

SUPPORTING INFORMATION

1S: Table 1: Dissociation channels and its corresponding energies ΔE in eV for the most stable V_xO_y cluster models. The smallest fragments have the following ground electronic states: $VO^+(^3\Sigma)$, $VO_2^+(^1A_1)$, $VO_3^+(^1A_1)$, $VO(^4\Sigma)$, $VO_2(^2A_1)$, $VO_3(^2A_1)$, $O_2(^3\Sigma_g^-)$, $O(^3P)$, $V(^5D)$ and $V(^4F)$.

2S: Vibrational frequency values (cm^{-1}) and the corresponding intensities in parentheses for $V_2O_y^+$ and V_2O_y clusters ($y=2-7$).

3S: Vibrational frequency values (cm^{-1}) and the corresponding intensities in parentheses for $V_{3-4}O_y^+$ and $V_{3-4}O_y$ clusters ($y=6-10$).

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Compound	Dissociation channel	ΔE
$V_2O_2^+$ Model A ($^4A'$) Model B ($^2A'$) Model C (4A)	$VO_2 + V^+$	4.38
	$VO^+ + VO$	3.35
	$VO_2 + V^+$	5.42
	$VO^+ + VO$	4.39
	$VO_2 + V^+$	-2.30
	$VO^+ + VO$	-3.33
V_2O_2 Model B (3A_1) Model C (3A)	$VO_2 + V$	3.80
	$2 VO$	-2.48
	$VO_2 + V$	2.49
	$2 VO$	-3.78
$V_2O_3^+$ Model A (4A_2) Model B ($^2A'$)	$V_2O_2^+ + O$	4.87
	$VO_2^+ + VO$	4.87
	$VO_2 + VO^+$	3.61
	$V_2O_2^+ + O$	6.12
	$VO_2^+ + VO$	6.11
	$VO_2 + VO^+$	4.86
V_2O_3 Model A (3B) Model B ($^3A'$)	$V_2O_2 + O$	6.34
	$VO_3 + V$	5.69
	$VO_2 + VO$	3.19
	$V_2O_2 + O$	7.40
	$VO_3 + V$	6.75
	$VO_2 + VO$	4.24
$V_2O_4^+$ Model A (2A) Model B ($^2A'$) Model C (2B_2)	$V_2O_3^+ + O$	6.78
	$V_2O_2 + O_2$	4.68
	$VO_2^+ + VO_2$	4.44
	$VO^+ + VO_3$	4.39
	$V_2O_3^+ + O$	8.07
	$V_2O_2^+ + O_2$	5.97
	$VO_2^+ + VO_2$	5.73
	$VO^+ + VO_3$	5.68
	$V_2O_3^+ + O$	6.32
	$V_2O_2 + O_2$	4.22
	$VO_2^+ + VO_2$	3.98
	$VO^+ + VO_3$	3.93
V_2O_4 Model A (3A) Model B (3B_2) Model C (3B_1)	$V_2O_3 + O$	7.83
	$V_2O_2 + O_2$	7.01
	$VO_2 + VO_2$	3.62
	$VO^+ + VO_3$	4.82
	$V_2O_3 + O$	9.69
	$V_2O_2 + O_2$	8.87
	$VO_2 + VO_2$	5.48
	$VO^+ + VO_3$	6.22
	$V_2O_3 + O$	8.89
	$V_2O_2 + O_2$	8.07
	$VO_2 + VO_2$	4.67
	$VO^+ + VO_3$	5.87

$V_2O_5^+$ Model A (2A)	$V_2O_4^+ + O$	2.15
	$V_2O_3^+ + O_2$	2.00
	$VO_2^+ + VO_3$	3.43
	$VO_2 + VO_3^+$	5.30
Model B ($^2A''$)	$V_2O_4^+ + O$	3.44
	$V_2O_3^+ + O_2$	3.29
	$VO_2^+ + VO_3$	4.72
	$VO_2 + VO_3^+$	6.59
V_2O_5 Model A (1A)	$V_2O_4 + O$	4.08
	$V_2O_3 + O_2$	5.55
	$VO_2 + VO_3$	5.11
Model B ($^1A'$)	$V_2O_4 + O$	5.05
	$V_2O_3 + O_2$	6.53
	$VO_2 + VO_3$	6.08
$V_2O_6^+$ Model A ($^2A''$)	$V_2O_5^+ + O$	1.40
	$V_2O_4^+ + O_2$	-0.57
	$VO_3^+ + VO_3$	3.54
	$VO_2^+ + VO_2 + O_2$	5.15
Model B (2A)	$V_2O_5^+ + O$	2.74
	$V_2O_4^+ + O_2$	0.77
	$VO_3^+ + VO_3$	4.88
	$VO_2^+ + VO_2 + O_2$	6.50
Model C (2A)	$V_2O_5^+ + O$	1.65
	$V_2O_4^+ + O_2$	-0.33
	$VO_3^+ + VO_3$	3.78
	$VO_2^+ + VO_2 + O_2$	5.40
V_2O_6 Model A (3A)	$V_2O_5 + O$	2.52
	$V_2O_4 + O_2$	0.95
	$2 VO_3$	2.94
	$2 VO_2 + O_2$	6.42
Model B (3A)	$V_2O_5 + O$	1.74
	$V_2O_4 + O_2$	1.39
	$2 VO_3$	3.38
	$2 VO_2 + O_2$	6.87
Model C (3A)	$V_2O_5 + O$	0.33
	$V_2O_4 + O_2$	-0.03
	$2 VO_3$	1.96
	$2 VO_2 + O_2$	5.45
$V_2O_7^+$ Model A ($^2A''$)	$V_2O_6^+ + O$	3.45
	$V_2O_5^+ + O_2$	0.78
	$V_2O_4^+ + O_2 + O$	4.22
	$VO_3^+ + VO_2 + O_2$	5.50
Model B (2A)	$V_2O_6^+ + O$	1.45
	$V_2O_5^+ + O_2$	-1.22
	$V_2O_4^+ + O_2 + O$	2.22
	$VO_3^+ + VO_2 + O_2$	3.50
V_2O_7 Model A ($^3A''$)	$V_2O_6 + O$	3.95
	$V_2O_5 + O_2$	1.06
	$V_2O_4 + O_2 + O$	6.11
	$VO_2 + VO + O_2$	0.43
Model B (3A)	$V_2O_6 + O$	0.67
	$V_2O_5 + O_2$	-2.22
	$V_2O_4 + O_2 + O$	2.83
	$VO_2 + VO + O_2$	0.31

$V_3O_6^+$ Model A ($^3A''$) Model B (3A) Model C (3A)	$V_2O_5 + VO^+$	4.21
	$V_2O_4^+ + VO_2$	3.55
	$VO_3 + VO_2 + VO^+$	10.30
	$VO_2^+ + 2 VO_2$	10.17
	$V_2O_5 + VO^+$	1.83
	$V_2O_4^+ + VO_2$	5.92
	$VO_3 + VO_2^+ + VO$	7.92
	$VO_2^+ + 2 VO_2$	7.97
	$V_2O_5 + VO^+$	3.51
	$V_2O_4^+ + VO_2$	4.25
	$VO_3 + VO_2^+ + VO$	9.59
	$VO_2^+ + 2 VO_2$	9.64
V_3O_6 Model A (4A) Model B (4A) Model C (4A)	$V_2O_5 + VO$	5.31
	$V_2O_4 + VO_2$	4.71
	$VO_3 + VO_2 + VO$	11.39
	$3VO_2$	10.19
	$V_2O_5 + VO$	1.90
	$V_2O_4 + VO_2$	1.31
	$VO_3 + VO_2 + VO$	7.98
	$3VO_2$	6.78
	$V_2O_5 + VO$	3.65
	$V_2O_4 + VO_2$	3.05
	$VO_3 + VO_2 + VO$	9.73
	$3 VO_2$	8.53
$V_3O_7^+$ Model A (1A) Model B ($^1A''$) Model C1 ($^1A''$) Model C2 ($^1A''$)	$V_3O_6^+ + O$	6.02
	$V_2O_5 + VO_2^+$	5.84
	$V_2O_4^+ + VO_3$	6.20
	$2VO_3 + VO^+$	11.87
	$V_3O_6^+ + O$	3.01
	$V_2O_5 + VO_2^+$	2.83
	$V_2O_4^+ + VO_3$	3.19
	$2VO_3 + VO^+$	8.86
	$V_3O_6^+ + O$	3.28
	$V_2O_5 + VO_2^+$	3.10
	$V_2O_4^+ + VO_3$	3.46
	$2VO_3 + VO^+$	9.13
	$V_3O_6^+ + O$	4.33
	$V_2O_5 + VO_2^+$	4.15
	$V_2O_4^+ + VO_3$	4.50
	$2VO_3 + VO^+$	10.18
V_3O_7 Model A ($^2A''$) Model B (2A) Model C1 (2A)	$V_3O_6 + O$	6.73
	$V_2O_5 + VO_2$	6.38
	$V_2O_4 + VO_3$	6.99
	$VO_3 + 2VO$	12.47
	$V_3O_6 + O$	3.03
	$V_2O_5 + VO_2$	2.68
	$V_2O_4 + VO_3$	3.29
	$VO_3 + 2VO$	8.77
	$V_3O_6 + O$	3.96
	$V_2O_5 + VO_2$	3.62
	$V_2O_4 + VO_3$	4.23
	$VO_3 + 2VO$	9.70

Model C2 ($^2A'$)	$V_3O_6 + O$	4.54
	$V_2O_5 + VO_2$	4.19
	$V_2O_4 + VO_3$	4.80
	$VO_3 + 2VO$	10.28
V_4O_{10} (1T_2)	$V_3O_7 + VO_3$	6.86
	$V_3O_6 + VO_2 + O_2$	12.62
	$2 V_2O_5$	7.16
	$2 V_2O_4 + O_2$	11.86

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Compound	Frequencies/cm ⁻¹
V ₂ O ₂ ⁺ Model A (⁴ A)	62(3.1), 117(10.8), 198(3.8), 385(4.2), 890(100), 1131(21.9)
V ₂ O ₂ ⁺ Model B (² A)	194(29.3), 313(0.5), 412(1.1), 590(100), 762(66.6), 876(76.9)
(⁴ B ₂)	221(41.2), 343(0.0), 393(0.3), 494(78.4), 734(100), 817(25.1)
V ₂ O ₂ ⁺ Model C (² A)	78(1.57), 129(3.23), 422(5.26), 518(11.91), 759(1.39), 1146(100)
(⁴ A)	90(17.34), 133(0.40), 462(0.55), 489(34.05), 770(1.27), 1208(100)
V ₂ O ₂ Model B (¹ B _{1u})	226(0.56), 281(0.00), 422(4.86), 648(0.00), 861(100), 876(0.05)
(¹ A _g)	141(18.36), 460(29.51), 466(0.00), 534(0.00), 694(100), 779(0.00)
(³ A ₁)	105(13.16), 216(6.50), 328(4.08), 478(38.54), 864(100), 895(61.40)
V ₂ O ₂ Model C (² A)	62(0.64), 182(2.86), 541(6.55), 594(9.10), 795(47.28), 902(100)
(⁴ A)	108(2.48), 133(1.69), 286(8.97), 522(7.03), 704(2.20), 927(100)
V ₂ O ₃ ⁺ Model A (² A)	31(7.11), 55(5.89), 118(32.22), 210(29.14), 287(4.92), 403(9.64), 838(32.45), 1127(100), 1145(79.19)
(⁴ A ₂)	46(0.00), 65(1.23), 170(23.83), 178(29.57), 292(2.77), 381(100), 453(4.38), 1122(50.42), 1146(42.34)
V ₂ O ₃ ⁺ Model B (² A)	128(5.35), 236(1.26), 273(18.24), 372(0.53), 391(0.00), 659(100), 765(52.36), 856(46.86), 1159(55.66)
(⁴ A ^{''})	138(5.14), 207(0.45), 295(20.58), 343(0.38), 364(1.22), 659(100), 750(58.20), 858(53.05), 1156(58.20)
V ₂ O ₃ Model A (³ B)	98(5.38), 109(0.62), 185(6.39), 299(3.51), 320(1.52), 557(22.44), 769(25.93), 1078(100), 1093(7.88)
V ₂ O ₃ Model B (¹ A)	186(10.68), 241(3.02), 283(16.07), 311(4.40), 437(0.21), 464(12.22), 826(100), 840(19.06), 1087(96.15)
(³ A)	90(1.38), 233(6.73), 250(0.59), 284(0.93), 462(0.11), 610(100), 732(3.92), 760(34.39), 1087(66.36)
V ₂ O ₄ ⁺ Model A (² A)	33(1.38), 58(3.46), 88(11.11), 165(1.22), 259(32.51), 285(9.22), 360(0.72), 458(1.10), 959(100), 1120(25.31), 1127(10.65), 1155(15.50)
(⁴ A)	35(15.56), 58(4.84), 87(12.89), 177(0.67), 200(37.33), 206(19.56), 311(18.67), 359(29.33), 584(95.55), 677(13.33), 1093(93.78), 1149(100)
V ₂ O ₄ ⁺ Model B (² A)	103(0.40), 198(16.72), 224(0.56), 325(0.00), 357(1.56), 371(12.96), 441(0.59), 660(100), 802(57.63), 878(60.37), 1141(68.34), 1171(47.78)
(⁴ A ^{''})	81(0.51), 178(0.00), 193(7.34), 250(2.26), 266(0.89), 336(5.81), 410(0.30), 526(0.00), 674(3.01), 680(100), 1142(21.55), 1159(32.54)
V ₂ O ₄ ⁺ Model C (² B ₂)	53(6.01), 156(39.09), 175(4.78), 201(0.00), 208(2.25), 314(5.09), 330(9.77), 419(0.00), 483(3.46), 756(100), 785(18.05), 952
(⁴ A)	106(0.80), 165(1.36), 204(1.12), 221(0.49), 272(12.17), 394(0.26), 395(0.00), 532(0.23), 689(100), 755(45.39), 847(43.09), 1018(49.67)
V ₂ O ₄ Model A (³ A)	34(1.81), 39(0.13), 54(3.62), 165(0.54), 197(9.05), 297(0.71), 355(0.27), 479(4.52), 879(100), 1074(35.75), 1096(2.12), 1101(34.48)
V ₂ O ₄ Model B (¹ A ₁)	121(0.00), 209(15.35), 238(0.00), 315(1.95), 361(7.55), 434(2.40), 490(0.65), 493(39.00), 806(6.64), 826(76.35), 1091(100), 1130(86.31)
(³ A)	94(0.31), 156(4.43), 244(0.45), 245(0.00), 310(5.74), 372(3.44), 501(0.00), 702(100), 746(24.92), 759(0.00), 1091(81.31), 1122(19.06)
V ₂ O ₄ Model C (¹ A ₁)	122(3.96), 198(0.83), 202(6.15), 257(12.70), 296(1.58), 416(2.61), 449(0.0), 601(54.76), 863(81.35), 936(100), 1088(72.62), 1100(87.30)
(³ B ₁)	110(2.46), 202(0.42), 210(6.36), 277(9.74), 293(0.59), 393(3.35), 437(1.25), 581(88.98), 823(76.27), 907(96.12), 1087(66.95), 1099(100)
V ₂ O ₅ ⁺ Model A (² A)	29(1.02), 56(0.61), 61(1.63), 162(0.71), 184(7.93), 221(1.59), 294(5.99), 319(3.53), 369(4.04), 461(3.19), 559(0.86), 945(100), 1019(6.17), 1122(31.39), 1135(7.23)
(⁴ A)	25(4.34), 55(2.19), 64(14.64), 130(2.68), 170(12.31), 207(9.42),

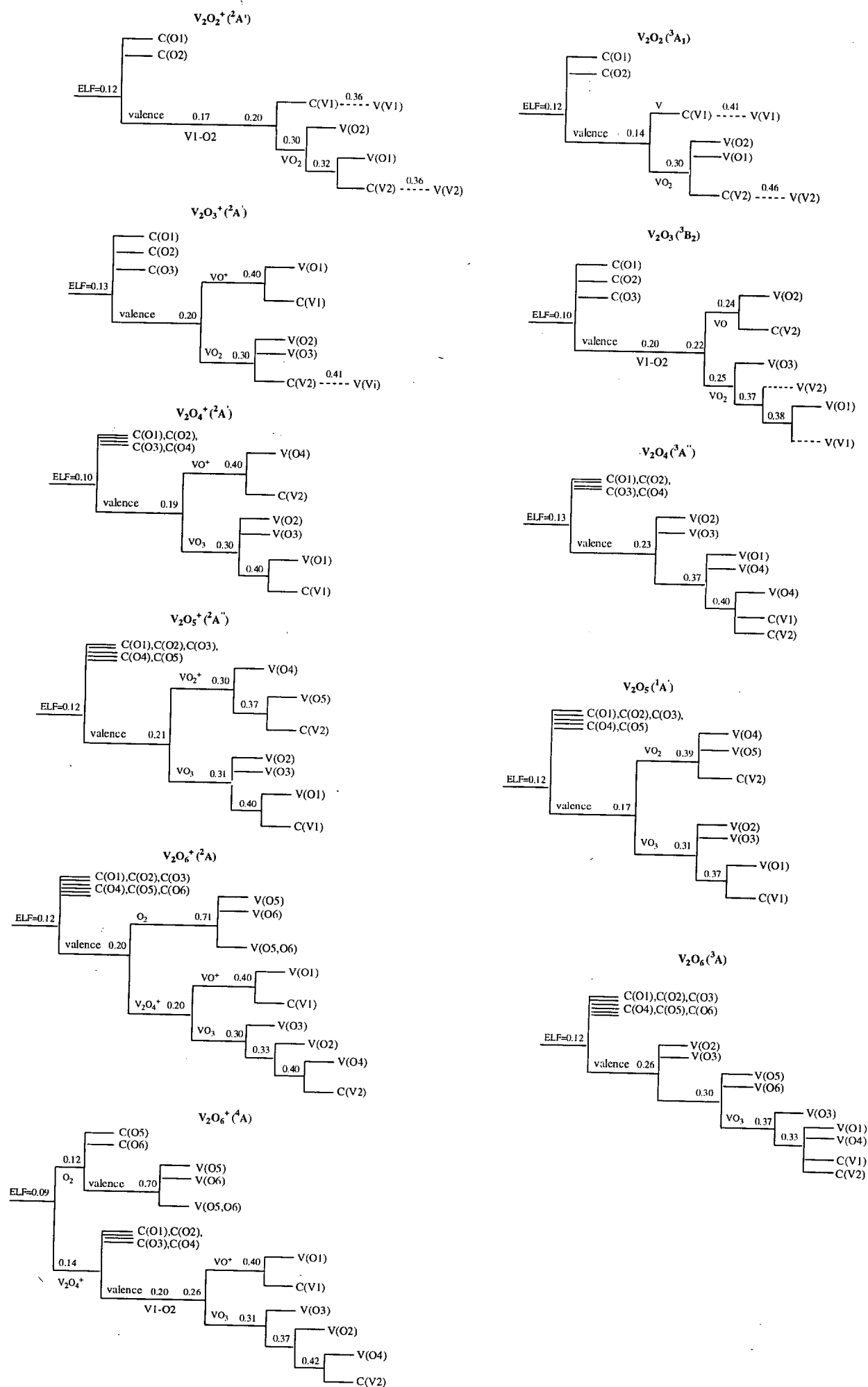
	219(12.32), 277(31.88), 325(6.52), 363(9.56), 546(21.01), 676(46.29), 827(9.78), 1025(100), 1108(93.47)
$V_2O_5^+$ Model B ($^2A''$)	97(1.37), 160(0.85), 186(4.11), 205(2.39), 219(1.03), 333(0.00), 362(5.48), 427(0.40), 468(0.55), 626(0.07), 701(100), 787(43.84), 881(69.86), 1040(51.37), 1158(46.92),
(4A)	77(0.80), 130(5.60), 152(0.66), 171(0.20), 188(3.45), 242(0.20), 262(2.40), 308(12.40), 396(0.78), 513(0.11), 588(9.48), 642(100), 695(54.8), 954(16.00), 1149(44.00)
V_2O_5 Model A (1A)	41(0.07), 46(1.02), 46(0.92), 134(8.81), 139(3.73), 260(3.27), 284(3.84), 322(0.45), 382(0.75), 495(0.34), 943(100), 1082(37.51), 1105(0.05), 1112(27.00), 1113(30.85)
(3A)	33(0.42), 40(0.53), 48(0.74), 96(2.33), 125(3.70), 185(4.24), 271(2.65), 281(1.38), 335(0.26), 463(0.95), 665(3.60), 928(100), 1069(21.82), 1099(11.86), 1112(25.42)
V_2O_5 Model B (1A)	85(2.38), 175(5.10), 190(4.07), 196(3.73), 280(0.47), 331(0.57), 363(9.83), 400(2.60), 433(1.09), 582(54.24), 878(55.93), 932(61.02), 1088(100), 1104(57.29), 1120(50.85)
(3A)	86(1.20), 177(2.26), 192(1.90), 208(1.34), 210(0.96), 298(0.08), 333(4.64), 378(1.56), 504(0.11), 599(0.08), 717(100), 758(28.29), 780(6.38), 1000(57.00), 1119(44.52)
$V_2O_6^+$ Model A ($^2A''$)	66(1.18), 116(0.39), 119(1.84), 161(3.11), 171(0.79), 194(0.08), 212(0.02), 262(0.09), 319(7.93), 378(0.52), 424(0.05), 520(11.33), 594(0.07), 667(100), 745(10.79), 781(28.24), 841(25.78), 1036(43.91)
(4B_1)	58(0.51), 112(11.12), 131(0.00), 132(0.14), 143(0.01), 168(0.00), 221(0.02), 246(0.64), 253(0.46), 302(4.58), 360(4.76), 492(0.00), 549(20.74), 630(0.51), 643(100), 671(0.79), 926(5.27), 930(0.31)
$V_2O_6^+$ Model B (2A)	59(1.08), 65(0.63), 117(0.40), 147(5.78), 190(1.15), 243(13.93), 243(0.17), 289(10.17), 324(0.09), 375(4.95), 417(7.93), 444(1.01), 661(61.20), 796(22.07), 883(31.03), 1144(37.07), 1171(27.76), 1331(100)
(4A)	48(0.78), 62(2.31), 93(0.20), 130(0.68), 155(0.50), 199(10.78), 243(1.04), 278(7.17), 327(0.05), 365(6.08), 374(13.68), 443(3.05), 636(100), 817(60.00), 885(60.78), 1137(74.51), 1166(51.37), 1628(6.78)
$V_2O_6^+$ Model C (2A)	25(2.77), 38(0.14), 50(0.40), 90(0.20), 107(1.12), 157(1.57), 202(5.59), 248(0.74), 283(2.92), 311(2.29), 323(13.31), 377(3.51), 477(5.27), 926(100), 1122(20.40), 1128(4.67), 1159(16.67), 1378(58.00)
(4A)	26(8.94), 37(0.10), 50(0.38), 65(0.10), 94(1.61), 126(0.37), 178(6.31), 190(2.94), 265(1.59), 282(4.96), 334(5.87), 375(1.72), 482(3.55), 922(100), 1121(24.93), 1123(12.04), 1150(19.53), 1619(2.69)
V_2O_6 Model A ($^1B_{2g}$)	90(5.41), 149(0.00), 175(0.00), 176(65.20), 214(0.00), 223(11.24), 249(0.00), 264(0.00), 331(21.90), 395(0.00), 439(7.02), 497(0.00), 628(100), 717(0.00), 773(0.06), 785(49.24), 904(9.62), 977(0.00)
(3A)	90(0.21), 157(0.61), 185(0.01), 196(3.42), 202(0.34), 234(0.67), 237(0.09), 303(0.00), 341(1.51), 392(0.00), 483(0.01), 563(0.25), 638(5.73), 747(24.77), 760(100), 793(11.79), 996(50.46), 1086(22.36)
V_2O_6 Model B (1A)	60(20.00), 90(30.13), 140(0.33), 183(0.13), 187(3.25), 260(5.67), 291(0.72), 327(19.97), 332(0.18), 405(4.48), 419(3.20), 538(39.34), 680(8.01), 862(54.06), 890(10.06), 1105(85.72), 1136(69.73), 1261(100)
(3A)	9(0.13), 75(0.71), 136(1.23), 153(2.31), 179(1.91), 245(1.41), 261(0.07), 290(0.36), 346(2.14), 386(2.57), 494(0.33), 604(11.65), 715(100), 756(26.26), 792(21.56), 1111(57.74), 1139(31.30), 1165(0.84)
V_2O_6 Model C (1A)	27(1.97), 42(0.74), 48(0.94), 81(2.63), 111(1.27), 161(4.30), 242(1.54), 271(0.84), 282(3.20), 301(0.92), 369(1.48), 486(0.25), 718(3.67), 929(100), 1093(21.35), 1112(22.67), 1141(18.81), 1275(14.30)
(3A)	24(0.71), 33(0.37), 41(0.03), 62(0.30), 79(1.07), 127(4.28),

	194(2.98), 228(0.23), 278(1.06), 295(2.12), 327(0.41), 446(1.17), 587(5.44), 926(100), 1092(18.29), 1113(22.60), 1129(17.70), 1318(0.16)
$V_2O_7^+$ Model A (2A)	34(0.00), 45(0.24), 86(0.85), 105(0.33), 162(0.14), 172(0.79), 189(3.32), 202(1.60), 215(0.01), 273(1.84), 324(0.00), 363(4.83), 451(7.02), 473(0.57), 635(0.23), 709 (100), 783(36.25), 869(64.95), 1041(49.55), 1153(41.24), 1630(6.25)
(4A)	39(0.04), 46(0.24), 87(0.79), 105(0.37), 163(0.15), 173(0.54), 189(3.58), 201(1.60), 214(0.00), 273(1.82), 322(0.00), 361(4.85), 450(6.88), 472(0.63), 625(0.03), 708(100), 781(36.36), 868(65.45), 1039(49.39), 1152(40.61), 1631(6.06)
$V_2O_7^+$ Model B (2A)	12(1.12), 35(0.10), 46(0.36), 81(0.27), 88(1.77), 114(1.76), 150(0.73), 187(1.51), 230(0.81), 257(0.84), 277(2.58), 311(2.99), 315(13.55), 383(7.15), 516(0.27), 607(10.41), 821(29.71), 1151(30.78), 1162(32.62), 1228(12.40), 1382(100)
(4A)	17(0.03), 24(0.21), 34(0.17), 70(0.17), 93(0.81), 108(2.54), 150(1.10), 212(1.15), 229(0.62), 239(2.85), 270(2.23), 306(10.11), 316(5.21), 375(8.82), 511(0.38), 604(10.93), 918(100), 1153(20.87), 1163(15.77), 1227(9.56), 1362(81.24)
V_2O_7 Model A (1A)	126(0.00), 143(0.21), 181(2.28), 184(2.43), 200(0.07), 238(0.26), 248(0.11), 266(0.66), 326(0.36), 413(0.03), 417(1.12), 484(0.63), 586(6.08), 648(7.84), 666(20.28), 717(45.33), 793(23.26), 810(6.26), 935(7.55), 1129(100), 1158(12.60)
(3A)	74(0.19), 76(1.03), 124(0.10), 165(0.11), 201(0.57), 216(0.03), 220(1.77), 240(0.39), 306(0.00), 341 (0.98), 377(0.40), 453(0.18), 478(0.50), 540(0.43), 586(4.77), 736(21.15), 757(100), 791(4.26), 988(43.77), 1141(27.87), 1229(8.03)
V_2O_7 Model B (1A)	17(1.24), 29(0.44), 37(0.31), 77(1.62), 123(0.33), 164(1.18), 210(0.53), 223(0.41), 255(2.37), 277(2.20), 282(0.55), 328(0.45), 451(0.35), 651(1.09), 688(1.70), 721(3.22), 936(100), 969(16.17), 1131(18.21), 1143(15.23), 1287(12.17)
(3A)	17(0.26), 25(0.08), 30(0.34), 64(0.03), 72(0.80), 149(0.83), 183(0.53), 214(0.14), 227(0.89), 256(1.48), 274(0.93), 299(1.17), 399(0.61), 581(4.90), 658(1.01), 689(1.58), 932(100), 970(11.92), 1125(16.82), 1134(15.03), 1318(0.17)

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Compound	Frequencies/cm ⁻¹
V ₃ O ₆ ⁺ Model A (¹ A ₁)	76(0.23), 81(0.32), 96(0.61), 194(8.21), 195(9.18), 204(20.77), 205(21.73), 276(0.00), 318(6.28), 337(6.76), 352(4.59), 354(4.64), 622(0.00), 678(17.68), 679(17.87), 696(19.81), 792(75.36), 794(75.36), 1150(50.57), 1150(50.77), 1174(100)
(³ A ₁)	37(0.14), 44(0.12), 54(0.09), 143(4.79), 181(0.38), 184(1.875), 189(7.08), 235(0.21), 265(2.08), 280(1.32), 337(0.20), 349(5.28), 483(4.00), 486(0.40), 564(9.85), 737(1.67), 898(35.21), 902(100), 1139(11.98), 1141(18.12), 1160(19.53)
V ₃ O ₆ ⁺ Model B (¹ A)	14(0.17), 23(0.44), 27(0.16), 52(0.19), 59(0.66), 83(1.15), 116(1.75), 223(2.71), 259(0.22), 273(2.20), 276(5.89), 331(0.31), 386(1.63), 452(0.38), 506(2.49), 888(100), 976(4.02), 1117(3.08), 1121(16.61), 1122(3.81), 1125(2.28)
(³ A)	11(0.30), 14(0.26), 20(0.09), 55(0.11), 59(0.37), 81(1.00), 105(1.32), 222(1.85), 253(3.62), 261(1.72), 276(1.80), 315(1.89), 377(1.65), 446(0.15), 494(1.89), 887(100), 973(6.76), 1118(4.92), 1121(11.86), 1124(2.98), 1125(1.80)
V ₃ O ₆ ⁺ Model C (¹ A)	23(0.54), 30(0.21), 44(1.20), 104(0.01), 151(2.91), 204(1.24), 249(3.38), 270(3.60), 303(2.81), 345(2.64), 382(0.99), 435(2.18), 466(0.34), 472(7.82), 517(6.06), 856(2.76), 867(16.11), 949(100), 1123(18.87), 1130(5.52), 1154(23.13)
(³ A)	20(0.22), 31(0.40), 51(0.98), 87(0.09), 148(2.49), 162(1.21), 224(0.17), 245(5.64), 264(1.69), 313(1.49), 348(2.68), 391(4.41), 432(0.19), 479(4.36), 657(36.09), 788 (12.87), 861(25.78), 943(100), 1123(16.89), 1128(5.04), 1158(15.20)
V ₃ O ₆ Model A (² A)	55(2.05), 112(0.47), 115(0.41), 166(0.15), 182(0.97), 189(2.41), 201 (3.95), 225(0.01), 293(7.60), 302(1.25), 333(0.05), 344(0.80), 583(1.48), 619(1.37), 687(0.23), 705(20.05), 776(16.15), 851(100), 1107(77.95), 1109(27.08), 1136(25.00)
(⁴ A)	40(1.03), 45(0.56), 58(1.15), 140(2.51), 143 (3.08), 163(0.05), 165(0.13), 219(0.69), 234(1.98), 257(7.12), 269(0.01), 302(0.15), 536(0.02), 625(2.02), 626(1.69), 670(0.26), 852(100), 855(97.06), 1102(39.15), 1106(55.35), 1125(1.94)
V ₃ O ₆ Model B (² A)	20(0.09), 23(0.07), 24(0.06), 54(1.59), 55(0.07), 85(0.61), 124(0.02), 153(4.74), 157(5.28), 246(3.78), 280(0.03), 301(0.69), 334(1.11), 422(0.19), 492(0.19), 881(100), 908(7.10), 1082(27.56), 1091(7.37), 1108(0.35), 1109(32.53)
(⁴ A)	14(0.19), 21(0.28), 22(0.09), 39(0.15), 46(0.98), 78(0.57), 91(0.24), 181(7.26), 182(7.12), 285(1.31), 288(0.56), 336(0.72), 365(0.69), 440(2.18), 535(2.49), 841(100), 881(10.08), 1079(32.20), 1087(4.04), 1102(13.38), 1104(22.77)
V ₃ O ₆ Model C (² A)	13(0.13), 31(0.24), 37(0.17), 64(0.24), 105(1.59), 133(0.97), 202(6.32), 239(0.01), 258(0.04), 276(0.07), 301(3.23), 381 (1.34), 431(0.54), 487(0.27), 705(47.15), 744(10.37), 763(0.67), 924(100), 1091(19.86), 1106(8.18), 1111(18.14)
(⁴ A)	14(0.12), 31(0.21), 37(0.19), 66(0.25), 106(1.55), 126(0.99), 200(6.10), 238(0.03), 257(0.98), 277(0.06), 297(3.38), 380(1.05), 443(0.42), 482(0.16), 672(33.67), 745(10.15), 763(0.31), 921(100), 1090(21.64), 1103(7.77), 1111 (17.14)
V ₃ O ₇ ⁺ Model A (¹ E)	113(7.67), 141(0.21), 141(0.18), 167(2.16), 168(2.21), 226(0.00), 238(0.12), 240(0.09), 295(9.43), 341(2.55), 341(2.53), 376(0.02), 464(0.02), 464(0.01), 492(0.00), 663(20.60), 729(38.80), 730(56.72), 731(35.22), 807(64.48), 808(64.18), 1160(100), 1160(100), 1186(14.63)

$(^3A'')$	95(2.76), 118(4.43), 139(0.93), 150(1.89), 178(2.27), 204(0.03), 208(0.76), 237(0.18), 267(0.00), 290(7.08), 331(2.56), 377(0.35), 391(5.98), 452(0.51), 465(0.93), 658(21.46), 703(21.47), 719(81.04), 736(20.84), 758(30.61), 758(34.40), 811(59.47), 1153(100), 1172(36.16)
$V_3O_7^+$ Model B (1A)	23(0.09), 26(0.02), 41(0.90), 46(0.74), 55(1.04), 62(0.66), 154(2.48), 172(0.33), 176(3.50), 234(6.08), 295(2.80), 298(3.80), 306(3.27), 352(0.78), 401(1.70), 452(1.75), 503(1.95), 930(100), 980(43.13), 1118(11.59), 1124(26.97), 1129(17.14), 1129(0.11), 1151(12.46)
$V_3O_7^+$ Model C1 (1A)	16(0.68), 28(0.35), 42(0.77), 75(0.32), 117(2.29), 137(0.94), 141(0.83), 186(4.83), 234(1.53), 250(2.75), 291(3.78), 330(3.36), 356(3.56), 373(3.13), 435(0.33), 465(5.89), 538(9.91), 956(100), 962(43.51), 1011(21.12), 1122(18.57), 1126(20.23), 1128(17.04), 1135(4.96)
$V_3O_7^+$ Model C2 (1A)	20(0.22), 22(0.38), 37(0.74), 93(1.82), 133(0.01), 168(2.12), 201(1.45), 215(0.65), 258(1.60), 283(9.26), 287(0.50), 338(0.01), 400(0.45), 429(0.65), 453(0.39), 504(4.96), 687(32.46), 803(13.40), 892(33.44), 970(100), 1123(21.89), 1127(8.71), 1149(32.35), 1156(1.09)
V_3O_7 Model A (2A)	135(1.22), 137(1.57), 155(3.65), 186(1.79), 193(0.98), 232(1.08), 237(0.06), 282(0.37), 296(5.47), 308(0.07), 328(1.12), 374(1.12), 428(1.27), 436(0.73), 478(0.35), 593(28.8), 678(20.37), 708(88.52), 752(88.52), 822(2.22), 872(80.56), 1119(100), 1121(97.19), 1151(14.75)
(^4A)	108(0.94), 127(0.13), 137(3.05), 179(2.39), 188(1.53), 199(0.34), 230(0.87), 257(0.16), 285(4.46), 306(0.35), 314(0.60), 367(0.64), 416(2.03), 430(1.11), 485(0.45), 593(27.47), 657(19.78), 676(30.16), 697(61.74), 757(18.99), 805(9.26), 860(79.11), 1113(100), 1136(37.56)
V_3O_7 Model B (2A)	17(0.00), 26(1.42), 29(1.54), 48(0.52), 49(0.87), 54(0.15), 118(1.01), 130(1.38), 138(4.05), 228(0.73), 247(2.50), 274(0.02), 278(1.36), 292(1.29), 366(0.26), 433(0.03), 515(0.24), 914(100), 959(21.14), 1091(6.44), 1093(21.78), 1111(0.02), 1113(25.13), 1119(2.97)
V_3O_7 Model C1 (2A)	18(0.13), 28(0.21), 33(0.27), 73(0.12), 119(1.26), 137(0.13), 189(4.10), 198(0.52), 229(0.43), 259(0.72), 277(0.64), 318(1.47), 343(1.22), 388(0.55), 418(0.10), 497(1.169), 579(12.67), 878(10.41), 924(100), 933(10.90), 1096(8.33), 1103(3.98), 1106(11.94), 1115(16.78)
V_3O_7 Model C2 (2A)	5(0.00), 15(0.25), 23(0.17), 81(3.33), 129(2.49), 161(0.11), 183(1.35), 205(1.12), 256(2.62), 276(0.90), 283(0.86), 313(0.00), 361(0.89), 398(1.16), 506(0.21), 508(0.11), 712(59.73), 757(11.06), 786(4.91), 946(100), 1094(15.30), 1110(38.6), 1113(19.88), 1127(0.08)
V_4O_{10} (1T_2)	162(0.00), 163(0.00), 184(0.00), 185(0.00), 202(0.00), 202(0.00), 203(0.00), 207(0.88), 208(0.82), 208(0.84), 217(0.22), 217(0.23), 218(0.22), 291(3.88), 291(3.81), 292(3.93), 294(0.03), 294(0.08), 294(0.08), 316(0.00), 517(0.01), 519(0.00), 519(0.00), 588(0.00), 656(6.65), 657(3.95), 657(6.93), 691(0.00), 691(0.00), 875(100), 876(99.66), 876(99.66), 1135(67.50), 1135(67.50), 1135(67.48), 1157(0.00)



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