

Supplementary Material

Screening Possible Drug Molecules for Covid-19. The Example of Vanadium (III/IV/V) Complex Molecules with Computational Chemistry and Molecular Docking.

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Table A1. Calculated Huckel Charges of Vbicah, Vbdeah and Vtocdea complex molecules.

Vbicah	Huckel Charges	Vbdeah	Huckel Charges	Vtocdea	Huckel Charges
C(1)	0.580045	C(1)	0.49443	C(1)	0.482146
C(2)	0.348572	C(2)	0.446314	C(2)	0.0187917
C(3)	-0.0170939	C(3)	-0.0672	C(3)	0.10197
C(4)	0.522331	C(4)	0.462057	C(4)	0.468077
C(5)	0.19997	C(5)	0.210345	C(5)	0.213254
C(6)	0.0978725	C(6)	-0.0169052	C(6)	0.127701
O(7)	0.314848	C(7)	0.0917216	O(7)	1.30517
C(8)	0.17631	O(8)	-0.0899862	C(8)	0.400773
N(9)	1.29941	C(9)	0.156815	C(9)	0.0523533
V(10)	-5.01766	O(10)	0.311305	C(10)	0.00680537
O(11)	-0.399955	N(11)	1.13708	C(11)	0.0899916
O(12)	-0.381017	N(12)	1.10787	O(12)	-0.19116
O(13)	-0.0400305	C(13)	0.0199996	N(13)	1.03515
O(14)	-0.348098	C(14)	0.11513	C(14)	-0.0936385
C(15)	0.699344	O(15)	-0.788696	C(15)	-0.025997
C(16)	0.317369	V(16)	-0.154612	C(16)	-0.0619843
O(17)	0.273057	O(17)	-1.55762	C(17)	-0.0612044
C(18)	0.354431	C(18)	0.00473522	C(18)	0.0168623
C(19)	0.689275	C(19)	0.17356	C(19)	-0.136021
O(20)	0.502122	O(20)	-0.804517	C(20)	-0.0744028
C(21)	0.111418	V(21)	0.059237	C(21)	-0.063897
O(22)	-0.0847671	C(22)	0.0830728	C(22)	0.0122581
V(23)	-2.39426	C(23)	0.164087	C(23)	-0.137169
N(24)	0.965976	O(24)	-0.85131	C(24)	-0.0673531
O(25)	-0.261555	O(25)	-1.57602	C(25)	-0.0643827
O(26)	-0.259292	O(26)	-0.557166	C(26)	-0.0651897
C(27)	0.0379175	C(27)	0.12782	C(27)	0.0156634
C(28)	0.655078	C(28)	0.351004	C(28)	-0.139074

O(29)	-0.698073	H(29)	0.0413037	C(29)	-0.0575149
O(30)	-0.447761	H(30)	0.0483916	C(30)	-0.132214
C(31)	-0.00886097	H(31)	0.0768194	C(31)	0.0187057
C(32)	0.628706	H(32)	0.0528134	C(32)	0.0134052
O(33)	-0.729699	H(33)	0.146213	C(33)	0.15689
O(34)	-0.50866	H(34)	0.0734207	O(34)	-0.901521
H(35)	0.0539011	H(35)	0.0261517	C(35)	0.159022
H(36)	0.0489056	H(36)	0.0538303	O(36)	-0.812782
H(37)	0.0501808	H(37)	0.0177339	V(37)	-2.03729
H(38)	0.0990761	H(38)	0.0126372	O(38)	-1.34839
H(39)	0.299025	H(39)	0.0606808	H(39)	0.0423643
H(40)	0.297901	H(40)	0.0204521	H(40)	0.0460513
H(41)	0.306115	H(41)	0.00467896	H(41)	0.0314613
H(42)	0.276179	H(42)	0.00705491	H(42)	0.039438
H(43)	0.0668951	H(43)	0.103364	H(43)	0.0479422
H(44)	0.0926314	H(44)	0.0729022	H(44)	0.0599681
H(45)	0.0487188	H(45)	0.0224795	H(45)	0.0714341
H(46)	0.0358278	H(46)	0.0103498	H(46)	0.040044
H(47)	0.0538782	H(47)	0.0102592	H(47)	0.0424324
H(48)	0.0476171	H(48)	0.0118923	H(48)	0.0397421
H(49)	0.199338	H(49)	0.0399236	H(49)	0.0415473
H(50)	0.203885	H(50)	0.0340878	H(50)	0.0358497
H(51)	0.201079			H(51)	0.036166
H(52)	0.206134			H(52)	0.035693
H(53)	0.0469772			H(53)	0.0312486
H(54)	0.0578191			H(54)	0.0295127
H(55)	0.0753729			H(55)	0.0296784
H(56)	0.0552683			H(56)	0.0236452
				H(57)	0.0378934
				H(58)	0.0378401
				H(59)	0.0389607
				H(60)	0.0322053
				H(61)	0.0303026
				H(62)	0.0292396
				H(63)	0.0289748
				H(64)	0.0246851
				H(65)	0.0389941
				H(66)	0.0381981
				H(67)	0.0392517
				H(68)	0.0299387
				H(69)	0.0293381

				H(70)	0.0314082
				H(71)	0.0314451
				H(72)	0.0287001
				H(73)	0.0289565
				H(74)	0.0240962
				H(75)	0.0396736
				H(76)	0.0400008
				H(77)	0.0384639
				H(78)	0.0300364
				H(79)	0.0310464
				H(80)	0.0394725
				H(81)	0.0404754
				H(82)	0.0391249
				H(83)	0.0362754
				H(84)	0.039634
				H(85)	0.0452334
				H(86)	0.0251958
				H(87)	0.00891232
				H(88)	0.00663621
				H(89)	0.0073135
				H(90)	0.00405208

Table A2. Calculated Huckel Charges of Vtcdpa, VXn and Xn molecules.

Vtcdpa	Huckel Charges	VXn	Huckel Charges	Xn	Huckel Charges
C(1)	0.419798	C(1)	0.515337	C(1)	0.489453
C(2)	0.0204756	C(2)	0.346823	C(2)	-0.449828
C(3)	0.463504	C(3)	0.561402	C(3)	0.328341
C(4)	0.563787	C(4)	0.650781	C(4)	-0.347411
C(5)	0.06304	C(5)	0.58501	C(5)	0.249433
C(6)	0.316265	C(6)	0.758488	C(6)	-0.322414
O(7)	0.784132	C(7)	0.118211	O(7)	-0.102596
C(8)	0.355164	C(8)	0.082692	O(8)	-0.235126
C(9)	0.0214997	C(9)	0.576125	O(9)	-0.220966
C(10)	8.95E-05	C(10)	0.709052	C(10)	0.0999393
C(11)	-0.06714	C(11)	-0.0818696	C(11)	0.00318307
O(12)	-0.328968	C(12)	-0.0750682	C(12)	-0.19478
C(13)	0.0673721	C(13)	0.332415	C(13)	0.10463
N(14)	0.521475	C(14)	0.348918	C(14)	-0.129989
C(15)	0.0421974	C(15)	0.140068	C(15)	-0.112219
C(16)	0.279718	C(16)	0.297491	C(16)	0.432155
C(17)	0.0546019	C(17)	0.0593446	C(17)	-0.199775
C(18)	0.59186	C(18)	0.0183381	O(18)	-0.822967

C(19)	0.305166	C(19)	0.485274	C(19)	0.0805369
C(20)	0.189072	C(20)	0.142736	C(20)	0.0911981
C(21)	0.420933	C(21)	0.0690432	C(21)	0.00335463
C(22)	0.330746	O(22)	-0.9204	C(22)	-0.16994
N(23)	0.513953	O(23)	0.629645	C(23)	0.408585
C(24)	-0.0607976	O(24)	0.36391	C(24)	-0.28603
C(25)	0.00291174	O(25)	0.89508	C(25)	0.0161162
C(26)	-0.0500697	O(26)	-0.326282	O(26)	-0.156392
C(27)	0.119293	O(27)	0.618078	H(27)	0.0454828
N(28)	0.438243	V(28)	-6.36927	H(28)	0.205006
C(29)	-0.133838	O(29)	-1.55507	H(29)	0.203054
C(30)	-0.0493508	H(30)	0.0526822	H(30)	0.0278997
C(31)	-0.0632754	O(31)	-0.971041	H(31)	0.0239943
C(32)	-0.0616841	H(32)	0.062907	H(32)	0.0221532
C(33)	0.0107518	H(33)	0.209558	H(33)	0.0304406
C(34)	-0.0688325	H(34)	0.0305389	H(34)	0.0328133
C(35)	-0.0684232	H(35)	0.0461123	H(35)	0.0289073
C(36)	-0.0602353	H(36)	0.0577836	H(36)	0.0413601
C(37)	0.0097369	H(37)	0.0722673	H(37)	0.0456956
C(38)	-0.0691869	H(38)	0.0618072	H(38)	0.0583437
C(39)	-0.0648734	H(39)	0.0509276	H(39)	0.0508024
C(40)	-0.0642284	H(40)	0.0928256	H(40)	0.0459865
C(41)	0.0238063	H(41)	0.0459481	H(41)	0.0375112
C(42)	-0.137351	H(42)	0.052778	H(42)	0.0456858
C(43)	-0.130275	H(43)	0.0959013	H(43)	0.0460971
C(44)	-0.130442	H(44)	0.0546055	H(44)	0.0468322
C(45)	-0.133905	H(45)	0.110531	H(45)	0.0734013
V(46)	-5.92233	H(46)	0.0413938	H(46)	0.061105
O(47)	-1.44939	H(47)	0.0474735	H(47)	0.0647153
H(48)	0.0628903	H(48)	0.0475419	H(48)	0.20622
H(49)	0.0377695	H(49)	0.0521658	Lp(49)	
H(50)	0.0302968	H(50)	0.0554939	Lp(50)	
H(51)	0.0373463	H(51)	0.0514366	Lp(51)	
H(52)	0.0494727	H(52)	0.206622	Lp(52)	
H(53)	0.0514549	H(53)	0.196543	Lp(53)	
H(54)	0.0744793	H(54)	0.198889	Lp(54)	
H(55)	0.0472077			Lp(55)	
H(56)	0.0536293			Lp(56)	
H(57)	0.0442329			Lp(57)	
H(58)	0.0334623			Lp(58)	
H(59)	0.0338931				
H(60)	0.0636614				
H(61)	0.0514705				

H(62)	0.0233667				
H(63)	0.0370249				
H(64)	0.0472213				
H(65)	0.0163073				
H(66)	0.0423585				
H(67)	0.0503505				
H(68)	0.042647				
H(69)	0.0411613				
H(70)	0.0427254				
H(71)	0.0410222				
H(72)	0.0394789				
H(73)	0.0395465				
H(74)	0.0345641				
H(75)	0.0321036				
H(76)	0.0361535				
H(77)	0.0311012				
H(78)	0.0282446				
H(79)	0.0224237				
H(80)	0.0301435				
H(81)	0.0300629				
H(82)	0.0296185				
H(83)	0.0372681				
H(84)	0.02838				
H(85)	0.0279846				
H(86)	0.0225794				
H(87)	0.0304569				
H(88)	0.0304633				
H(89)	0.0294534				
H(90)	0.0340172				
H(91)	0.0308375				
H(92)	0.0284354				
H(93)	0.0230726				
H(94)	0.0384691				
H(95)	0.0395383				
H(96)	0.0393306				
H(97)	0.0368726				
H(98)	0.0368197				
H(99)	0.0374599				
H(100)	0.036831				
H(101)	0.0368054				
H(102)	0.037387				
H(103)	0.0374827				
H(104)	0.0374453				

H(105)	0.0387288				
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Table B. Calculated bond lengths and bond angles in angstroms for the studies molecules.

Vtodeca	Actual A	Vtodeca	Actual A	Vtodeca	Actual A	Vtodeca	Actual A	VXn	Actual A	VXn	Actual A
O(39)-Lp(101)	0.6087	H(82)-C(28)-H(81)	109.2602	O(48)-Lp(114)	0.5812	H(105)-C(43)-H(103)	108.8083	O(32)-Lp(70)	0.6363	Lp(68)-O(28)-Lp(67)	106.9009
O(39)-Lp(100)	0.6556	H(82)-C(28)-H(80)	117.8848	O(48)-Lp(113)	0.6002	H(105)-C(43)-H(104)	109.2252	O(32)-Lp(69)	0.6242	Lp(68)-O(28)-H(52)	94.3858
O(37)-Lp(99)	0.64	H(82)-C(28)-C(27)	104.33	O(46)-Lp(112)	0.6108	H(105)-C(43)-C(39)	100.5237	O(28)-Lp(68)	0.6208	Lp(68)-O(28)-C(19)	113.4661
O(37)-Lp(98)	0.6129	H(81)-C(28)-H(80)	104.257	O(46)-Lp(111)	0.6049	H(103)-C(43)-H(104)	111.5541	O(28)-Lp(67)	0.6407	Lp(67)-O(28)-H(52)	111.538
O(36)-Lp(97)	0.6013	H(81)-C(28)-C(27)	117.4597	O(45)-Lp(110)	0.5741	H(103)-C(43)-C(39)	114.2585	O(27)-Lp(66)	0.5801	Lp(67)-O(28)-C(19)	109.0908
O(36)-Lp(96)	0.5428	H(80)-C(28)-C(27)	104.1814	O(45)-Lp(109)	0.5658	H(104)-C(43)-C(39)	111.7972	O(27)-Lp(65)	0.5838	H(52)-O(28)-C(19)	120.14
O(35)-Lp(95)	0.6391	H(79)-C(27)-H(78)	104.5149	N(26)-Lp(108)	0.5557	H(95)-C(40)-H(96)	99.0777	O(26)-Lp(64)	0.5929	H(50)-C(20)-C(21)	110.2846
O(35)-Lp(94)	0.6366	H(79)-C(27)-C(28)	100.8536	N(21)-Lp(107)	0.5575	H(95)-C(40)-H(94)	112.951	O(26)-Lp(63)	0.5824	H(50)-C(20)-C(19)	110.6856
O(34)-Lp(93)	0.666	H(79)-C(27)-C(25)	108.4351	N(12)-Lp(106)	0.5974	H(95)-C(40)-C(39)	105.9014	O(25)-Lp(62)	0.6177	C(21)-C(20)-C(19)	108.9745
O(34)-Lp(92)	0.5849	H(78)-C(27)-C(28)	111.7498	V(47)-O(48)	1.8431	H(96)-C(40)-H(94)	111.8079	O(25)-Lp(61)	0.637	O(28)-C(19)-C(20)	106.4634
N(11)-Lp(91)	0.687	H(78)-C(27)-C(25)	108.4099	O(46)-V(47)	1.8641	H(96)-C(40)-C(39)	106.9929	O(24)-Lp(60)	0.5466	O(28)-C(19)-C(18)	110.141
V(38)-O(39)	1.8468	C(28)-C(27)-C(25)	121.3264	C(43)-H(105)	1.1222	H(94)-C(40)-C(39)	118.2108	O(24)-Lp(59)	0.5731	C(20)-C(19)-C(18)	106.6548
O(37)-V(38)	1.8537	H(77)-C(26)-H(76)	111.3373	C(43)-H(103)	1.1253	H(93)-C(39)-C(40)	114.0841	O(23)-Lp(58)	0.6081	H(51)-C(21)-C(20)	110.985
O(36)-V(38)	1.8915	H(77)-C(26)-H(75)	106.1848	C(43)-H(104)	1.1228	H(93)-C(39)-C(43)	104.6968	O(23)-Lp(57)	0.6548	H(51)-C(21)-C(16)	104.0613
O(35)-V(38)	1.8509	H(77)-C(26)-C(25)	118.5644	C(42)-H(101)	1.1079	H(93)-C(39)-C(38)	105.5641	O(22)-Lp(56)	0.5623	C(20)-C(21)-C(16)	108.0972
C(32)-H(90)	1.0837	H(76)-C(26)-H(75)	99.8573	C(42)-H(102)	1.1334	C(40)-C(39)-C(43)	110.7406	O(22)-Lp(55)	0.603	H(49)-C(18)-C(19)	91.5317
C(32)-H(89)	1.0944	H(76)-C(26)-C(25)	108.6409	C(42)-H(100)	1.0718	C(40)-C(39)-C(38)	111.857	O(32)-H(54)	0.9325	H(49)-C(18)-C(17)	105.5448
C(32)-O(37)	1.4489	H(75)-C(26)-C(25)	110.6252	C(41)-H(98)	1.0922	C(43)-C(39)-C(38)	109.5157	V(29)-O(32)	1.8881	C(19)-C(18)-C(17)	113.9392
C(31)-H(88)	1.0887	H(74)-C(25)-C(27)	106.6581	C(41)-H(97)	1.0661	H(91)-C(38)-H(92)	107.9712	O(28)-H(52)	0.9207	Lp(70)-O(32)-Lp(69)	113.7532
C(31)-H(87)	1.1143	H(74)-C(25)-C(26)	113.7361	C(41)-H(99)	1.0497	H(91)-C(38)-C(39)	113.2283	O(27)-V(29)	1.8785	Lp(70)-O(32)-H(54)	111.8959

C(31)-O(36)	1.4313	H(74)-C(25)-C(24)	101.7749	C(40)-H(95)	1.1833	H(91)-C(38)-C(37)	114.1112	O(25)-V(29)	1.8545	Lp(70)-O(32)-V(29)	105.4456
C(30)-H(86)	1.1533	C(27)-C(25)-C(26)	110.5571	C(40)-H(96)	1.1268	H(92)-C(38)-C(39)	106.1736	O(24)-H(34)	0.9336	Lp(69)-O(32)-H(54)	110.4845
C(30)-H(85)	1.1562	C(27)-C(25)-C(24)	112.4737	C(40)-H(94)	1.0872	H(92)-C(38)-C(37)	100.8997	O(23)-H(53)	0.9958	Lp(69)-O(32)-V(29)	112.9687
C(30)-C(32)	1.5322	C(26)-C(25)-C(24)	111.3235	C(39)-H(93)	1.117	C(39)-C(38)-C(37)	113.2232	O(23)-V(29)	1.8908	H(54)-O(32)-V(29)	101.5699
C(29)-H(84)	1.0737	H(73)-C(24)-H(72)	116.3998	C(39)-C(40)	1.5553	H(101)-C(42)-H(102)	99.7182	O(22)-V(29)	1.8422	Lp(56)-O(22)-Lp(55)	106.6523
C(29)-H(83)	1.1248	H(73)-C(24)-C(25)	99.168	C(39)-C(43)	1.5325	H(101)-C(42)-H(100)	108.8602	C(21)-H(51)	1.1278	Lp(56)-O(22)-V(29)	106.2453
C(29)-C(31)	1.4993	H(73)-C(24)-C(23)	105.4882	C(38)-H(91)	1.1443	H(101)-C(42)-C(35)	115.5768	C(20)-H(50)	1.1107	Lp(55)-O(22)-V(29)	113.8428
C(28)-H(82)	1.068	H(72)-C(24)-C(25)	118.9989	C(38)-H(92)	1.1258	H(102)-C(42)-H(100)	106.2766	C(20)-C(21)	1.5479	H(48)-C(17)-C(18)	117.1523
C(28)-H(81)	1.128	H(72)-C(24)-C(23)	99.8058	C(38)-C(39)	1.5074	H(102)-C(42)-C(35)	110.2244	C(19)-O(28)	1.4406	H(48)-C(17)-C(16)	105.8704
C(28)-H(80)	1.1303	C(25)-C(24)-C(23)	117.0422	C(37)-H(90)	1.1234	H(100)-C(42)-C(35)	114.7738	C(19)-C(20)	1.6176	C(18)-C(17)-C(16)	109.4571
C(27)-H(79)	1.1155	H(71)-C(23)-H(70)	115.6253	C(37)-H(89)	1.142	H(90)-C(37)-H(89)	104.2107	C(18)-H(49)	1.1208	H(44)-C(12)-H(43)	105.7494
C(27)-H(78)	1.1631	H(71)-C(23)-C(24)	103.7861	C(37)-C(38)	1.5535	H(90)-C(37)-C(38)	113.4093	C(18)-C(19)	1.5102	H(44)-C(12)-H(42)	108.1308
C(27)-C(28)	1.5436	H(71)-C(23)-C(22)	104.0506	C(36)-H(87)	1.0981	H(90)-C(37)-C(36)	98.3806	C(17)-H(48)	1.1351	H(44)-C(12)-C(10)	107.4742
C(26)-H(77)	1.1168	H(70)-C(23)-C(24)	113.8074	C(36)-H(88)	1.0546	H(89)-C(37)-C(38)	112.1036	C(17)-C(18)	1.506	H(43)-C(12)-H(42)	112.1339
C(26)-H(76)	1.1202	H(70)-C(23)-C(22)	108.1135	C(36)-C(37)	1.5631	H(89)-C(37)-C(36)	111.368	C(16)-C(21)	1.5346	H(43)-C(12)-C(10)	114.2391
C(26)-H(75)	1.099	C(24)-C(23)-C(22)	111.0304	C(35)-H(86)	1.1045	C(38)-C(37)-C(36)	116.0194	C(16)-C(17)	1.5755	H(42)-C(12)-C(10)	108.8093
C(25)-H(74)	1.1646	H(69)-C(22)-H(68)	101.2205	C(35)-C(42)	1.533	H(87)-C(36)-H(88)	101.0455	C(15)-H(47)	1.1059	Lp(58)-O(23)-Lp(57)	109.9878
C(25)-C(27)	1.5732	H(69)-C(22)-C(23)	112.6027	C(35)-C(36)	1.5358	H(87)-C(36)-C(37)	109.3961	C(15)-C(16)	1.4817	Lp(58)-O(23)-H(53)	104.2118
C(25)-C(26)	1.5056	H(69)-C(22)-C(20)	102.0044	C(34)-H(85)	1.147	H(87)-C(36)-C(35)	115.9719	C(14)-H(46)	1.1271	Lp(58)-O(23)-V(29)	97.2061
C(24)-H(73)	1.09	H(68)-C(22)-C(23)	110.2216	C(34)-H(84)	1.1584	H(88)-C(36)-C(37)	109.9994	C(14)-C(15)	1.5564	Lp(57)-O(23)-H(53)	110.8813
C(24)-H(72)	1.0652	H(68)-C(22)-C(20)	114.4831	C(34)-C(35)	1.5168	H(88)-C(36)-C(35)	106.0391	C(13)-H(45)	1.0911	Lp(57)-O(23)-V(29)	113.7465
C(24)-C(25)	1.5224	C(23)-C(22)-C(20)	115.1788	C(33)-H(82)	1.0481	C(37)-C(36)-C(35)	113.4993	C(13)-O(27)	1.4099	H(53)-O(23)-V(29)	119.1169
C(23)-H(71)	1.1305	H(67)-C(21)-H(66)	110.4944	C(33)-H(83)	1.0653	H(86)-C(35)-C(42)	109.1623	C(13)-C(14)	1.5348	C(21)-C(16)-C(17)	111.6978

C(23)-H(70)	1.1161	H(67)-C(21)-H(65)	112.0267	C(33)-C(34)	1.5604	H(86)-C(35)-C(36)	109.0347	C(12)-H(44)	1.1289	C(21)-C(16)-C(15)	118.4134
C(23)-C(24)	1.5383	H(67)-C(21)-C(20)	107.7876	C(32)-H(81)	1.1411	H(86)-C(35)-C(34)	102.9017	C(12)-H(43)	1.1766	C(17)-C(16)-C(15)	117.6047
C(22)-H(69)	1.075	H(66)-C(21)-H(65)	109.0873	C(32)-H(80)	1.1129	C(42)-C(35)-C(36)	105.7943	C(12)-H(42)	1.0772	H(41)-C(11)-H(40)	111.9724
C(22)-H(68)	1.0454	H(66)-C(21)-C(20)	109.4694	C(32)-C(33)	1.5851	C(42)-C(35)-C(34)	119.6677	C(11)-H(41)	1.1529	H(41)-C(11)-H(39)	100.0336
C(22)-C(23)	1.5366	H(65)-C(21)-C(20)	107.908	C(31)-H(79)	1.0878	C(36)-C(35)-C(34)	110.0012	C(11)-H(40)	1.1268	H(41)-C(11)-C(10)	105.2171
C(21)-H(67)	1.1318	H(64)-C(20)-C(22)	101.7172	C(31)-C(41)	1.5469	H(85)-C(34)-H(84)	103.6445	C(11)-H(39)	1.1036	H(40)-C(11)-H(39)	108.6657
C(21)-H(66)	1.1059	H(64)-C(20)-C(21)	113.0341	C(31)-C(32)	1.5769	H(85)-C(34)-C(35)	115.6899	C(10)-C(12)	1.5734	H(40)-C(11)-C(10)	118.7998
C(21)-H(65)	1.103	H(64)-C(20)-C(19)	107.6715	C(30)-H(78)	1.108	H(85)-C(34)-C(33)	98.9023	C(10)-C(11)	1.5702	H(39)-C(11)-C(10)	110.521
C(20)-H(64)	1.1613	C(22)-C(20)-C(21)	110.065	C(30)-H(77)	1.0858	H(84)-C(34)-C(35)	114.5739	C(9)-H(38)	1.06	Lp(66)-O(27)-Lp(65)	125.2722
C(20)-C(22)	1.5732	C(22)-C(20)-C(19)	109.0214	C(30)-C(31)	1.4726	H(84)-C(34)-C(33)	104.134	C(9)-C(10)	1.5211	Lp(66)-O(27)-V(29)	109.2756
C(20)-C(21)	1.539	C(21)-C(20)-C(19)	114.5123	C(29)-H(60)	1.1264	C(35)-C(34)-C(33)	117.7294	C(8)-H(31)	1.0958	Lp(66)-O(27)-C(13)	104.0983
C(19)-H(63)	1.1039	H(63)-C(19)-H(48)	97.7547	C(29)-H(76)	1.1654	H(98)-C(41)-H(97)	101.7439	C(8)-H(30)	1.0778	Lp(65)-O(27)-V(29)	107.3179
C(19)-H(48)	1.1095	H(63)-C(19)-C(20)	110.5464	C(29)-C(30)	1.5444	H(98)-C(41)-H(99)	99.619	C(8)-C(9)	1.4937	Lp(65)-O(27)-C(13)	96.0817
C(19)-C(20)	1.5367	H(63)-C(19)-C(18)	107.9263	C(28)-H(75)	1.1538	H(98)-C(41)-C(31)	112.0768	C(7)-H(37)	1.1414	V(29)-O(27)-C(13)	114.3292
C(18)-H(62)	1.1313	H(48)-C(19)-C(20)	112.2968	C(28)-H(74)	1.2182	H(97)-C(41)-H(99)	106.1355	C(7)-H(36)	1.1082	H(47)-C(15)-C(16)	114.6566
C(18)-H(61)	1.1498	H(48)-C(19)-C(18)	112.8401	C(28)-C(29)	1.5464	H(97)-C(41)-C(31)	117.0192	C(7)-H(35)	1.1228	H(47)-C(15)-C(14)	115.8458
C(18)-C(19)	1.5992	C(20)-C(19)-C(18)	114.1636	C(27)-H(72)	1.1641	H(99)-C(41)-C(31)	117.7561	C(7)-O(26)	1.4458	C(16)-C(15)-C(14)	108.1699
C(17)-H(60)	1.1202	H(62)-C(18)-H(61)	113.7008	C(27)-H(71)	1.1189	H(82)-C(33)-H(83)	105.164	C(6)-C(8)	1.5871	C(12)-C(10)-C(11)	112.9002
C(17)-H(59)	1.1454	H(62)-C(18)-C(19)	111.9554	C(27)-H(73)	1.0879	H(82)-C(33)-C(34)	103.915	C(5)-O(25)	1.3735	C(12)-C(10)-C(9)	106.418
C(17)-H(58)	1.1678	H(62)-C(18)-C(16)	107.9592	N(26)-V(47)	1.9001	H(82)-C(33)-C(32)	115.4032	C(5)-C(6)	1.5617	C(11)-C(10)-C(9)	114.1427
C(16)-H(57)	1.0538	H(61)-C(18)-C(19)	103.6269	C(25)-H(70)	1.1007	H(83)-C(33)-C(34)	106.0008	C(4)-C(13)	1.5041	O(32)-V(29)-O(27)	153.0256
C(16)-C(18)	1.5572	H(61)-C(18)-C(16)	105.1165	C(25)-N(26)	1.4378	H(83)-C(33)-C(32)	108.8209	C(4)-C(5)	1.464	O(32)-V(29)-O(25)	110.6562
C(16)-C(17)	1.491	C(19)-C(18)-C(16)	114.3794	C(24)-H(69)	1.1302	C(34)-C(33)-C(32)	116.5786	C(3)-O(26)	1.37	O(32)-V(29)-O(23)	84.2806

C(15)- H(56)	1.1733	H(60)- C(17)- H(59)	115.2769	C(24)- C(25)	1.4982	H(81)- C(32)- H(80)	104.6365	C(3)- C(4)	1.5145	O(32)- V(29)- O(22)	82.6586
C(15)- H(55)	1.1012	H(60)- C(17)- H(58)	108.4532	C(23)- H(68)	1.1779	H(81)- C(32)- C(33)	109.0424	C(2)- H(33)	1.1428	O(27)- V(29)- O(25)	89.3452
C(15)- C(16)	1.614	H(60)- C(17)- C(16)	111.1314	C(23)- C(24)	1.5137	H(81)- C(32)- C(31)	108.2743	C(2)- C(3)	1.4879	O(27)- V(29)- O(23)	77.8419
C(14)- H(54)	1.0719	H(59)- C(17)- H(58)	97.8862	C(22)- H(67)	1.0473	H(80)- C(32)- C(33)	104.395	C(1)- O(24)	1.3824	O(27)- V(29)- O(22)	105.1864
C(14)- H(53)	1.0656	H(59)- C(17)- C(16)	107.6611	C(22)- C(23)	1.5039	H(80)- C(32)- C(31)	114.8312	C(1)- C(6)	1.4591	O(25)- V(29)- O(23)	89.3205
C(14)- C(15)	1.5487	H(58)- C(17)- C(16)	116.0103	N(21)- V(47)	1.9661	C(33)- C(32)- C(31)	115.0641	C(1)- C(2)	1.4764	O(25)- V(29)- O(22)	116.1534
C(13)- H(52)	1.1403	H(57)- C(16)- C(18)	108.4831	C(20)- H(66)	1.0987	H(65)- C(19)- C(20)	115.5016			O(23)- V(29)- O(22)	154.163
C(13)- H(51)	1.1103	H(57)- C(16)- C(17)	108.2208	C(20)- N(21)	1.6145	H(65)- C(19)- C(18)	112.6693			H(46)- C(14)- C(15)	113.8514
C(13)- C(14)	1.5018	H(57)- C(16)- C(15)	100.1019	C(19)- H(65)	1.0359	C(20)- C(19)- C(18)	60.4227			H(46)- C(14)- C(13)	113.3486
C(12)- H(50)	1.0929	C(18)- C(16)- C(17)	110.7474	C(19)- C(20)	1.4892	H(79)- C(31)- C(41)	110.9735			C(15)- C(14)- C(13)	124.473
C(12)- H(49)	1.0756	C(18)- C(16)- C(15)	119.3353	C(18)- H(64)	1.0782	H(79)- C(31)- C(32)	101.6908			H(38)- C(9)- C(10)	114.8306
C(12)- H(33)	1.1178	C(17)- C(16)- C(15)	109.0264	C(18)- C(20)	1.4963	H(79)- C(31)- C(30)	110.8341			H(38)- C(9)- C(8)	110.4653
N(11)- V(38)	1.9521	H(56)- C(15)- H(55)	95.8398	C(18)- C(19)	1.4844	C(41)- C(31)- C(32)	113.6392			C(10)- C(9)- C(8)	107.6351
N(11)- C(30)	1.6009	H(56)- C(15)- C(16)	112.854	C(17)- H(63)	1.1057	C(41)- C(31)- C(30)	109.3271			Lp(62)- O(25)- Lp(61)	110.5758
N(11)- C(29)	1.5781	H(56)- C(15)- C(14)	106.498	C(17)- N(21)	1.6717	C(32)- C(31)- C(30)	110.2046			Lp(62)- O(25)- V(29)	112.1578
C(10)- H(47)	1.1289	H(55)- C(15)- C(16)	112.8045	C(17)- C(18)	1.5039	H(69)- C(24)- C(25)	119.1926			Lp(62)- O(25)- C(5)	96.7689
C(10)- H(46)	1.1412	H(55)- C(15)- C(14)	100.6948	C(16)- N(21)	1.6724	H(69)- C(24)- C(23)	107.3422			Lp(61)- O(25)- V(29)	110.8359
C(10)- N(11)	1.6562	C(16)- C(15)- C(14)	123.9817	C(16)- C(17)	1.6122	C(25)- C(24)- C(23)	117.9176			Lp(61)- O(25)- C(5)	105.0925
C(9)- H(45)	1.1407	H(90)- C(32)- H(89)	109.6039	C(15)- H(62)	1.1353	H(68)- C(23)- C(24)	107.6801			V(29)- O(25)- C(5)	120.4172
C(9)- H(44)	1.0989	H(90)- C(32)- O(37)	108.5449	C(15)- H(61)	1.1633	H(68)- C(23)- C(22)	113.5932			H(45)- C(13)- O(27)	108.0566
C(8)- H(43)	1.1017	H(90)- C(32)- C(30)	107.7182	C(15)- C(16)	1.4821	C(24)- C(23)- C(22)	109.3353			H(45)- C(13)- C(14)	109.4663
C(8)- H(42)	1.0729	H(89)- C(32)- O(37)	109.359	C(14)- C(22)	1.5045	H(66)- C(20)- N(21)	112.3469			H(45)- C(13)- C(4)	117.5777
C(8)- C(9)	1.5213	H(89)- C(32)- C(30)	115.8944	C(14)- N(26)	1.4849	H(66)- C(20)- C(19)	132.1362			O(27)- C(13)- C(14)	109.9937

C(7)-O(34)	1.3562	O(37)-C(32)-C(30)	105.4513	C(13)-H(59)	1.146	H(66)-C(20)-C(18)	129.2946			O(27)-C(13)-C(4)	112.4164
C(7)-C(8)	1.575	H(54)-C(14)-H(53)	99.224	C(13)-H(44)	1.1716	N(21)-C(20)-C(19)	113.1959			C(14)-C(13)-C(4)	98.902
C(7)-C(13)	1.4883	H(54)-C(14)-C(15)	114.4457	C(13)-C(14)	1.54	N(21)-C(20)-C(18)	94.8038			H(31)-C(8)-H(30)	119.0857
C(7)-C(12)	1.5943	H(54)-C(14)-C(13)	105.5365	N(12)-V(47)	1.9643	C(19)-C(20)-C(18)	59.6313			H(31)-C(8)-C(9)	100.7551
C(6)-C(10)	1.5691	H(53)-C(14)-C(15)	111.2183	N(12)-C(13)	1.7124	H(64)-C(18)-C(20)	134.2366			H(31)-C(8)-C(6)	110.5211
C(5)-C(9)	1.5108	H(53)-C(14)-C(13)	112.9979	N(12)-C(15)	1.6337	H(64)-C(18)-C(19)	129.3398			H(30)-C(8)-C(9)	109.4762
C(5)-C(6)	1.5366	C(15)-C(14)-C(13)	112.6312	C(11)-H(58)	1.1323	H(64)-C(18)-C(17)	113.5028			H(30)-C(8)-C(6)	107.2785
C(4)-O(34)	1.405	H(88)-C(31)-H(87)	114.2179	C(11)-H(57)	1.105	C(20)-C(18)-C(19)	59.946			C(9)-C(8)-C(6)	109.3698
C(4)-C(5)	1.5171	H(88)-C(31)-O(36)	106.8064	C(11)-N(12)	1.6154	C(20)-C(18)-C(17)	91.3217			H(37)-C(7)-H(36)	114.7615
C(3)-H(41)	1.075	H(88)-C(31)-C(29)	101.7385	C(10)-H(56)	1.0777	C(19)-C(18)-C(17)	114.0999			H(37)-C(7)-H(35)	108.9344
C(3)-C(4)	1.5229	H(87)-C(31)-O(36)	113.852	C(10)-H(54)	1.0374	H(78)-C(30)-H(77)	97.4762			H(37)-C(7)-O(26)	106.4877
C(2)-H(40)	1.1421	H(87)-C(31)-C(29)	114.5152	C(10)-H(55)	1.1215	H(78)-C(30)-C(31)	114.9111			H(36)-C(7)-H(35)	104.894
C(2)-C(3)	1.5911	O(36)-C(31)-C(29)	104.5072	C(9)-H(52)	1.154	H(78)-C(30)-C(29)	106.9136			H(36)-C(7)-O(26)	115.7814
C(1)-O(35)	1.395	H(86)-C(30)-H(85)	108.3189	C(9)-H(53)	1.1182	H(77)-C(30)-C(31)	110.943			H(35)-C(7)-O(26)	105.4476
C(1)-C(2)	1.5176	H(86)-C(30)-C(32)	109.6571	C(8)-H(50)	1.1589	H(77)-C(30)-C(29)	113.676			Lp(64)-O(26)-Lp(63)	123.4879
C(1)-C(6)	1.5344	H(86)-C(30)-N(11)	117.3589	C(8)-H(51)	1.0935	C(31)-C(30)-C(29)	112.1257			Lp(64)-O(26)-C(7)	112.5334
		H(85)-C(30)-C(32)	106.4253	C(8)-C(9)	1.5247	H(70)-C(25)-N(26)	121.1269			Lp(64)-O(26)-C(3)	103.8659
		H(85)-C(30)-N(11)	104.9267	C(7)-O(45)	1.4311	H(70)-C(25)-C(24)	110.791			Lp(63)-O(26)-C(7)	103.0841
		C(32)-C(30)-N(11)	109.5264	C(7)-C(28)	1.5638	N(26)-C(25)-C(24)	106.8839			Lp(63)-O(26)-C(3)	96.3492
		H(52)-C(13)-H(51)	112.0893	C(7)-C(27)	1.5135	H(67)-C(22)-C(23)	117.187			C(7)-O(26)-C(3)	117.334
		H(52)-C(13)-C(14)	106.9304	C(7)-C(8)	1.5513	H(67)-C(22)-C(14)	110.9535			Lp(60)-O(24)-Lp(59)	113.233
		H(52)-C(13)-C(7)	95.473	C(6)-C(11)	1.5137	C(23)-C(22)-C(14)	110.4415			Lp(60)-O(24)-H(34)	105.3704
		H(51)-C(13)-C(14)	104.0708	C(5)-C(9)	1.5474	H(63)-C(17)-N(21)	103.8732			Lp(60)-O(24)-C(1)	109.2172

		H(51)- C(13)- C(7)	119.7201	C(5)- C(6)	1.5064	H(63)- C(17)- C(18)	124.5097			Lp(59)- O(24)- H(34)	115.3431
		C(14)- C(13)- C(7)	117.8954	C(4)- O(45)	1.3475	H(63)- C(17)- C(16)	113.968			Lp(59)- O(24)- C(1)	105.7432
		Lp(101)- O(39)- Lp(100)	102.6587	C(4)- C(5)	1.4872	N(21)- C(17)- C(18)	92.2116			H(34)- O(24)- C(1)	107.7543
		Lp(101)- O(39)- V(38)	107.6737	C(3)- C(10)	1.4903	N(21)- C(17)- C(16)	61.1976			O(25)- C(5)- C(6)	105.8177
		Lp(100)- O(39)- V(38)	110.5081	C(3)- C(4)	1.5208	C(18)- C(17)- C(16)	120.2176			O(25)- C(5)- C(4)	111.2794
		Lp(99)- O(37)- Lp(98)	128.4513	C(2)- H(49)	1.1035	H(60)- C(29)- H(76)	110.3606			C(6)- C(5)- C(4)	120.7533
		Lp(99)- O(37)- V(38)	100.9398	C(2)- C(3)	1.6245	H(60)- C(29)- C(30)	108.4833			C(8)- C(6)- C(5)	108.7792
		Lp(99)- O(37)- C(32)	105.8686	C(1)- O(46)	1.3919	H(60)- C(29)- C(28)	108.2266			C(8)- C(6)- C(1)	114.9137
		Lp(98)- O(37)- V(38)	100.797	C(1)- C(2)	1.5759	H(76)- C(29)- C(30)	109.9052			C(5)- C(6)- C(1)	111.7353
		Lp(98)- O(37)- C(32)	100.6107	C(1)- C(6)	1.5227	H(76)- C(29)- C(28)	107.8372			C(13)- C(4)- C(5)	113.6076
		V(38)- O(37)- C(32)	122.4632			C(30)- C(29)- C(28)	112.0173			C(13)- C(4)- C(3)	106.8028
		Lp(97)- O(36)- Lp(96)	130.6954			N(21)- C(16)- C(17)	61.1556			C(5)- C(4)- C(3)	117.2912
		Lp(97)- O(36)- V(38)	100.5367			N(21)- C(16)- C(15)	107.7194			O(26)- C(3)- C(4)	113.8774
		Lp(97)- O(36)- C(31)	95.4351			C(17)- C(16)- C(15)	121.6345			O(26)- C(3)- C(2)	111.0579
		Lp(96)- O(36)- V(38)	114.1154			C(22)- C(14)- N(26)	117.3082			C(4)- C(3)- C(2)	104.3905
		Lp(96)- O(36)- C(31)	104.0407			C(22)- C(14)- C(13)	111.7757			H(33)- C(2)- C(3)	107.4754
		V(38)- O(36)- C(31)	109.6106			N(26)- C(14)- C(13)	110.5214			H(33)- C(2)- C(1)	114.1261
		H(84)- C(29)- H(83)	102.8481			Lp(114)- O(48)- Lp(113)	108.9667			C(3)- C(2)- C(1)	118.0182
		H(84)- C(29)- C(31)	109.4431			Lp(114)- O(48)- V(47)	105.0933			O(24)- C(1)- C(6)	110.7891
		H(84)- C(29)- N(11)	119.107			Lp(113)- O(48)- V(47)	102.3427			O(24)- C(1)- C(2)	109.3416
		H(83)- C(29)- C(31)	113.1464			H(75)- C(28)- H(74)	104.9359			C(6)- C(1)- C(2)	115.4407
		H(83)- C(29)- N(11)	108.2998			H(75)- C(28)- C(29)	109.4893				
		C(31)- C(29)- N(11)	104.2991			H(75)- C(28)- C(7)	109.2994				

		H(50)- C(12)- H(49)	116.1583			H(74)- C(28)- C(29)	105.3994				
		H(50)- C(12)- H(33)	111.5131			H(74)- C(28)- C(7)	110.8725				
		H(50)- C(12)- C(7)	114.1095			C(29)- C(28)- C(7)	116.2122				
		H(49)- C(12)- H(33)	109.2996			Lp(108)- N(26)- V(47)	108.3433				
		H(49)- C(12)- C(7)	109.0722			Lp(108)- N(26)- C(25)	101.2925				
		H(33)- C(12)- C(7)	94.5626			Lp(108)- N(26)- C(14)	113.6835				
		Lp(91)- N(11)- V(38)	177.0948			V(47)- N(26)- C(25)	116.0543				
		Lp(91)- N(11)- C(30)	73.1666			V(47)- N(26)- C(14)	108.375				
		Lp(91)- N(11)- C(29)	75.7478			C(25)- N(26)- C(14)	109.1356				
		Lp(91)- N(11)- C(10)	62.1786			H(62)- C(15)- H(61)	102.2471				
		V(38)- N(11)- C(30)	109.2315			H(62)- C(15)- C(16)	119.3638				
		V(38)- N(11)- C(29)	104.055			H(62)- C(15)- N(12)	101.3141				
		V(38)- N(11)- C(10)	115.37			H(61)- C(15)- C(16)	117.3592				
		C(30)- N(11)- C(29)	119.6794			H(61)- C(15)- N(12)	109.5733				
		C(30)- N(11)- C(10)	101.3109			C(16)- C(15)- N(12)	105.7056				
		C(29)- N(11)- C(10)	107.756			H(72)- C(27)- H(71)	102.654				
		H(43)- C(8)- H(42)	107.7279			H(72)- C(27)- H(73)	115.6165				
		H(43)- C(8)- C(9)	111.8495			H(72)- C(27)- C(7)	111.9112				
		H(43)- C(8)- C(7)	105.9436			H(71)- C(27)- H(73)	97.9442				
		H(42)- C(8)- C(9)	108.871			H(71)- C(27)- C(7)	116.4436				
		H(42)- C(8)- C(7)	106.9444			H(73)- C(27)- C(7)	111.4438				
		C(9)- C(8)- C(7)	115.1565			Lp(107)- N(21)- V(47)	116.0809				
		O(34)- C(7)- C(8)	106.6377			Lp(107)- N(21)- C(20)	82.2074				

		O(34)- C(7)- C(13)	110.6437			Lp(107)- N(21)- C(17)	114.9605				
		O(34)- C(7)- C(12)	99.5758			Lp(107)- N(21)- C(16)	70.7552				
		C(8)- C(7)- C(13)	115.4429			V(47)- N(21)- C(20)	131.7141				
		C(8)- C(7)- C(12)	103.0041			V(47)- N(21)- C(17)	121.4431				
		C(13)- C(7)- C(12)	119.7351			V(47)- N(21)- C(16)	117.7772				
		O(39)- V(38)- O(37)	86.6932			C(20)- N(21)- C(17)	81.5085				
		O(39)- V(38)- O(36)	90.5477			C(20)- N(21)- C(16)	110.3837				
		O(39)- V(38)- O(35)	109.9562			C(17)- N(21)- C(16)	57.6468				
		O(39)- V(38)- N(11)	154.9069			H(59)- C(13)- H(44)	115.509				
		O(37)- V(38)- O(36)	144.8552			H(59)- C(13)- C(14)	102.6951				
		O(37)- V(38)- O(35)	95.5865			H(59)- C(13)- N(12)	111.5967				
		O(37)- V(38)- N(11)	80.6065			H(44)- C(13)- C(14)	101.4893				
		O(36)- V(38)- O(35)	118.1078			H(44)- C(13)- N(12)	117.9034				
		O(36)- V(38)- N(11)	87.6092			C(14)- C(13)- N(12)	105.1886				
		O(35)- V(38)- N(11)	92.8472			Lp(106)- N(12)- V(47)	147.0134				
		Lp(93)- O(34)- Lp(92)	139.456			Lp(106)- N(12)- C(13)	53.4913				
		Lp(93)- O(34)- C(7)	108.7266			Lp(106)- N(12)- C(15)	69.9451				
		Lp(93)- O(34)- C(4)	102.9893			Lp(106)- N(12)- C(11)	95.0011				
		Lp(92)- O(34)- C(7)	95.3336			V(47)- N(12)- C(13)	104.4836				
		Lp(92)- O(34)- C(4)	97.8075			V(47)- N(12)- C(15)	116.2959				
		C(7)- O(34)- C(4)	111.0466			V(47)- N(12)- C(11)	114.5896				
		H(47)- C(10)- H(46)	106.0921			C(13)- N(12)- C(15)	121.2032				
		H(47)- C(10)- N(11)	107.9786			C(13)- N(12)- C(11)	100.281				

		H(47)- C(10)- C(6)	111.1957			C(15)- N(12)- C(11)	99.109				
		H(46)- C(10)- N(11)	112.2693			H(50)- C(8)- H(51)	106.9702				
		H(46)- C(10)- C(6)	111.2132			H(50)- C(8)- C(9)	110.5631				
		N(11)- C(10)- C(6)	108.0715			H(50)- C(8)- C(7)	112.7591				
		H(45)- C(9)- H(44)	105.3691			H(51)- C(8)- C(9)	109.9518				
		H(45)- C(9)- C(8)	112.756			H(51)- C(8)- C(7)	111.258				
		H(45)- C(9)- C(5)	110.7999			C(9)- C(8)- C(7)	105.3731				
		H(44)- C(9)- C(8)	103.1854			O(45)- C(7)- C(28)	112.2712				
		H(44)- C(9)- C(5)	115.3451			O(45)- C(7)- C(27)	107.6925				
		C(8)- C(9)- C(5)	109.2232			O(45)- C(7)- C(8)	106.2602				
		Lp(95)- O(35)- Lp(94)	130.1833			C(28)- C(7)- C(27)	109.7607				
		Lp(95)- O(35)- V(38)	110.0048			C(28)- C(7)- C(8)	115.1572				
		Lp(95)- O(35)- C(1)	99.9149			C(27)- C(7)- C(8)	105.2181				
		Lp(94)- O(35)- V(38)	107.2565			O(48)- V(47)- O(46)	108.9599				
		Lp(94)- O(35)- C(1)	94.1248			O(48)- V(47)- N(26)	93.6983				
		V(38)- O(35)- C(1)	113.6578			O(48)- V(47)- N(21)	91.5613				
		C(9)- C(5)- C(6)	118.7321			O(48)- V(47)- N(12)	148.0438				
		C(9)- C(5)- C(4)	121.3776			O(46)- V(47)- N(26)	92.6145				
		C(6)- C(5)- C(4)	111.2597			O(46)- V(47)- N(21)	94.0162				
		C(10)- C(6)- C(5)	115.5032			O(46)- V(47)- N(12)	102.0567				
		C(10)- C(6)- C(1)	118.4238			N(26)- V(47)- N(21)	169.7248				
		C(5)- C(6)- C(1)	108.4267			N(26)- V(47)- N(12)	92.3718				
		O(34)- C(4)- C(5)	114.4138			N(21)- V(47)- N(12)	78.5726				

		O(34)- C(4)- C(3)	103.0361			Lp(110)- O(45)- Lp(109)	125.2456				
		C(5)- C(4)- C(3)	105.2148			Lp(110)- O(45)- C(7)	114.3777				
		H(41)- C(3)- C(4)	114.3808			Lp(110)- O(45)- C(4)	101.2956				
		H(41)- C(3)- C(2)	112.116			Lp(109)- O(45)- C(7)	108.6795				
		C(4)- C(3)- C(2)	113.3737			Lp(109)- O(45)- C(4)	99.5762				
		H(40)- C(2)- C(3)	118.5748			C(7)- O(45)- C(4)	103.7792				
		H(40)- C(2)- C(1)	109.012			H(58)- C(11)- H(57)	106.3229				
		C(3)- C(2)- C(1)	110.5741			H(58)- C(11)- N(12)	104.5078				
		O(35)- C(1)- C(2)	112.5904			H(58)- C(11)- C(6)	111.7462				
		O(35)- C(1)- C(6)	108.7072			H(57)- C(11)- N(12)	113.4222				
		C(2)- C(1)- C(6)	113.8516			H(57)- C(11)- C(6)	109.6549				
						N(12)- C(11)- C(6)	111.0256				
						H(52)- C(9)- H(53)	104.631				
						H(52)- C(9)- C(8)	109.651				
						H(52)- C(9)- C(5)	115.3488				
						H(53)- C(9)- C(8)	103.5982				
						H(53)- C(9)- C(5)	109.0394				
						C(8)- C(9)- C(5)	113.5233				
						Lp(112)- O(46)- Lp(111)	119.6283				
						Lp(112)- O(46)- V(47)	104.8797				
						Lp(112)- O(46)- C(1)	104.0545				
						Lp(111)- O(46)- V(47)	108.9594				
						Lp(111)- O(46)- C(1)	104.9981				

						V(47)- O(46)- C(1)	114.6588						
						H(56)- C(10)- H(54)	106.0365						
						H(56)- C(10)- H(55)	104.5661						
						H(56)- C(10)- C(3)	118.6336						
						H(54)- C(10)- H(55)	108.3701						
						H(54)- C(10)- C(3)	112.5787						
						H(55)- C(10)- C(3)	106.0289						
						C(9)- C(5)- C(6)	111.0769						
						C(9)- C(5)- C(4)	109.1877						
						C(6)- C(5)- C(4)	113.9578						
						C(11)- C(6)- C(5)	124.1736						
						C(11)- C(6)- C(1)	100.4916						
						C(5)- C(6)- C(1)	109.2343						
						O(45)- C(4)- C(5)	117.9441						
						O(45)- C(4)- C(3)	111.7761						
						C(5)- C(4)- C(3)	112.4239						
						C(10)- C(3)- C(4)	109.7825						
						C(10)- C(3)- C(2)	104.7664						
						C(4)- C(3)- C(2)	116.4556						
						H(49)- C(2)- C(3)	105.832						
						H(49)- C(2)- C(1)	105.4882						
						C(3)- C(2)- C(1)	109.0221						
						O(46)- C(1)- C(2)	104.755						

						O(46)- C(1)- C(6)	112.1162				
						C(2)- C(1)- C(6)	119.4953				