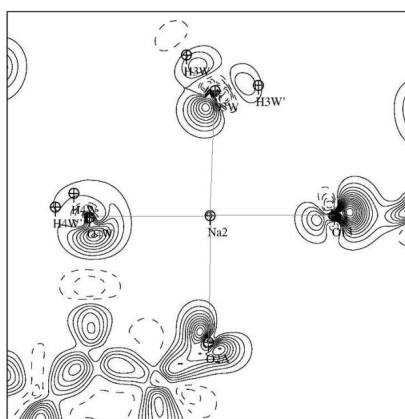
a)



b)



c)



d)

Figure S-9.

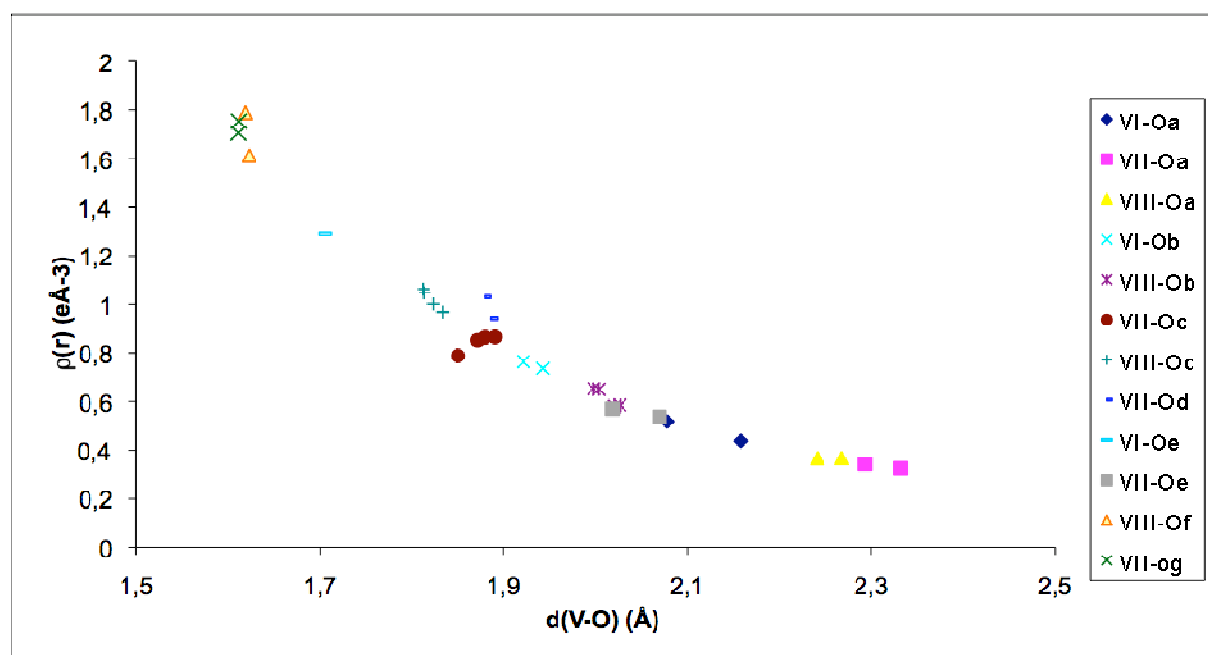


Figure S-10.