

Electronic Supplementary Information

Relativistic Effects in Triphenylbismuth and Their Consequences on Molecular Structure and Spectroscopic Properties

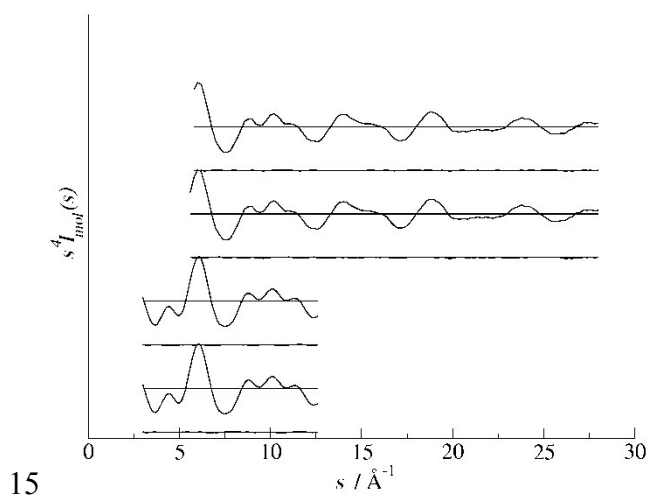
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S1 Gas-phase electron diffraction data details

10 **Table S1** Experimental details for the gas electron diffraction experiment of BiPh₃. The calibrated electron wavelength was 0.04816 nm for all datasets.

Data set	R_g %	R_d %	K	e.s.d	Corr. Parameter	s [nm ⁻¹]	s_{\min} [nm ⁻¹]	s_{w1} [nm ⁻¹]	s_{w2} [nm ⁻¹]	s_{\max} [nm ⁻¹]	d [mm]
1	7.37	3.53	0.8089	0.0074	0.4932	1.00	30.0	47.0	113.0	126.0	500.0
2	6.56	3.07	0.8081	0.0075	0.4879	1.00	30.0	49.0	114.0	126.0	500.0
3	10.94	8.04	0.6882	0.0074	0.3125	2.00	56.0	76.0	258.0	280.0	250.0
4	10.79	8.05	0.6895	0.0079	0.2984	2.00	58.0	78.0	240.8	280.0	250.0

S2 Gas-phase electron diffraction molecular scattering intensity curves



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S3 Refined structure parameters and restraints

parameter	short description	restraint(uncertainty)	value(e.s.d.)
<i>p</i> [1]	rBiC	–	2.263(3)
<i>p</i> [2]	tors	43.5(20)	43.6(20)
<i>p</i> [3]	wiC3	–	31.9(7)
<i>p</i> [4]	dwBi	–4.0(10)	–3.70(96)
<i>p</i> [5]	rC1C4	1.390(14)	1.398(10)
<i>p</i> [6]	rC4C2	1.390(14)	1.400(10)
<i>p</i> [7]	rC2C6	1.390(14)	1.400(11)
<i>p</i> [8]	rC6C3	1.390(14)	1.398(11)
<i>p</i> [9]	rC3C5	1.390(14)	1.401(09)
<i>p</i> [10]	rC5C1	1.390(14)	1.392(10)
<i>p</i> [11]	wC1C4C2	120.0(10)	119.84(87)
<i>p</i> [12]	wC3C5C1	120.0(10)	119.78(83)
<i>p</i> [13]	wC2C6C3	120.0(10)	119.16(51)
<i>p</i> [14]	rH5	1.070(10)	1.065(10)
<i>p</i> [15]	rH1	1.070(10)	1.065(09)
<i>p</i> [16]	rH4	1.070(10)	1.065(09)
<i>p</i> [17]	rH2	1.070(10)	1.064(09)
<i>p</i> [18]	rH6	1.070(10)	1.067(09)
<i>p</i> [19]	dwH5	3.6(10)	3.7(10)
<i>p</i> [20]	dwH1	1.4(20)	1.3(20)
<i>p</i> [21]	dwH4	–1.6(20)	–1.4(19)
<i>p</i> [22]	dwH2	1.6(20)	1.6(20)
<i>p</i> [23]	dwH6	–0.1(20)	–0.1(20)

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S4 Independently refined amplitudes of vibration

Table 4 Independently refined vibrational amplitudes from the structure refinement of BiPh3

amplitude	description	$r_{h,1}$	u	orig. u	area	k
u_4	Bi(1)···C(5)	4.493(16)	0.125(15)	0.101	0.4	-0.011
u_{15}	Bi(1)···C(16)	4.518(13)	0.091(9)	0.091	0.1	-0.018
u_{23}	Bi(1)-C(24)	2.264(3)	0.071(4)	0.068	100.0	0.003
u_{28}	Bi(1)···C(29)	5.040(7)	0.105(8)	0.090	44.9	-0.025
u_{29}	Bi(1)···H(30)	6.091(11)	0.119(10)	0.116	6.2	-0.041
u_{34}	C(2)-C(3)	1.398(10)	0.037(1)	0.049	11.7	0.001
u_{35}	C(2)···H(4)	2.115(16)	0.082(5)	0.101	1.3	-0.013
u_{36}	C(2)···C(5)	2.423(13)	0.058(3)	0.064	6.8	0.004
u_{350}	C(13)···C(33)	3.898(32)	0.461(49)	0.469	4.2	-0.036
u_{361}	C(14)···C(24)	3.449(36)	0.327(17)	0.280	4.7	0.129
u_{363}	C(14)···H(26)	3.997(91)	0.965(89)	0.965	0.7	0.055
u_{364}	C(14)···C(27)	4.898(64)	0.586(49)	0.585	3.3	0.158
u_{380}	H(15)···C(24)	2.893(43)	0.543(24)	0.454	0.9	0.298
u_{382}	H(15)···H(26)	3.338(118)	1.159(87)	1.100	0.1	0.147
u_{385}	H(15)···C(29)	4.430(56)	0.679(68)	0.677	0.6	0.412
u_{389}	H(15)···C(33)	2.954(87)	1.031(30)	0.825	0.9	0.241
u_{398}	C(16)···C(24)	4.780(38)	0.288(29)	0.289	3.4	0.087
u_{407}	C(16)···C(33)	4.986(60)	0.727(79)	0.729	3.3	0.051
u_{469}	C(20)···C(33)	6.048(32)	0.629(59)	0.628	2.7	-0.141
u_{485}	C(22)···C(24)	4.571(22)	0.176(16)	0.172	3.6	-0.095
u_{527}	H(26)···H(28)	2.402(25)	0.164(20)	0.167	0.2	-0.002
u_{556}	C(31)-H(32)	1.061(9)	0.088(5)	0.077	2.6	0.004

^a Footnote text.

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S5 Complete Table of amplitude refinement

Amplitude	Distance (ra)	e.s.d.	u -Value	e.s.d.	Mult. k -Value	Area	Orig. u -Value		
$u[458]$	C(20)-C(22)	1.4007	0.0106	0.0354	Tied to $u[34]$	1.00	0.0014	11.7	0.0465
$u[557]$	C(31)-C(33)	1.4007	0.0106	0.0355	Tied to $u[34]$	1.00	0.0014	11.7	0.0466
10 $u[67]$	C(3)-C(5)	1.4007	0.0106	0.0355	Tied to $u[34]$	1.00	0.0014	11.7	0.0466
$u[238]$	C(9)-C(11)	1.4013	0.0096	0.0355	Tied to $u[34]$	1.00	0.0014	11.7	0.0466
$u[518]$	C(25)-C(27)	1.4013	0.0096	0.0356	Tied to $u[34]$	1.00	0.0014	11.7	0.0466
$u[353]$	C(14)-C(16)	1.4013	0.0096	0.0357	Tied to $u[34]$	1.00	0.0014	11.7	0.0467
15 $u[128]$	C(5)-C(7)	1.4004	0.0113	0.0366	Tied to $u[34]$	1.00	0.0013	11.7	0.0480
$u[535]$	C(27)-C(29)	1.3986	0.0113	0.0368	Tied to $u[34]$	1.00	0.0013	11.7	0.0483
$u[185]$	C(7)-C(9)	1.3985	0.0113	0.0368	Tied to $u[34]$	1.00	0.0012	11.7	0.0483
$u[427]$	C(18)-C(20)	1.4004	0.0113	0.0369	Tied to $u[34]$	1.00	0.0013	11.7	0.0482
$u[392]$	C(16)-C(18)	1.3986	0.0113	0.0369	Tied to $u[34]$	1.00	0.0013	11.7	0.0484
$u[548]$	C(29)-C(31)	1.4004	0.0113	0.0369	Tied to $u[34]$	1.00	0.0013	11.7	0.0483
20 $u[42]$	C(2)-C(11)	1.3925	0.0099	0.0371	Tied to $u[34]$	1.00	0.0011	11.8	0.0487
$u[507]$	C(24)-C(25)	1.3925	0.0099	0.0373	Tied to $u[34]$	1.00	0.0011	11.8	0.0489
$u[331]$	C(13)-C(14)	1.3925	0.0099	0.0373	Tied to $u[34]$	1.00	0.0011	11.8	0.0490
$u[34]$	C(2)-C(3)	1.3979	0.0103	0.0374	0.0012	1.00	0.0012	11.7	0.0491
25 $u[515]$	C(24)-C(33)	1.3977	0.0103	0.0375	Tied to $u[34]$	1.00	0.0011	11.7	0.0492
$u[339]$	C(13)-C(22)	1.3977	0.0103	0.0376	Tied to $u[34]$	1.00	0.0011	11.7	0.0493
$u[537]$	C(27)···C(31)	2.4001	0.0120	0.0552	Tied to $u[36]$	1.00	-0.0117	6.8	0.0608
$u[394]$	C(16)···C(20)	2.4026	0.0120	0.0552	Tied to $u[36]$	1.00	-0.0092	6.8	0.0608
$u[130]$	C(5)···C(9)	2.3983	0.0120	0.0552	Tied to $u[36]$	1.00	-0.0135	6.8	0.0609
$u[69]$	C(3)···C(7)	2.4311	0.0120	0.0556	Tied to $u[36]$	1.00	0.0020	6.7	0.0613
30 $u[359]$	C(14)···C(22)	2.4091	0.0097	0.0558	Tied to $u[36]$	1.00	-0.0079	6.8	0.0615
$u[524]$	C(25)···C(33)	2.4066	0.0097	0.0559	Tied to $u[36]$	1.00	-0.0104	6.8	0.0616
$u[429]$	C(18)···C(22)	2.4304	0.0120	0.0559	Tied to $u[36]$	1.00	0.0013	6.7	0.0616
$u[73]$	C(3)···C(11)	2.4052	0.0097	0.0559	Tied to $u[36]$	1.00	-0.0118	6.8	0.0616
35 $u[550]$	C(29)···C(33)	2.4313	0.0120	0.0561	Tied to $u[36]$	1.00	0.0022	6.7	0.0618
$u[520]$	C(25)···C(29)	2.4337	0.0121	0.0564	Tied to $u[36]$	1.00	0.0034	6.7	0.0622

	u[355]	C(14)...C(18)	2.4318	0.0121	0.0564	Tied to u[36]	1.00	0.0015	6.7	0.0622
	u[187]	C(7)...C(11)	2.4354	0.0121	0.0565	Tied to u[36]	1.00	0.0051	6.7	0.0623
	u[40]	C(2)...C(9)	2.4156	0.0118	0.0566	Tied to u[36]	1.00	0.0006	6.8	0.0624
	u[333]	C(13)...C(16)	2.4149	0.0118	0.0570	Tied to u[36]	1.00	-0.0001	6.8	0.0628
5	u[509]	C(24)...C(27)	2.4156	0.0118	0.0571	Tied to u[36]	1.00	0.0007	6.8	0.0629
	u[337]	C(13)...C(20)	2.4198	0.0134	0.0574	Tied to u[36]	1.00	0.0001	6.8	0.0633
	u[513]	C(24)...C(31)	2.4216	0.0134	0.0575	Tied to u[36]	1.00	0.0019	6.8	0.0634
	u[36]	C(2)...C(5)	2.4234	0.0134	0.0576	0.0026	1.00	0.0037	6.8	0.0635
	u[1]	Bi(1)-C(2)	2.2637	0.0031	0.0709	Tied to u[23]	1.00	0.0029	100.0	0.0680
10	u[23]	Bi(1)-C(24)	2.2637	0.0031	0.0710	0.0039	1.00	0.0029	100.0	0.0681
	u[12]	Bi(1)-C(13)	2.2637	0.0031	0.0710	Tied to u[23]	1.00	0.0029	100.0	0.0681
	u[35]	C(2)...H(4)	2.1152	0.0159	0.0819	0.0048	1.00	-0.0128	1.3	0.1014
	u[442]	H(19)...C(20)	2.1451	0.0166	0.0821	Tied to u[35]	1.00	0.0000	1.3	0.1016
	u[516]	C(24)...H(34)	2.1166	0.0159	0.0822	Tied to u[35]	1.00	-0.0114	1.3	0.1017
15	u[129]	C(5)...H(8)	2.1461	0.0166	0.0822	Tied to u[35]	1.00	0.0010	1.3	0.1017
	u[340]	C(13)...H(23)	2.1189	0.0159	0.0822	Tied to u[35]	1.00	-0.0091	1.3	0.1017
	u[552]	H(30)...C(31)	2.1461	0.0166	0.0823	Tied to u[35]	1.00	0.0010	1.3	0.1019
	u[332]	C(13)...H(15)	2.1426	0.0143	0.0824	Tied to u[35]	1.00	-0.0088	1.3	0.1020
	u[541]	H(28)...C(29)	2.1328	0.0163	0.0824	Tied to u[35]	1.00	-0.0119	1.3	0.1020
20	u[186]	C(7)...H(10)	2.1312	0.0163	0.0824	Tied to u[35]	1.00	-0.0135	1.3	0.1020
	u[43]	C(2)...H(12)	2.1397	0.0143	0.0825	Tied to u[35]	1.00	-0.0117	1.3	0.1021
	u[409]	H(17)...C(18)	2.1350	0.0163	0.0825	Tied to u[35]	1.00	-0.0097	1.3	0.1021
	u[508]	C(24)...H(26)	2.1406	0.0143	0.0825	Tied to u[35]	1.00	-0.0108	1.3	0.1021
	u[393]	C(16)...H(19)	2.1425	0.0166	0.0827	Tied to u[35]	1.00	0.0000	1.3	0.1024
25	u[211]	H(8)...C(9)	2.1458	0.0166	0.0827	Tied to u[35]	1.00	0.0033	1.3	0.1024
	u[536]	C(27)...H(30)	2.1443	0.0166	0.0827	Tied to u[35]	1.00	0.0018	1.3	0.1024
	u[38]	C(2)...C(7)	2.7952	0.0075	0.0828	Tied to u[380]	1.00	-0.0071	5.9	0.0693
	u[428]	C(18)...H(21)	2.1335	0.0181	0.0829	Tied to u[35]	1.00	-0.0100	1.3	0.1026
	u[549]	C(29)...H(32)	2.1315	0.0181	0.0829	Tied to u[35]	1.00	-0.0120	1.3	0.1026
30	u[511]	C(24)...C(29)	2.7948	0.0075	0.0829	Tied to u[380]	1.00	-0.0074	5.9	0.0694
	u[335]	C(13)...C(18)	2.7953	0.0075	0.0829	Tied to u[380]	1.00	-0.0069	5.9	0.0694
	u[156]	H(6)...C(7)	2.1302	0.0181	0.0831	Tied to u[35]	1.00	-0.0133	1.3	0.1028
	u[372]	H(15)...C(16)	2.1203	0.0142	0.0832	Tied to u[35]	1.00	-0.0002	1.3	0.1029
	u[526]	H(26)...C(27)	2.1218	0.0142	0.0833	Tied to u[35]	1.00	0.0013	1.3	0.1031
35	u[239]	C(9)...H(12)	2.1230	0.0142	0.0833	Tied to u[35]	1.00	0.0025	1.3	0.1031
	u[97]	H(4)...C(5)	2.1481	0.0194	0.0836	Tied to u[35]	1.00	0.0004	1.3	0.1034
	u[558]	C(31)...H(34)	2.1485	0.0194	0.0838	Tied to u[35]	1.00	0.0008	1.3	0.1037
	u[459]	C(20)...H(23)	2.1478	0.0194	0.0838	Tied to u[35]	1.00	0.0001	1.3	0.1037
	u[471]	H(21)...C(22)	2.1263	0.0174	0.0839	Tied to u[35]	1.00	-0.0001	1.3	0.1038
40	u[262]	H(10)...C(11)	2.1235	0.0185	0.0840	Tied to u[35]	1.00	-0.0001	1.3	0.1039
	u[559]	H(32)...C(33)	2.1279	0.0174	0.0840	Tied to u[35]	1.00	0.0015	1.3	0.1040
	u[519]	C(25)...H(28)	2.1237	0.0185	0.0840	Tied to u[35]	1.00	0.0001	1.3	0.1040
	u[354]	C(14)...H(17)	2.1231	0.0185	0.0840	Tied to u[35]	1.00	-0.0005	1.3	0.1040
	u[68]	C(3)...H(6)	2.1295	0.0174	0.0843	Tied to u[35]	1.00	0.0032	1.3	0.1043
45	u[547]	C(29)-H(30)	1.0642	0.0093	0.0869	Tied to u[556]	1.00	0.0038	2.6	0.0764
	u[426]	C(18)-H(19)	1.0642	0.0093	0.0869	Tied to u[556]	1.00	0.0038	2.6	0.0764
	u[184]	C(7)-H(8)	1.0642	0.0093	0.0869	Tied to u[556]	1.00	0.0038	2.6	0.0764
	u[132]	C(5)...C(11)	2.7845	0.0144	0.0870	Tied to u[380]	1.00	-0.0068	5.9	0.0728
	u[391]	C(16)-H(17)	1.0615	0.0093	0.0878	Tied to u[556]	1.00	0.0039	2.6	0.0772
50	u[286]	C(11)-H(12)	1.0616	0.0094	0.0878	Tied to u[556]	1.00	0.0038	2.6	0.0772
	u[352]	C(14)-H(15)	1.0616	0.0094	0.0878	Tied to u[556]	1.00	0.0038	2.6	0.0772
	u[237]	C(9)-H(10)	1.0615	0.0093	0.0878	Tied to u[556]	1.00	0.0039	2.6	0.0772
	u[517]	C(25)-H(26)	1.0616	0.0094	0.0879	Tied to u[556]	1.00	0.0038	2.6	0.0773
	u[534]	C(27)-H(28)	1.0615	0.0093	0.0879	Tied to u[556]	1.00	0.0039	2.6	0.0773
55	u[522]	C(25)...C(31)	2.7871	0.0144	0.0879	Tied to u[380]	1.00	-0.0042	5.9	0.0736
	u[556]	C(31)-H(32)	1.0605	0.0094	0.0880	0.0047	1.00	0.0039	2.6	0.0774
	u[457]	C(20)-H(21)	1.0605	0.0094	0.0880	Tied to u[556]	1.00	0.0039	2.6	0.0774
	u[127]	C(5)-H(6)	1.0604	0.0094	0.0881	Tied to u[556]	1.00	0.0039	2.6	0.0775
	u[357]	C(14)...C(20)	2.7881	0.0144	0.0882	Tied to u[380]	1.00	-0.0031	5.9	0.0738
60	u[66]	C(3)-H(4)	1.0614	0.0094	0.0883	Tied to u[556]	1.00	0.0039	2.6	0.0776
	u[71]	C(3)...C(9)	2.7893	0.0150	0.0883	Tied to u[380]	1.00	0.0015	5.9	0.0739
	u[484]	C(22)-H(23)	1.0613	0.0094	0.0884	Tied to u[556]	1.00	0.0038	2.6	0.0777
	u[561]	C(33)-H(34)	1.0613	0.0094	0.0884	Tied to u[556]	1.00	0.0038	2.6	0.0777
	u[539]	C(27)...C(33)	2.7868	0.0150	0.0887	Tied to u[380]	1.00	-0.0009	5.9	0.0742
65	u[396]	C(16)...C(22)	2.7853	0.0150	0.0888	Tied to u[380]	1.00	-0.0024	5.9	0.0743
	u[8]	Bi(1)...C(9)	4.5186	0.0130	0.0905	Tied to u[15]	1.00	-0.0175	50.1	0.0905
	u[26]	Bi(1)...C(27)	4.5196	0.0130	0.0907	Tied to u[15]	1.00	-0.0165	50.1	0.0907
	u[15]	Bi(1)...C(16)	4.5182	0.0130	0.0909	0.0092	1.00	-0.0179	50.1	0.0909
	u[39]	C(2)...H(8)	3.8509	0.0119	0.1052	Tied to u[382]	1.00	-0.0184	0.7	0.0998
70	u[336]	C(13)...H(19)	3.8511	0.0119	0.1052	Tied to u[382]	1.00	-0.0182	0.7	0.0998
	u[512]	C(24)...H(30)	3.8507	0.0119	0.1053	Tied to u[382]	1.00	-0.0186	0.7	0.0999
	u[28]	Bi(1)...C(29)	5.0399	0.0069	0.1054	0.0079	1.00	-0.0251	44.9	0.0896
	u[6]	Bi(1)...C(7)	5.0396	0.0069	0.1054	Tied to u[28]	1.00	-0.0254	44.9	0.0896
	u[17]	Bi(1)...C(18)	5.0392	0.0069	0.1059	Tied to u[28]	1.00	-0.0258	44.9	0.0900

	u[133]	C(5)...H(12)	3.8376	0.0170	0.1106	Tied to u[382]	1.00	-0.0179	0.7	0.1049
	u[160]	H(6)...C(11)	3.8365	0.0170	0.1112	Tied to u[382]	1.00	-0.0180	0.7	0.1055
	u[530]	H(23)...C(31)	3.8402	0.0170	0.1116	Tied to u[382]	1.00	-0.0152	0.7	0.1059
	u[72]	C(3)...H(10)	3.8424	0.0175	0.1117	Tied to u[382]	1.00	-0.0096	0.7	0.1060
5	u[376]	H(15)...C(20)	3.8412	0.0170	0.1119	Tied to u[382]	1.00	-0.0142	0.7	0.1062
	u[523]	C(25)...H(32)	3.8391	0.0170	0.1120	Tied to u[382]	1.00	-0.0154	0.7	0.1063
	u[101]	H(4)...C(9)	3.8425	0.0176	0.1122	Tied to u[382]	1.00	-0.0096	0.7	0.1065
	u[358]	C(14)...H(21)	3.8401	0.0170	0.1123	Tied to u[382]	1.00	-0.0144	0.7	0.1066
	u[545]	H(28)...C(33)	3.8398	0.0175	0.1123	Tied to u[382]	1.00	-0.0121	0.7	0.1066
10	u[413]	H(17)...C(22)	3.8384	0.0175	0.1124	Tied to u[382]	1.00	-0.0135	0.7	0.1067
	u[540]	C(27)...H(34)	3.8398	0.0176	0.1129	Tied to u[382]	1.00	-0.0122	0.7	0.1071
	u[397]	C(16)...H(23)	3.8383	0.0176	0.1131	Tied to u[382]	1.00	-0.0137	0.7	0.1073
	u[444]	H(19)...C(22)	3.8861	0.0156	0.1142	Tied to u[361]	1.00	-0.0087	0.8	0.0979
	u[70]	C(3)...H(8)	3.3857	0.0156	0.1143	Tied to u[361]	1.00	-0.0091	0.8	0.0980
15	u[554]	H(30)...C(33)	3.3865	0.0156	0.1146	Tied to u[361]	1.00	-0.0083	0.8	0.0982
	u[521]	C(25)...H(30)	3.3884	0.0157	0.1153	Tied to u[361]	1.00	-0.0065	0.8	0.0988
	u[356]	C(14)...H(19)	3.3865	0.0157	0.1153	Tied to u[361]	1.00	-0.0084	0.8	0.0988
	u[213]	H(8)...C(11)	3.3906	0.0157	0.1155	Tied to u[361]	1.00	-0.0043	0.8	0.0990
	u[131]	C(5)...H(10)	3.3569	0.0147	0.1160	Tied to u[361]	1.00	-0.0246	0.8	0.0994
20	u[543]	H(28)...C(31)	3.3586	0.0147	0.1162	Tied to u[361]	1.00	-0.0229	0.8	0.0996
	u[103]	H(4)...C(11)	3.3495	0.0134	0.1162	Tied to u[361]	1.00	-0.0231	0.8	0.0996
	u[411]	H(17)...C(20)	3.3613	0.0147	0.1163	Tied to u[361]	1.00	-0.0202	0.8	0.0997
	u[525]	C(25)...H(34)	3.3508	0.0134	0.1164	Tied to u[361]	1.00	-0.0218	0.8	0.0998
	u[360]	C(14)...H(23)	3.3535	0.0134	0.1165	Tied to u[361]	1.00	-0.0191	0.8	0.0999
25	u[532]	H(26)...C(33)	3.3692	0.0139	0.1167	Tied to u[361]	1.00	-0.0219	0.8	0.1000
	u[378]	H(15)...C(22)	3.3725	0.0139	0.1167	Tied to u[361]	1.00	-0.0186	0.8	0.1000
	u[74]	C(3)...H(12)	3.3671	0.0139	0.1167	Tied to u[361]	1.00	-0.0240	0.8	0.1000
	u[538]	C(27)...H(32)	3.3553	0.0166	0.1168	Tied to u[361]	1.00	-0.0237	0.8	0.1001
	u[395]	C(16)...H(21)	3.3585	0.0166	0.1168	Tied to u[361]	1.00	-0.0205	0.8	0.1001
30	u[158]	H(6)...C(9)	3.3525	0.0166	0.1170	Tied to u[361]	1.00	-0.0265	0.8	0.1003
	u[29]	Bi(1)...H(30)	6.0909	0.0113	0.1191	0.0095	1.00	-0.0414	6.2	0.1163
	u[7]	Bi(1)...H(8)	6.0905	0.0113	0.1191	Tied to u[29]	1.00	-0.0418	6.2	0.1163
	u[10]	Bi(1)...C(11)	3.2094	0.0117	0.1191	Tied to u[389]	1.00	-0.0043	70.5	0.0954
	u[18]	Bi(1)...H(19)	6.0900	0.0113	0.1194	Tied to u[29]	1.00	-0.0423	6.2	0.1166
35	u[24]	Bi(1)...C(25)	3.2099	0.0117	0.1197	Tied to u[389]	1.00	-0.0038	70.5	0.0959
	u[13]	Bi(1)...C(14)	3.2086	0.0117	0.1199	Tied to u[389]	1.00	-0.0050	70.5	0.0960
	u[188]	C(7)...H(12)	3.3762	0.0155	0.1217	Tied to u[361]	1.00	-0.0013	0.8	0.1043
	u[99]	H(4)...C(7)	3.3917	0.0183	0.1219	Tied to u[361]	1.00	-0.0030	0.8	0.1045
	u[374]	H(15)...C(18)	3.3719	0.0155	0.1219	Tied to u[361]	1.00	-0.0056	0.8	0.1045
40	u[41]	C(2)...H(10)	3.3620	0.0182	0.1220	Tied to u[361]	1.00	-0.0047	0.8	0.1046
	u[528]	H(26)...C(29)	3.3745	0.0155	0.1220	Tied to u[361]	1.00	-0.0030	0.8	0.1046
	u[551]	C(29)...H(34)	3.3913	0.0183	0.1228	Tied to u[361]	1.00	-0.0034	0.8	0.1053
	u[430]	C(18)...H(23)	3.3894	0.0183	0.1228	Tied to u[361]	1.00	-0.0053	0.8	0.1053
	u[510]	C(24)...H(28)	3.3615	0.0182	0.1230	Tied to u[361]	1.00	-0.0052	0.8	0.1054
45	u[334]	C(13)...H(17)	3.3599	0.0182	0.1230	Tied to u[361]	1.00	-0.0068	0.8	0.1054
	u[338]	C(13)...H(21)	3.3667	0.0178	0.1237	Tied to u[361]	1.00	-0.0066	0.8	0.1060
	u[37]	C(2)...H(6)	3.3714	0.0178	0.1238	Tied to u[361]	1.00	-0.0019	0.8	0.1061
	u[514]	C(24)...H(32)	3.3692	0.0178	0.1238	Tied to u[361]	1.00	-0.0041	0.8	0.1061
	u[4]	Bi(1)...C(5)	4.4925	0.0160	0.1254	0.0147	1.00	-0.0113	50.4	0.1007
50	u[30]	Bi(1)...C(31)	4.4905	0.0160	0.1257	Tied to u[4]	1.00	-0.0133	50.4	0.1009
	u[19]	Bi(1)...C(20)	4.4882	0.0160	0.1264	Tied to u[4]	1.00	-0.0156	50.4	0.1015
	u[161]	H(6)...H(12)	4.8873	0.0187	0.1309	(fixed)	1.00	-0.0317	0.1	0.1309
	u[102]	H(4)...H(10)	4.8929	0.0193	0.1319	(fixed)	1.00	-0.0234	0.1	0.1319
	u[531]	H(26)...H(32)	4.8899	0.0187	0.1320	(fixed)	1.00	-0.0290	0.1	0.1320
55	u[377]	H(15)...H(21)	4.8909	0.0187	0.1324	(fixed)	1.00	-0.0280	0.1	0.1324
	u[546]	H(28)...H(34)	4.8904	0.0193	0.1329	(fixed)	1.00	-0.0259	0.1	0.1329
	u[414]	H(17)...H(23)	4.8889	0.0193	0.1332	(fixed)	1.00	-0.0274	0.1	0.1332
	u[2]	Bi(1)...C(3)	3.1696	0.0136	0.1333	Tied to u[389]	1.00	0.0014	71.4	0.1068
	u[32]	Bi(1)...C(33)	3.1674	0.0136	0.1340	Tied to u[389]	1.00	-0.0007	71.5	0.1073
60	u[104]	H(4)...H(12)	4.2284	0.0172	0.1348	(fixed)	1.00	-0.0393	0.1	0.1348
	u[379]	H(15)...H(23)	4.2352	0.0172	0.1349	(fixed)	1.00	-0.0325	0.1	0.1349
	u[21]	Bi(1)...C(22)	3.1656	0.0136	0.1350	Tied to u[389]	1.00	-0.0025	71.5	0.1081
	u[533]	H(26)...H(34)	4.2306	0.0172	0.1350	(fixed)	1.00	-0.0370	0.1	0.1350
	u[544]	H(28)...H(32)	4.2337	0.0194	0.1359	(fixed)	1.00	-0.0389	0.1	0.1359
65	u[412]	H(17)...H(21)	4.2381	0.0194	0.1360	(fixed)	1.00	-0.0345	0.1	0.1360
	u[159]	H(6)...H(10)	4.2307	0.0194	0.1361	(fixed)	1.00	-0.0419	0.1	0.1361
	u[100]	H(4)...H(8)	4.2682	0.0224	0.1377	(fixed)	1.00	-0.0131	0.1	0.1377
	u[375]	H(15)...H(19)	4.2405	0.0195	0.1381	(fixed)	1.00	-0.0147	0.1	0.1381
	u[529]	H(26)...H(30)	4.2439	0.0195	0.1382	(fixed)	1.00	-0.0113	0.1	0.1382
70	u[214]	H(8)...H(12)	4.2466	0.0195	0.1383	(fixed)	1.00	-0.0086	0.1	0.1383
	u[445]	H(19)...H(23)	4.2667	0.0224	0.1383	(fixed)	1.00	-0.0146	0.1	0.1383
	u[555]	H(30)...H(34)	4.2683	0.0224	0.1384	(fixed)	1.00	-0.0129	0.1	0.1384
	u[9]	Bi(1)...H(10)	5.3160	0.0237	0.1420	(fixed)	1.00	-0.0238	7.1	0.1420
	u[27]	Bi(1)...H(28)	5.3169	0.0237	0.1426	(fixed)	1.00	-0.0229	7.1	0.1426

	u[16]	Bi(1)...H(17)	5.3146	0.0237	0.1427	(fixed)	1.00	-.0252	7.1	0.1427
	u[31]	Bi(1)...H(32)	5.2770	0.0239	0.1541	(fixed)	1.00	-.0178	7.1	0.1541
	u[5]	Bi(1)...H(6)	5.2806	0.0239	0.1541	(fixed)	1.00	-.0142	7.1	0.1541
	u[20]	Bi(1)...H(21)	5.2730	0.0239	0.1546	(fixed)	1.00	-.0218	7.2	0.1546
5	u[373]	H(15)...H(17)	2.4023	0.0251	0.1634	Tied to u[527]	1.00	-.0016	0.2	0.1672
	u[98]	H(4)...H(6)	2.4499	0.0289	0.1634	Tied to u[527]	1.00	-.0019	0.2	0.1672
	u[472]	H(21)...H(23)	2.4500	0.0289	0.1634	Tied to u[527]	1.00	-.0018	0.2	0.1672
	u[263]	H(10)...H(12)	2.4020	0.0251	0.1636	Tied to u[527]	1.00	-.0019	0.2	0.1674
	u[527]	H(26)...H(28)	2.4021	0.0251	0.1636	0.0196	1.00	-.0018	0.2	0.1674
10	u[560]	H(32)...H(34)	2.4498	0.0289	0.1636	Tied to u[527]	1.00	-.0020	0.2	0.1674
	u[212]	H(8)...H(10)	2.4664	0.0262	0.1654	Tied to u[527]	1.00	-.0057	0.2	0.1693
	u[410]	H(17)...H(19)	2.4692	0.0262	0.1655	Tied to u[527]	1.00	-.0029	0.2	0.1694
	u[542]	H(28)...H(30)	2.4685	0.0262	0.1656	Tied to u[527]	1.00	-.0036	0.2	0.1695
	u[553]	H(30)...H(32)	2.4706	0.0277	0.1659	Tied to u[527]	1.00	-.0011	0.2	0.1698
15	u[443]	H(19)...H(21)	2.4694	0.0277	0.1659	Tied to u[527]	1.00	-.0023	0.2	0.1698
	u[157]	H(6)...H(8)	2.4726	0.0277	0.1661	Tied to u[527]	1.00	0.0009	0.2	0.1700
	u[485]	C(22)...C(24)	4.5711	0.0222	0.1762	0.0164	1.00	-.0947	3.6	0.1723
	u[75]	C(3)...C(13)	4.5738	0.0222	0.1864	Tied to u[485]	1.00	-.0912	3.6	0.1823
	u[460]	C(20)...C(24)	5.6336	0.0256	0.1918	(fixed)	1.00	-.0840	2.9	0.1918
20	u[64]	C(2)...C(33)	4.5675	0.0222	0.1930	Tied to u[485]	1.00	-.0970	3.6	0.1888
	u[341]	C(13)...C(24)	3.3178	0.0240	0.1934	Tied to u[389]	1.00	-.0002	4.9	0.1549
	u[44]	C(2)...C(13)	3.3174	0.0240	0.1963	Tied to u[389]	1.00	-.0002	4.9	0.1572
	u[55]	C(2)...C(24)	3.3163	0.0240	0.2004	Tied to u[389]	1.00	-.0008	4.9	0.1605
	u[134]	C(5)...C(13)	5.6303	0.0256	0.2050	(fixed)	1.00	-.0864	2.9	0.2050
25	u[62]	C(2)...C(31)	5.6246	0.0256	0.2118	(fixed)	1.00	-.0916	2.9	0.2118
	u[473]	H(21)...C(24)	6.5653	0.0275	0.2138	(fixed)	1.00	-.1340	0.4	0.2138
	u[11]	Bi(1)...H(12)	3.2924	0.0195	0.2286	Tied to u[389]	1.00	0.0057	11.5	0.1831
	u[162]	H(6)...C(13)	6.5665	0.0275	0.2291	(fixed)	1.00	-.1318	0.4	0.2291
	u[25]	Bi(1)...H(26)	3.2906	0.0195	0.2302	Tied to u[389]	1.00	0.0041	11.5	0.1844
30	u[14]	Bi(1)...H(15)	3.2887	0.0195	0.2304	Tied to u[389]	1.00	0.0023	11.5	0.1845
	u[431]	C(18)...C(24)	5.7266	0.0325	0.2331	(fixed)	1.00	-.0124	2.9	0.2331
	u[496]	H(23)...C(24)	4.8978	0.0266	0.2358	Tied to u[407]	1.00	-.1581	0.6	0.2363
	u[189]	C(7)...C(13)	5.7156	0.0325	0.2369	(fixed)	1.00	-.0231	2.9	0.2369
	u[63]	C(2)...H(32)	6.5579	0.0275	0.2382	(fixed)	1.00	-.1397	0.4	0.2382
35	u[105]	H(4)...C(13)	4.9078	0.0266	0.2412	Tied to u[407]	1.00	-.1476	0.6	0.2417
	u[3]	Bi(1)...H(4)	3.1636	0.0290	0.2427	Tied to u[389]	1.00	0.0080	11.9	0.1944
	u[60]	C(2)...C(29)	5.7134	0.0325	0.2439	(fixed)	1.00	-.0247	2.9	0.2439
	u[33]	Bi(1)...H(34)	3.1628	0.0290	0.2452	Tied to u[389]	1.00	0.0076	11.9	0.1964
	u[22]	Bi(1)...H(23)	3.1601	0.0290	0.2463	Tied to u[389]	1.00	0.0051	11.9	0.1973
40	u[65]	C(2)...H(34)	4.8987	0.0266	0.2521	Tied to u[407]	1.00	-.1557	0.6	0.2526
	u[446]	H(19)...C(24)	6.7100	0.0375	0.2651	(fixed)	1.00	-.0268	0.4	0.2651
	u[215]	H(8)...C(13)	6.6970	0.0375	0.2692	(fixed)	1.00	-.0394	0.4	0.2692
	u[61]	C(2)...H(30)	6.6949	0.0375	0.2762	(fixed)	1.00	-.0410	0.4	0.2762
	u[240]	C(9)...C(13)	4.7662	0.0383	0.2783	Tied to u[398]	1.00	0.0722	3.4	0.2790
45	u[346]	C(13)...C(29)	5.6655	0.0325	0.2862	(fixed)	1.00	-.0347	2.9	0.2862
	u[398]	C(16)...C(24)	4.7796	0.0383	0.2884	0.0288	1.00	0.0868	3.4	0.2891
	u[58]	C(2)...C(27)	4.7673	0.0383	0.2895	Tied to u[398]	1.00	0.0747	3.4	0.2902
	u[49]	C(2)...C(18)	5.6688	0.0325	0.2900	(fixed)	1.00	-.0310	2.9	0.2900
	u[200]	C(7)...C(24)	5.6635	0.0325	0.2941	(fixed)	1.00	-.0359	2.9	0.2941
50	u[287]	C(11)...C(13)	3.4417	0.0355	0.3109	Tied to u[361]	1.00	0.1183	4.8	0.2665
	u[490]	C(22)...C(29)	6.9202	0.0323	0.3216	(fixed)	1.00	-.1768	2.4	0.3216
	u[361]	C(14)...C(24)	3.4494	0.0356	0.3266	0.0166	1.00	0.1290	4.7	0.2800
	u[56]	C(2)...C(25)	3.4420	0.0356	0.3278	Tied to u[361]	1.00	0.1218	4.8	0.2810
	u[347]	C(13)...H(30)	6.6393	0.0359	0.3302	(fixed)	1.00	-.0527	0.4	0.3302
55	u[50]	C(2)...H(19)	6.6431	0.0359	0.3341	(fixed)	1.00	-.0485	0.4	0.3341
	u[226]	H(8)...C(24)	6.6373	0.0359	0.3380	(fixed)	1.00	-.0539	0.4	0.3380
	u[80]	C(3)...C(18)	6.9231	0.0323	0.3415	(fixed)	1.00	-.1720	2.4	0.3415
	u[501]	H(23)...C(29)	7.3985	0.0315	0.3448	(fixed)	1.00	-.2787	0.4	0.3448
	u[209]	C(7)...C(33)	6.9108	0.0323	0.3540	(fixed)	1.00	-.1831	2.4	0.3540
60	u[108]	H(4)...C(16)	6.8898	0.0320	0.3547	(fixed)	1.00	-.2650	0.4	0.3547
	u[251]	C(9)...C(24)	5.2138	0.0409	0.3642	(fixed)	1.00	-.0243	3.1	0.3642
	u[264]	H(10)...C(13)	5.2198	0.0502	0.3652	(fixed)	1.00	0.1268	0.5	0.3652
	u[261]	C(9)...H(34)	6.8939	0.0320	0.3655	(fixed)	1.00	-.2598	0.4	0.3655
	u[110]	H(4)...C(18)	7.4092	0.0315	0.3660	(fixed)	1.00	-.2660	0.4	0.3660
65	u[491]	C(22)...H(30)	7.8787	0.0364	0.3747	(fixed)	1.00	-.2063	0.3	0.3747
	u[106]	H(4)...C(14)	5.6523	0.0293	0.3784	(fixed)	1.00	-.2174	0.5	0.3784
	u[59]	C(2)...H(28)	5.2214	0.0502	0.3804	(fixed)	1.00	0.1306	0.5	0.3804
	u[344]	C(13)...C(27)	5.2115	0.0409	0.3809	(fixed)	1.00	-.0242	3.1	0.3809
	u[415]	H(17)...C(24)	5.2346	0.0502	0.3826	(fixed)	1.00	0.1442	0.5	0.3826
70	u[502]	H(23)...H(30)	8.3861	0.0342	0.3863	(fixed)	1.00	-.3182	0.1	0.3863
	u[260]	C(9)...C(33)	6.4470	0.0382	0.3866	(fixed)	1.00	-.1673	2.5	0.3866
	u[210]	C(7)...H(34)	7.3938	0.0315	0.3868	(fixed)	1.00	-.2794	0.4	0.3868
	u[47]	C(2)...C(16)	5.1983	0.0409	0.3925	(fixed)	1.00	-.0357	3.1	0.3925
	u[308]	C(11)...H(34)	5.6614	0.0293	0.3925	(fixed)	1.00	-.2065	0.5	0.3925

	u[81]	C(3)...H(19)	7.8818	0.0364	0.3953	(fixed)	1.00	-.2013	0.3	0.3953
	u[298]	C(11)...C(24)	4.0654	0.0408	0.4027	Tied to u[385]	1.00	-.0133	4.0	0.4015
	u[78]	C(3)...C(16)	6.4358	0.0382	0.4030	(fixed)	1.00	-.1766	2.5	0.4030
5	u[235]	H(8)...C(33)	7.8686	0.0364	0.4084	(fixed)	1.00	-.2132	0.3	0.4084
	u[111]	H(4)...H(19)	8.3971	0.0342	0.4096	(fixed)	1.00	-.3051	0.1	0.4096
	u[465]	C(20)...C(29)	7.7085	0.0409	0.4124	(fixed)	1.00	-.1660	2.1	0.4124
	u[307]	C(11)...C(33)	5.2882	0.0344	0.4149	(fixed)	1.00	-.1322	3.1	0.4149
	u[76]	C(3)...C(14)	5.2719	0.0344	0.4209	(fixed)	1.00	-.1475	3.1	0.4209
	u[45]	C(2)...C(14)	4.0443	0.0408	0.4210	Tied to u[385]	1.00	-.0307	4.0	0.4198
10	u[342]	C(13)...C(25)	4.0600	0.0408	0.4229	Tied to u[385]	1.00	-.0146	4.0	0.4217
	u[488]	C(22)...C(27)	6.4517	0.0382	0.4282	(fixed)	1.00	-.1575	2.5	0.4282
	u[499]	H(23)...C(27)	6.8943	0.0320	0.4285	(fixed)	1.00	-.2524	0.4	0.4285
	u[236]	H(8)...H(34)	8.3806	0.0342	0.4319	(fixed)	1.00	-.3194	0.1	0.4319
	u[478]	H(21)...C(29)	8.6739	0.0413	0.4350	(fixed)	1.00	-.2519	0.3	0.4350
15	u[139]	C(5)...C(18)	7.7026	0.0409	0.4366	(fixed)	1.00	-.1693	2.1	0.4366
	u[207]	C(7)...C(31)	7.6889	0.0410	0.4500	(fixed)	1.00	-.1815	2.1	0.4500
	u[53]	C(2)...C(22)	3.9179	0.0321	0.4501	Tied to u[350]	1.00	-.0186	4.2	0.4581
	u[350]	C(13)...C(33)	3.8978	0.0322	0.4610	0.0485	1.00	-.0362	4.2	0.4692
	u[486]	C(22)...C(25)	5.2888	0.0344	0.4630	(fixed)	1.00	-.1238	3.1	0.4630
20	u[497]	H(23)...C(25)	5.6582	0.0294	0.4633	(fixed)	1.00	-.1994	0.5	0.4633
	u[167]	H(6)...C(18)	8.6706	0.0413	0.4689	(fixed)	1.00	-.2517	0.3	0.4689
	u[86]	C(3)...C(24)	3.8925	0.0322	0.4800	Tied to u[350]	1.00	-.0370	4.2	0.4886
	u[51]	C(2)...C(20)	5.0929	0.0327	0.4863	Tied to u[28]	1.00	-.0237	3.2	0.4133
	u[208]	C(7)...H(32)	8.6530	0.0413	0.4883	(fixed)	1.00	-.2673	0.3	0.4883
25	u[466]	C(20)...H(30)	8.5929	0.0463	0.4897	(fixed)	1.00	-.1970	0.3	0.4897
	u[258]	C(9)...C(31)	7.2769	0.0485	0.4926	(fixed)	1.00	-.1640	2.2	0.4926
	u[305]	C(11)...C(31)	6.2455	0.0435	0.4998	(fixed)	1.00	-.1271	2.6	0.4998
	u[259]	C(9)...H(32)	8.2315	0.0478	0.5022	(fixed)	1.00	-.2444	0.3	0.5022
	u[306]	C(11)...H(32)	7.1829	0.0422	0.5058	(fixed)	1.00	-.1892	0.4	0.5058
30	u[306]	C(11)...H(32)	7.1829	0.0422	0.5058	(fixed)	1.00	-.1892	0.4	0.5058
	u[348]	C(13)...C(31)	5.0723	0.0327	0.5074	Tied to u[28]	1.00	-.0402	3.2	0.4312
	u[309]	H(12)...C(13)	2.8918	0.0430	0.5088	Tied to u[380]	1.00	0.2832	0.9	0.4258
	u[109]	H(4)...H(17)	7.5531	0.0402	0.5094	(fixed)	1.00	-.3038	0.1	0.5094
	u[492]	C(22)...C(31)	6.3065	0.0295	0.5105	(fixed)	1.00	-.1741	2.6	0.5105
35	u[436]	C(18)...C(29)	7.4315	0.0553	0.5143	(fixed)	1.00	-.0384	2.2	0.5143
	u[140]	C(5)...H(19)	8.5862	0.0463	0.5151	(fixed)	1.00	-.2008	0.3	0.5151
	u[479]	H(21)...H(30)	9.5551	0.0466	0.5169	(fixed)	1.00	-.2937	0.0	0.5169
	u[163]	H(6)...C(14)	7.1623	0.0422	0.5179	(fixed)	1.00	-.2081	0.4	0.5179
	u[135]	C(5)...C(14)	6.2214	0.0435	0.5209	(fixed)	1.00	-.1479	2.6	0.5209
40	u[194]	C(7)...C(18)	7.4182	0.0553	0.5226	(fixed)	1.00	-.0506	2.2	0.5226
	u[285]	H(10)...H(34)	7.5675	0.0402	0.5236	(fixed)	1.00	-.2875	0.1	0.5236
	u[503]	H(23)...C(31)	6.7624	0.0343	0.5256	(fixed)	1.00	-.2643	0.4	0.5256
	u[275]	H(10)...C(24)	5.9316	0.0517	0.5261	(fixed)	1.00	-.0348	0.5	0.5261
	u[165]	H(6)...C(16)	8.2161	0.0478	0.5263	(fixed)	1.00	-.2569	0.3	0.5263
45	u[137]	C(5)...C(16)	7.2579	0.0486	0.5277	(fixed)	1.00	-.1783	2.3	0.5277
	u[233]	H(8)...C(31)	8.5710	0.0463	0.5296	(fixed)	1.00	-.2143	0.3	0.5296
	u[145]	C(5)...C(24)	5.0667	0.0328	0.5322	Tied to u[28]	1.00	-.0408	3.2	0.4523
	u[82]	C(3)...C(20)	6.3321	0.0295	0.5323	(fixed)	1.00	-.1451	2.6	0.5323
	u[293]	C(11)...H(19)	6.1359	0.0526	0.5328	(fixed)	1.00	0.1450	0.4	0.5328
50	u[205]	C(7)...C(29)	7.4067	0.0554	0.5333	(fixed)	1.00	-.0605	2.2	0.5333
	u[463]	C(20)...C(27)	7.2889	0.0486	0.5341	(fixed)	1.00	-.1463	2.2	0.5341
	u[494]	C(22)...C(33)	5.1103	0.0274	0.5358	(fixed)	1.00	-.1447	3.2	0.5358
	u[380]	H(15)...C(24)	2.8931	0.0432	0.5425	0.0244	1.00	0.2976	0.9	0.4540
	u[367]	C(14)...H(30)	6.1424	0.0526	0.5439	(fixed)	1.00	0.1535	0.4	0.5439
55	u[227]	H(8)...C(25)	6.1318	0.0526	0.5454	(fixed)	1.00	0.1431	0.4	0.5454
	u[57]	C(2)...H(26)	2.8840	0.0432	0.5457	Tied to u[380]	1.00	0.2898	0.9	0.4567
	u[461]	C(20)...C(25)	6.2524	0.0436	0.5469	(fixed)	1.00	-.1126	2.6	0.5469
	u[345]	C(13)...H(28)	5.9272	0.0517	0.5471	(fixed)	1.00	-.0354	0.5	0.5471
	u[505]	H(23)...C(33)	5.4963	0.0338	0.5503	(fixed)	1.00	-.2145	0.5	0.5503
60	u[48]	C(2)...H(17)	5.9065	0.0517	0.5519	(fixed)	1.00	-.0552	0.5	0.5519
	u[168]	H(6)...H(19)	9.5507	0.0466	0.5534	(fixed)	1.00	-.2942	0.0	0.5534
	u[84]	C(3)...C(22)	5.1390	0.0274	0.5571	(fixed)	1.00	-.1116	3.2	0.5571
	u[476]	H(21)...C(27)	8.2444	0.0478	0.5583	(fixed)	1.00	-.2245	0.3	0.5583
	u[292]	C(11)...C(18)	5.2408	0.0496	0.5590	Tied to u[28]	1.00	0.1527	3.1	0.4751
65	u[252]	C(9)...C(25)	4.9078	0.0643	0.5650	Tied to u[364]	1.00	0.1625	3.3	0.5639
	u[474]	H(21)...C(25)	7.1905	0.0422	0.5682	(fixed)	1.00	-.1725	0.4	0.5682
	u[154]	C(5)...C(33)	6.2976	0.0295	0.5701	(fixed)	1.00	-.1732	2.6	0.5701
	u[366]	C(14)...C(29)	5.2465	0.0496	0.5743	Tied to u[28]	1.00	0.1618	3.1	0.4880
	u[234]	H(8)...H(32)	9.5312	0.0466	0.5747	(fixed)	1.00	-.3112	0.0	0.5747
70	u[201]	C(7)...C(25)	5.2361	0.0496	0.5755	Tied to u[28]	1.00	0.1517	3.1	0.4892
	u[284]	H(10)...C(33)	7.1139	0.0484	0.5776	(fixed)	1.00	-.1885	0.4	0.5776
	u[112]	H(4)...C(20)	6.7927	0.0344	0.5791	(fixed)	1.00	-.2256	0.4	0.5791
	u[303]	C(11)...C(29)	6.2206	0.0595	0.5813	(fixed)	1.00	-.0372	2.6	0.5813
	u[52]	C(2)...H(21)	5.7628	0.0422	0.5831	(fixed)	1.00	-.0362	0.5	0.5831

	u[95]	C(3)...C(33)	5.1040	0.0274	0.5848	(fixed)	1.00	-.1407	3.2	0.5848
	u[451]	H(19)...C(29)	8.2427	0.0649	0.5858	(fixed)	1.00	-.0494	0.3	0.5858
	u[364]	C(14)...C(27)	4.8981	0.0644	0.5859	0.0491	1.00	0.1578	3.3	0.5847
	u[245]	C(9)...C(18)	6.2472	0.0603	0.5869	Tied to u[29]	1.00	0.1118	2.6	0.5732
5	u[79]	C(3)...H(17)	7.0906	0.0484	0.5906	(fixed)	1.00	-.2097	0.4	0.5906
	u[220]	H(8)...C(18)	8.2249	0.0649	0.5953	(fixed)	1.00	-.0658	0.3	0.5953
	u[114]	H(4)...C(22)	5.5310	0.0339	0.5965	(fixed)	1.00	-.1706	0.5	0.5965
	u[403]	C(16)...C(29)	6.2620	0.0604	0.5990	Tied to u[29]	1.00	0.1289	2.6	0.5851
	u[203]	C(7)...C(27)	6.2407	0.0604	0.6005	Tied to u[29]	1.00	0.1079	2.6	0.5866
10	u[256]	C(9)...C(29)	7.0728	0.0669	0.6008	(fixed)	1.00	-.0483	2.3	0.6008
	u[349]	C(13)...H(32)	5.7353	0.0422	0.6038	(fixed)	1.00	-.0595	0.5	0.6038
	u[206]	C(7)...H(30)	8.2126	0.0649	0.6073	(fixed)	1.00	-.0764	0.3	0.6073
	u[155]	C(5)...H(34)	6.7594	0.0344	0.6077	(fixed)	1.00	-.2541	0.4	0.6077
	u[437]	C(18)...H(30)	8.2252	0.0617	0.6106	(fixed)	1.00	-.0561	0.3	0.6106
15	u[299]	C(11)...C(25)	3.9891	0.0653	0.6112	Tied to u[382]	1.00	0.1399	4.1	0.5799
	u[432]	C(18)...C(25)	6.2279	0.0595	0.6136	(fixed)	1.00	-.0237	2.6	0.6136
	u[290]	C(11)...C(16)	4.8712	0.0645	0.6156	Tied to u[364]	1.00	0.1383	3.4	0.6143
	u[500]	H(23)...H(28)	7.5660	0.0403	0.6174	(fixed)	1.00	-.2755	0.1	0.6174
20	u[96]	C(3)...H(34)	5.4965	0.0339	0.6180	(fixed)	1.00	-.2006	0.5	0.6180
	u[195]	C(7)...H(19)	8.2112	0.0617	0.6198	(fixed)	1.00	-.0688	0.3	0.6198
	u[304]	C(11)...H(30)	7.1512	0.0658	0.6238	(fixed)	1.00	-.0516	0.4	0.6238
	u[190]	C(7)...C(14)	6.1853	0.0596	0.6250	(fixed)	1.00	-.0641	2.6	0.6250
	u[294]	C(11)...C(20)	4.7372	0.0560	0.6267	Tied to u[485]	1.00	0.1206	3.5	0.6129
	u[173]	H(6)...C(24)	5.7311	0.0423	0.6277	(fixed)	1.00	-.0587	0.5	0.6277
25	u[469]	C(20)...C(33)	6.0479	0.0315	0.6287	0.0589	1.00	-.1406	2.7	0.6278
	u[467]	C(20)...C(31)	7.1129	0.0368	0.6293	(fixed)	1.00	-.1704	2.3	0.6293
	u[231]	H(8)...C(29)	8.1980	0.0617	0.6309	(fixed)	1.00	-.0803	0.3	0.6309
	u[434]	C(18)...C(27)	7.0860	0.0669	0.6313	(fixed)	1.00	-.0299	2.3	0.6313
	u[362]	C(14)...C(25)	3.9728	0.0654	0.6315	Tied to u[382]	1.00	0.1300	4.1	0.5992
30	u[301]	C(11)...C(27)	5.2070	0.0698	0.6339	(fixed)	1.00	0.0916	3.1	0.6339
	u[489]	C(22)...H(28)	7.1166	0.0485	0.6375	(fixed)	1.00	-.1759	0.4	0.6375
	u[141]	C(5)...C(20)	7.1365	0.0368	0.6458	(fixed)	1.00	-.1439	2.3	0.6458
	u[143]	C(5)...C(22)	6.0753	0.0315	0.6468	Tied to u[469]	1.00	-.1095	2.7	0.6458
	u[314]	H(12)...C(18)	4.4229	0.0561	0.6497	Tied to u[385]	1.00	0.3959	0.6	0.6478
35	u[288]	C(11)...C(14)	3.9443	0.0655	0.6537	Tied to u[382]	1.00	0.1088	4.1	0.6203
	u[447]	H(19)...C(25)	7.1615	0.0658	0.6578	(fixed)	1.00	-.0353	0.4	0.6578
	u[399]	C(16)...C(25)	5.2029	0.0699	0.6589	(fixed)	1.00	0.0938	3.1	0.6589
	u[482]	H(21)...C(33)	6.9847	0.0305	0.6594	(fixed)	1.00	-.1991	0.4	0.6594
	u[192]	C(7)...C(16)	7.0415	0.0670	0.6610	(fixed)	1.00	-.0690	2.3	0.6610
40	u[254]	C(9)...C(27)	5.9565	0.0751	0.6615	(fixed)	1.00	0.1148	2.7	0.6615
	u[368]	C(14)...C(31)	4.7300	0.0561	0.6638	Tied to u[485]	1.00	0.1236	3.5	0.6493
	u[246]	C(9)...H(19)	7.0168	0.0657	0.6649	(fixed)	1.00	0.1083	0.4	0.6649
	u[257]	C(9)...H(30)	7.9168	0.0762	0.6663	(fixed)	1.00	-.0635	0.3	0.6663
	u[480]	H(21)...C(31)	8.0631	0.0358	0.6687	(fixed)	1.00	-.2481	0.3	0.6687
45	u[216]	H(8)...C(14)	7.1137	0.0658	0.6717	(fixed)	1.00	-.0806	0.4	0.6717
	u[296]	C(11)...C(22)	3.7700	0.0583	0.6727	Tied to u[382]	1.00	0.0829	4.3	0.6383
	u[404]	C(16)...H(30)	7.0322	0.0657	0.6758	(fixed)	1.00	0.1258	0.4	0.6758
	u[229]	H(8)...C(27)	7.0091	0.0657	0.6777	(fixed)	1.00	0.1031	0.4	0.6777
	u[385]	H(15)...C(29)	4.4299	0.0562	0.6791	0.0677	1.00	0.4124	0.6	0.6772
50	u[198]	C(7)...C(22)	6.0298	0.0446	0.6808	(fixed)	1.00	-.0425	2.7	0.6808
	u[107]	H(4)...H(15)	5.4764	0.0332	0.6816	(fixed)	1.00	-.2274	0.1	0.6816
	u[315]	H(12)...H(19)	5.2818	0.0575	0.6846	(fixed)	1.00	0.3868	0.1	0.6846
	u[93]	C(3)...C(31)	6.0324	0.0315	0.6849	Tied to u[469]	1.00	-.1443	2.7	0.6839
	u[241]	C(9)...C(14)	5.1607	0.0700	0.6862	(fixed)	1.00	0.0586	3.2	0.6862
55	u[202]	C(7)...H(26)	4.4173	0.0563	0.6871	Tied to u[385]	1.00	0.4025	0.6	0.6852
	u[401]	C(16)...C(27)	5.9584	0.0752	0.6888	(fixed)	1.00	0.1229	2.7	0.6888
	u[440]	C(18)...C(33)	6.0105	0.0446	0.6910	(fixed)	1.00	-.0595	2.7	0.6910
	u[370]	C(14)...C(33)	3.7680	0.0585	0.6933	Tied to u[382]	1.00	0.0883	4.3	0.6578
	u[146]	C(5)...C(25)	4.6979	0.0562	0.6955	Tied to u[485]	1.00	0.1006	3.5	0.6801
60	u[46]	C(2)...H(15)	4.0249	0.0548	0.6968	Tied to u[363]	1.00	-.0581	0.7	0.6970
	u[171]	H(6)...C(22)	7.0187	0.0305	0.6978	(fixed)	1.00	-.1579	0.4	0.6978
	u[196]	C(7)...C(20)	6.9118	0.0502	0.6988	(fixed)	1.00	-.0473	2.4	0.6988
	u[449]	H(19)...C(27)	7.9340	0.0762	0.6990	(fixed)	1.00	-.0408	0.3	0.6990
	u[152]	C(5)...C(31)	7.0915	0.0369	0.6994	(fixed)	1.00	-.1791	2.3	0.6994
65	u[452]	H(19)...H(30)	8.9726	0.0733	0.7009	(fixed)	1.00	-.0664	0.1	0.7009
	u[249]	C(9)...C(22)	4.9930	0.0596	0.7011	Tied to u[407]	1.00	0.0500	3.3	0.7026
	u[386]	H(15)...H(30)	5.2903	0.0576	0.7084	(fixed)	1.00	0.4019	0.1	0.7084
	u[221]	H(8)...H(19)	8.9531	0.0733	0.7118	(fixed)	1.00	-.0842	0.1	0.7118
	u[169]	H(6)...C(20)	8.0909	0.0358	0.7126	(fixed)	1.00	-.2131	0.3	0.7126
70	u[320]	H(12)...C(24)	4.0504	0.0548	0.7136	Tied to u[363]	1.00	-.0270	0.7	0.7137
	u[228]	H(8)...H(26)	5.2787	0.0576	0.7186	(fixed)	1.00	0.3932	0.1	0.7186
	u[330]	H(12)...H(34)	5.4958	0.0333	0.7190	(fixed)	1.00	-.1990	0.1	0.7190
	u[438]	C(18)...C(31)	6.8925	0.0502	0.7215	(fixed)	1.00	-.0620	2.4	0.7215
	u[247]	C(9)...C(20)	5.7765	0.0627	0.7220	(fixed)	1.00	0.0833	2.8	0.7220

	u[232]	H(8)...	H(30)	8.9386	0.0733	0.7245	(fixed)	1.00	-0.0967	0.1	0.7245
	u[87]	C(3)...	C(25)	3.7313	0.0586	0.7265	Tied to u[382]	1.00	0.0640	4.4	0.6894
	u[407]	C(16)...	C(33)	4.9862	0.0597	0.7271	0.0785	1.00	0.0506	3.3	0.7286
	u[243]	C(9)...	C(16)	5.9130	0.0753	0.7279	(fixed)	1.00	0.0869	2.8	0.7279
5	u[269]	H(10)...	C(18)	6.2711	0.0778	0.7297	(fixed)	1.00	0.2381	0.4	0.7297
	u[224]	H(8)...	C(22)	6.9568	0.0495	0.7301	(fixed)	1.00	-0.0564	0.4	0.7301
	u[218]	H(8)...	C(16)	7.8823	0.0763	0.7320	(fixed)	1.00	-0.0866	0.3	0.7320
	u[94]	C(3)...	H(32)	6.9720	0.0306	0.7326	(fixed)	1.00	-0.1977	0.4	0.7326
	u[302]	C(11)...	H(28)	5.5366	0.0842	0.7335	(fixed)	1.00	0.1793	0.5	0.7335
10	u[91]	C(3)...	C(29)	5.9846	0.0446	0.7336	(fixed)	1.00	-0.0755	2.7	0.7336
	u[493]	C(22)...	H(32)	6.8859	0.0370	0.7346	(fixed)	1.00	-0.2017	0.4	0.7346
	u[343]	C(13)...	H(26)	4.0376	0.0549	0.7365	Tied to u[363]	1.00	-0.0318	0.7	0.7367
	u[504]	H(23)...	H(32)	7.3557	0.0408	0.7369	(fixed)	1.00	-0.2937	0.1	0.7369
	u[455]	H(19)...	C(33)	6.9379	0.0495	0.7401	(fixed)	1.00	-0.0732	0.4	0.7401
15	u[77]	C(3)...	H(15)	5.1419	0.0430	0.7417	(fixed)	1.00	-0.1691	0.5	0.7417
	u[282]	H(10)...	C(31)	7.8739	0.0625	0.7422	(fixed)	1.00	-0.1908	0.3	0.7422
	u[204]	C(7)...	H(28)	6.2638	0.0778	0.7512	(fixed)	1.00	0.2360	0.4	0.7512
	u[83]	C(3)...	H(21)	6.9257	0.0370	0.7547	(fixed)	1.00	-0.1577	0.4	0.7547
	u[420]	H(17)...	C(29)	6.2897	0.0778	0.7559	(fixed)	1.00	0.2630	0.4	0.7559
20	u[89]	C(3)...	C(27)	4.9498	0.0598	0.7603	Tied to u[407]	1.00	0.0240	3.3	0.7619
	u[283]	H(10)...	H(32)	8.8099	0.0609	0.7611	(fixed)	1.00	-0.2795	0.1	0.7611
	u[416]	H(17)...	C(25)	5.5238	0.0844	0.7624	(fixed)	1.00	0.1744	0.5	0.7624
	u[153]	C(5)...	H(32)	8.0417	0.0359	0.7631	(fixed)	1.00	-0.2533	0.3	0.7631
	u[405]	C(16)...	C(31)	5.7649	0.0628	0.7685	(fixed)	1.00	0.0837	2.8	0.7685
25	u[253]	C(9)...	H(26)	4.1379	0.0766	0.7687	Tied to u[382]	1.00	0.4293	0.7	0.7294
	u[329]	H(12)...	C(33)	5.1671	0.0430	0.7696	(fixed)	1.00	-0.1361	0.5	0.7696
	u[150]	C(5)...	C(29)	6.8608	0.0503	0.7717	(fixed)	1.00	-0.0830	2.4	0.7717
	u[222]	H(8)...	C(20)	7.7465	0.0575	0.7739	(fixed)	1.00	-0.0623	0.4	0.7739
	u[138]	C(5)...	H(17)	7.8380	0.0625	0.7757	(fixed)	1.00	-0.2204	0.3	0.7757
30	u[276]	H(10)...	C(25)	5.5590	0.0810	0.7774	(fixed)	1.00	0.1503	0.5	0.7774
	u[166]	H(6)...	H(17)	8.7773	0.0609	0.7836	(fixed)	1.00	-0.3083	0.1	0.7836
	u[92]	C(3)...	H(30)	6.9093	0.0496	0.7868	(fixed)	1.00	-0.0918	0.4	0.7868
	u[265]	H(10)...	C(14)	5.4832	0.0845	0.7905	(fixed)	1.00	0.1418	0.5	0.7905
	u[365]	C(14)...	H(28)	5.5427	0.0811	0.7924	(fixed)	1.00	0.1383	0.5	0.7924
35	u[113]	H(4)...	H(21)	7.4004	0.0408	0.7947	(fixed)	1.00	-0.2376	0.1	0.7947
	u[312]	H(12)...	C(16)	4.0883	0.0768	0.7949	Tied to u[382]	1.00	0.3903	0.7	0.7542
	u[453]	H(19)...	C(31)	7.7282	0.0576	0.7967	(fixed)	1.00	-0.0761	0.4	0.7967
	u[383]	H(15)...	C(27)	4.0876	0.0768	0.7998	Tied to u[382]	1.00	0.3916	0.7	0.7589
	u[182]	H(6)...	C(33)	6.8781	0.0371	0.8005	(fixed)	1.00	-0.1954	0.4	0.8005
40	u[148]	C(5)...	C(27)	5.7256	0.0629	0.8027	(fixed)	1.00	0.0537	2.9	0.8027
	u[464]	C(20)...	H(28)	7.8830	0.0625	0.8028	(fixed)	1.00	-0.1701	0.3	0.8028
	u[273]	H(10)...	C(22)	5.2972	0.0778	0.8037	(fixed)	1.00	0.1075	0.5	0.8037
	u[498]	H(23)...	H(26)	5.4841	0.0334	0.8055	(fixed)	1.00	-0.1879	0.1	0.8055
	u[255]	C(9)...	H(28)	6.0747	0.0929	0.8075	(fixed)	1.00	0.2383	0.4	0.8075
45	u[351]	C(13)...	H(34)	3.6841	0.0506	0.8231	Tied to u[382]	1.00	-0.0687	0.7	0.7810
	u[487]	C(22)...	H(26)	5.1589	0.0432	0.8284	(fixed)	1.00	-0.1270	0.5	0.8284
	u[183]	H(6)...	H(34)	7.3550	0.0409	0.8301	(fixed)	1.00	-0.2755	0.1	0.8301
	u[54]	C(2)...	H(23)	3.7051	0.0507	0.8316	Tied to u[382]	1.00	-0.0441	0.7	0.7891
	u[291]	C(11)...	H(17)	5.5073	0.0812	0.8319	(fixed)	1.00	0.1145	0.5	0.8319
50	u[424]	H(17)...	C(33)	5.3021	0.0779	0.8330	(fixed)	1.00	0.1214	0.5	0.8330
	u[295]	C(11)...	H(21)	5.3028	0.0728	0.8345	(fixed)	1.00	0.0866	0.5	0.8345
	u[116]	H(4)...	C(24)	3.6769	0.0507	0.8400	Tied to u[382]	1.00	-0.0688	0.7	0.7970
	u[418]	H(17)...	C(27)	6.0673	0.0930	0.8429	(fixed)	1.00	0.2408	0.4	0.8429
	u[270]	H(10)...	H(19)	6.9189	0.0841	0.8438	(fixed)	1.00	0.2512	0.1	0.8438
55	u[477]	H(21)...	H(28)	8.8200	0.0610	0.8456	(fixed)	1.00	-0.2546	0.1	0.8456
	u[151]	C(5)...	H(30)	7.6910	0.0576	0.8528	(fixed)	1.00	-0.1016	0.4	0.8528
	u[316]	H(12)...	C(20)	3.8667	0.0767	0.8582	Tied to u[382]	1.00	0.2926	0.7	0.8143
	u[369]	C(14)...	H(32)	5.2957	0.0729	0.8632	(fixed)	1.00	0.0886	0.5	0.8632
	u[230]	H(8)...	H(28)	6.9102	0.0842	0.8653	(fixed)	1.00	0.2479	0.1	0.8653
60	u[421]	H(17)...	H(30)	6.9389	0.0842	0.8698	(fixed)	1.00	0.2777	0.1	0.8698
	u[387]	H(15)...	C(31)	3.8977	0.0769	0.8703	Tied to u[382]	1.00	0.3291	0.7	0.8258
	u[90]	C(3)...	H(28)	5.2515	0.0781	0.8708	(fixed)	1.00	0.0829	0.5	0.8708
	u[271]	H(10)...	C(20)	5.8588	0.0841	0.8712	(fixed)	1.00	0.1747	0.5	0.8712
	u[267]	H(10)...	C(16)	6.0193	0.0932	0.8771	(fixed)	1.00	0.2027	0.5	0.8771
65	u[280]	H(10)...	C(29)	7.6110	0.0851	0.8900	(fixed)	1.00	-0.0697	0.4	0.8900
	u[136]	C(5)...	H(15)	6.0753	0.0558	0.8947	(fixed)	1.00	-0.1806	0.4	0.8947
	u[506]	H(23)...	H(34)	5.1361	0.0514	0.8991	(fixed)	1.00	-0.2146	0.1	0.8991
	u[174]	H(6)...	C(25)	5.2549	0.0731	0.9030	(fixed)	1.00	0.0609	0.5	0.9030
	u[164]	H(6)...	H(15)	6.9753	0.0515	0.9092	(fixed)	1.00	-0.2349	0.1	0.9092
70	u[327]	H(12)...	C(31)	6.1112	0.0558	0.9130	(fixed)	1.00	-0.1395	0.4	0.9130
	u[277]	H(10)...	H(26)	4.8106	0.0963	0.9153	(fixed)	1.00	0.4039	0.1	0.9153
	u[468]	C(20)...	H(32)	7.5965	0.0448	0.9166	(fixed)	1.00	-0.2088	0.4	0.9166
	u[422]	H(17)...	C(31)	5.8556	0.0843	0.9255	(fixed)	1.00	0.1883	0.5	0.9255
	u[435]	C(18)...	H(28)	7.6202	0.0852	0.9292	(fixed)	1.00	-0.0513	0.4	0.9292

	u[300]	C(11)...H(26)	3.2665	0.0843	0.9308	Tied to u[389]	1.00	0.3647	0.8	0.7455
	u[384]	H(15)...H(28)	4.7459	0.0964	0.9323	(fixed)	1.00	0.3461	0.1	0.9323
	u[328]	H(12)...H(32)	7.0105	0.0515	0.9329	(fixed)	1.00	-0.1938	0.1	0.9329
	u[142]	C(5)...H(21)	7.6375	0.0448	0.9333	(fixed)	1.00	-0.1639	0.4	0.9333
5	u[147]	C(5)...H(26)	3.8185	0.0775	0.9366	Tied to u[382]	1.00	0.2817	0.7	0.8887
	u[278]	H(10)...C(27)	6.4944	0.0956	0.9447	(fixed)	1.00	0.1010	0.4	0.9447
	u[115]	H(4)...H(23)	5.1930	0.0515	0.9458	(fixed)	1.00	-0.1420	0.1	0.9458
	u[313]	H(12)...H(17)	4.7473	0.0966	0.9506	(fixed)	1.00	0.3550	0.1	0.9506
	u[193]	C(7)...H(17)	7.5580	0.0853	0.9533	(fixed)	1.00	-0.1077	0.4	0.9533
10	u[310]	H(12)...C(14)	3.2048	0.0847	0.9547	Tied to u[389]	1.00	0.3172	0.9	0.7647
	u[381]	H(15)...C(25)	3.2001	0.0847	0.9575	Tied to u[389]	1.00	0.3141	0.9	0.7669
	u[126]	H(4)...H(34)	5.1416	0.0516	0.9625	(fixed)	1.00	-0.1876	0.1	0.9625
	u[149]	C(5)...H(28)	5.7987	0.0845	0.9634	(fixed)	1.00	0.1437	0.5	0.9634
15	u[289]	C(11)...H(15)	3.9768	0.0914	0.9641	Tied to u[363]	1.00	0.0341	0.7	0.9642
	u[363]	C(14)...H(26)	3.9971	0.0914	0.9649	0.0885	1.00	0.0547	0.7	0.9651
	u[321]	H(12)...C(25)	4.0173	0.0915	0.9664	Tied to u[363]	1.00	0.0756	0.7	0.9666
	u[462]	C(20)...H(26)	6.1097	0.0560	0.9681	(fixed)	1.00	-0.1248	0.4	0.9681
	u[402]	C(16)...H(28)	6.4897	0.0957	0.9693	(fixed)	1.00	0.1035	0.4	0.9693
20	u[481]	H(21)...H(32)	8.5207	0.0435	0.9805	(fixed)	1.00	-0.2932	0.1	0.9805
	u[281]	H(10)...H(30)	8.4007	0.0962	0.9865	(fixed)	1.00	-0.0866	0.1	0.9865
	u[180]	H(6)...C(31)	7.5722	0.0449	0.9968	(fixed)	1.00	-0.2137	0.4	0.9968
	u[475]	H(21)...H(26)	7.0110	0.0517	1.0058	(fixed)	1.00	-0.1740	0.1	1.0058
	u[388]	H(15)...H(32)	4.4903	0.0985	1.0079	(fixed)	1.00	0.2663	0.1	1.0079
25	u[197]	C(7)...H(21)	7.3405	0.0633	1.0135	(fixed)	1.00	-0.0728	0.4	1.0135
	u[325]	H(12)...C(29)	6.1402	0.0788	1.0162	(fixed)	1.00	-0.0677	0.4	1.0162
	u[244]	C(9)...H(17)	6.4278	0.0960	1.0172	(fixed)	1.00	0.0562	0.4	1.0172
	u[191]	C(7)...H(15)	6.0929	0.0788	1.0174	(fixed)	1.00	-0.1146	0.4	1.0174
	u[248]	C(9)...H(21)	6.2028	0.0819	1.0183	(fixed)	1.00	0.0493	0.4	1.0183
30	u[317]	H(12)...H(21)	4.4379	0.0986	1.0219	(fixed)	1.00	0.2203	0.1	1.0219
	u[170]	H(6)...H(21)	8.5671	0.0435	1.0286	(fixed)	1.00	-0.2359	0.1	1.0286
	u[450]	H(19)...H(28)	8.4136	0.0963	1.0298	(fixed)	1.00	-0.0635	0.1	1.0298
	u[389]	H(15)...C(33)	2.9544	0.0872	1.0301	0.0298	1.00	0.2406	0.9	0.8250
	u[439]	C(18)...H(32)	7.3045	0.0633	1.0359	(fixed)	1.00	-0.1028	0.4	1.0359
35	u[318]	H(12)...C(22)	2.9063	0.0873	1.0376	Tied to u[389]	1.00	0.1976	0.9	0.8311
	u[433]	C(18)...H(26)	6.1391	0.0789	1.0481	(fixed)	1.00	-0.0584	0.4	1.0481
	u[470]	C(20)...H(34)	5.6996	0.0463	1.0485	(fixed)	1.00	-0.1742	0.5	1.0485
	u[371]	C(14)...H(34)	3.6098	0.0886	1.0570	Tied to u[382]	1.00	-0.0051	0.8	1.0029
	u[219]	H(8)...H(17)	8.3408	0.0964	1.0580	(fixed)	1.00	-0.1295	0.1	1.0580
40	u[406]	C(16)...H(32)	6.1828	0.0820	1.0597	(fixed)	1.00	0.0430	0.4	1.0597
	u[323]	H(12)...C(27)	5.1906	0.0962	1.0626	(fixed)	1.00	0.0345	0.5	1.0626
	u[495]	C(22)...H(34)	4.7255	0.0406	1.0628	Tied to u[28]	1.00	-0.1641	0.6	0.9029
	u[242]	C(9)...H(15)	5.1386	0.0962	1.0720	(fixed)	1.00	-0.0138	0.5	1.0720
	u[400]	C(16)...H(26)	5.1794	0.0962	1.0731	(fixed)	1.00	0.0275	0.5	1.0731
45	u[326]	H(12)...H(30)	7.0711	0.0848	1.0735	(fixed)	1.00	-0.0809	0.1	1.0735
	u[217]	H(8)...H(15)	7.0179	0.0848	1.0808	(fixed)	1.00	-0.1319	0.1	1.0808
	u[144]	C(5)...H(23)	5.7432	0.0464	1.0837	(fixed)	1.00	-0.1182	0.5	1.0837
	u[297]	C(11)...H(23)	3.5820	0.0889	1.0842	Tied to u[382]	1.00	-0.0180	0.8	1.0288
	u[117]	H(4)...C(25)	3.5660	0.0890	1.0861	Tied to u[382]	1.00	-0.0329	0.8	1.0305
50	u[175]	H(6)...H(26)	4.3973	0.0993	1.0863	(fixed)	1.00	0.2102	0.1	1.0863
	u[181]	H(6)...H(32)	8.4955	0.0436	1.0895	(fixed)	1.00	-0.2931	0.1	1.0895
	u[178]	H(6)...C(29)	7.2659	0.0635	1.0964	(fixed)	1.00	-0.1243	0.4	1.0964
	u[483]	H(21)...H(34)	6.5951	0.0422	1.0979	(fixed)	1.00	-0.2217	0.1	1.0979
	u[123]	H(4)...C(31)	5.6869	0.0465	1.0982	(fixed)	1.00	-0.1693	0.5	1.0982
55	u[85]	C(3)...H(23)	4.7655	0.0407	1.0983	Tied to u[28]	1.00	-0.1091	0.6	0.9331
	u[176]	H(6)...C(27)	6.1325	0.0822	1.1044	(fixed)	1.00	0.0080	0.4	1.1044
	u[448]	H(19)...H(26)	7.0732	0.0849	1.1071	(fixed)	1.00	-0.0687	0.1	1.1071
	u[88]	C(3)...H(26)	2.8515	0.0886	1.1074	Tied to u[389]	1.00	0.1917	1.0	0.8869
	u[125]	H(4)...C(33)	4.7165	0.0407	1.1133	Tied to u[28]	1.00	-0.1516	0.6	0.9460
60	u[441]	C(18)...H(34)	5.7231	0.0647	1.1206	(fixed)	1.00	-0.1192	0.5	1.1206
	u[223]	H(8)...H(21)	8.1089	0.0711	1.1256	(fixed)	1.00	-0.0902	0.1	1.1256
	u[279]	H(10)...H(28)	6.5228	0.1190	1.1291	(fixed)	1.00	0.2303	0.1	1.1291
	u[199]	C(7)...H(23)	5.7477	0.0648	1.1425	(fixed)	1.00	-0.0864	0.5	1.1425
	u[172]	H(6)...H(23)	6.6535	0.0423	1.1472	(fixed)	1.00	-0.1474	0.1	1.1472
65	u[454]	H(19)...H(32)	8.0715	0.0712	1.1479	(fixed)	1.00	-0.1216	0.1	1.1479
	u[419]	H(17)...H(28)	6.5040	0.1192	1.1574	(fixed)	1.00	0.2215	0.1	1.1574
	u[121]	H(4)...C(29)	5.6963	0.0648	1.1584	(fixed)	1.00	-0.1317	0.5	1.1584
	u[382]	H(15)...H(26)	3.3381	0.1177	1.1591	0.0865	1.00	0.1467	0.1	1.0998
	u[124]	H(4)...H(32)	6.5877	0.0423	1.1632	(fixed)	1.00	-0.2080	0.1	1.1632
70	u[324]	H(12)...H(28)	5.5608	0.1138	1.1711	(fixed)	1.00	0.1028	0.1	1.1711
	u[311]	H(12)...H(15)	3.3523	0.1180	1.1740	Tied to u[382]	1.00	0.1706	0.1	1.1139
	u[417]	H(17)...H(26)	5.5404	0.1138	1.1750	(fixed)	1.00	0.0840	0.1	1.1750
	u[456]	H(19)...H(34)	6.6497	0.0680	1.1860	(fixed)	1.00	-0.1337	0.1	1.1860
	u[266]	H(10)...H(15)	5.5006	0.1139	1.1892	(fixed)	1.00	0.0501	0.1	1.1892
	u[322]	H(12)...H(26)	3.3824	0.1185	1.1985	Tied to u[382]	1.00	0.2170	0.1	1.1372

	u[272]	H(10)...	H(21)	6.1710	0.1089	1.2063	(fixed)	1.00	0.1279	0.1	1.2063
	u[225]	H(8)...	H(23)	6.6783	0.0680	1.2074	(fixed)	1.00	-.0978	0.1	1.2074
	u[268]	H(10)...	H(17)	6.4374	0.1195	1.2097	(fixed)	1.00	0.1739	0.1	1.2097
	u[179]	H(6)...	H(30)	8.0249	0.0713	1.2166	(fixed)	1.00	-.1487	0.1	1.2166
5	u[425]	H(17)...	H(34)	5.1639	0.1085	1.2258	(fixed)	1.00	0.0048	0.1	1.2258
	u[122]	H(4)...	H(30)	6.6207	0.0681	1.2277	(fixed)	1.00	-.1483	0.1	1.2277
	u[274]	H(10)...	H(23)	5.1341	0.1087	1.2474	(fixed)	1.00	-.0152	0.1	1.2474
	u[423]	H(17)...	H(32)	6.1657	0.1092	1.2508	(fixed)	1.00	0.1400	0.1	1.2508
	u[120]	H(4)...	H(28)	5.1040	0.1088	1.2614	(fixed)	1.00	-.0388	0.1	1.2614
10	u[177]	H(6)...	H(28)	6.0893	0.1096	1.3029	(fixed)	1.00	0.0848	0.1	1.3029
	u[390]	H(15)...	H(34)	2.9302	0.1252	1.3034	Tied to u[361]	1.00	0.0714	0.2	1.1172
	u[408]	C(16)...	H(34)	4.6911	0.0893	1.3279	Tied to u[28]	1.00	-.0397	0.6	1.1279
	u[250]	C(9)...	H(23)	4.6796	0.0895	1.3500	Tied to u[28]	1.00	-.0396	0.6	1.1475
	u[118]	H(4)...	H(26)	2.8376	0.1267	1.3615	Tied to u[361]	1.00	0.0248	0.2	1.1672
15	u[119]	H(4)...	C(27)	4.6442	0.0896	1.3622	Tied to u[28]	1.00	-.0685	0.6	1.1578
	u[319]	H(12)...	H(23)	2.8171	0.1270	1.3701	Tied to u[361]	1.00	0.0113	0.2	1.1746