Supporting Information

Ethylene heterogeneous hydroformylation on Polymer Supported Rh-based Catalyst: A DFT analysis of Mechanism and Rh-P Effect

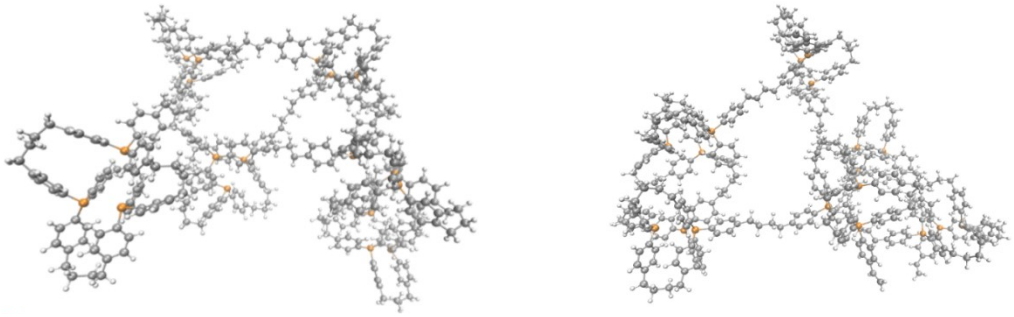
Jing Ma[1, 2], Meizhe Liu[1, 2], Mingxuan Zhu[1, 2], Yutong Wang [1, 2], Baohe Wang[1, 2]*

[1]Key Laboratory for Green Chemical Technology of Ministry of Education, R&D Center for Petrochemical Technology, Tianjin University, Tianjin 300072, China

[2]Collaborative Innovation Center of Chemical Science and Engineering, Tianjin University, Tianjin 300072, China

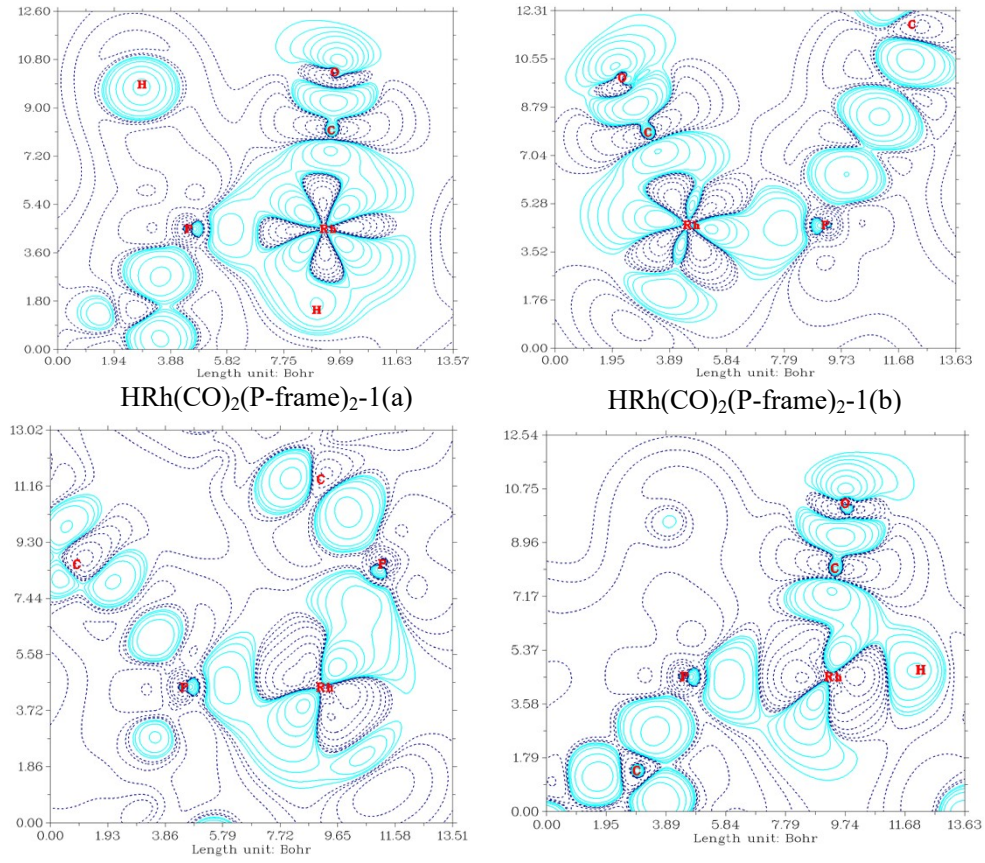
Corresponding Author

*E-mail for Baohe Wang: wangbh@tju.edu.cn



POL-1 POL-2

Fig. S1. Construction of 3V-PPh_3 polymer with different cross-linking methods



$HRh(CO)_2(P\text{-frame})_2$-1(a) $HRh(CO)_2(P\text{-frame})_2$-1(b)

$HRh(CO)_2(P\text{-frame})_2$-2(a) $HRh(CO)_2(P\text{-frame})_2$-2(b)

Fig. S2. Diagram of deformation density during the formation of $HRh(CO)_2(P\text{-frame})_2$, where (I), (II), (III) and (IV) represent the different cross-sections of $HRh(CO)_2(P\text{-frame})_2$-1(a), -1(b), -2(a) and -2(b), respectively (cyan and dark blue colors indicate regions with the increase and decrease of electron density, respectively)

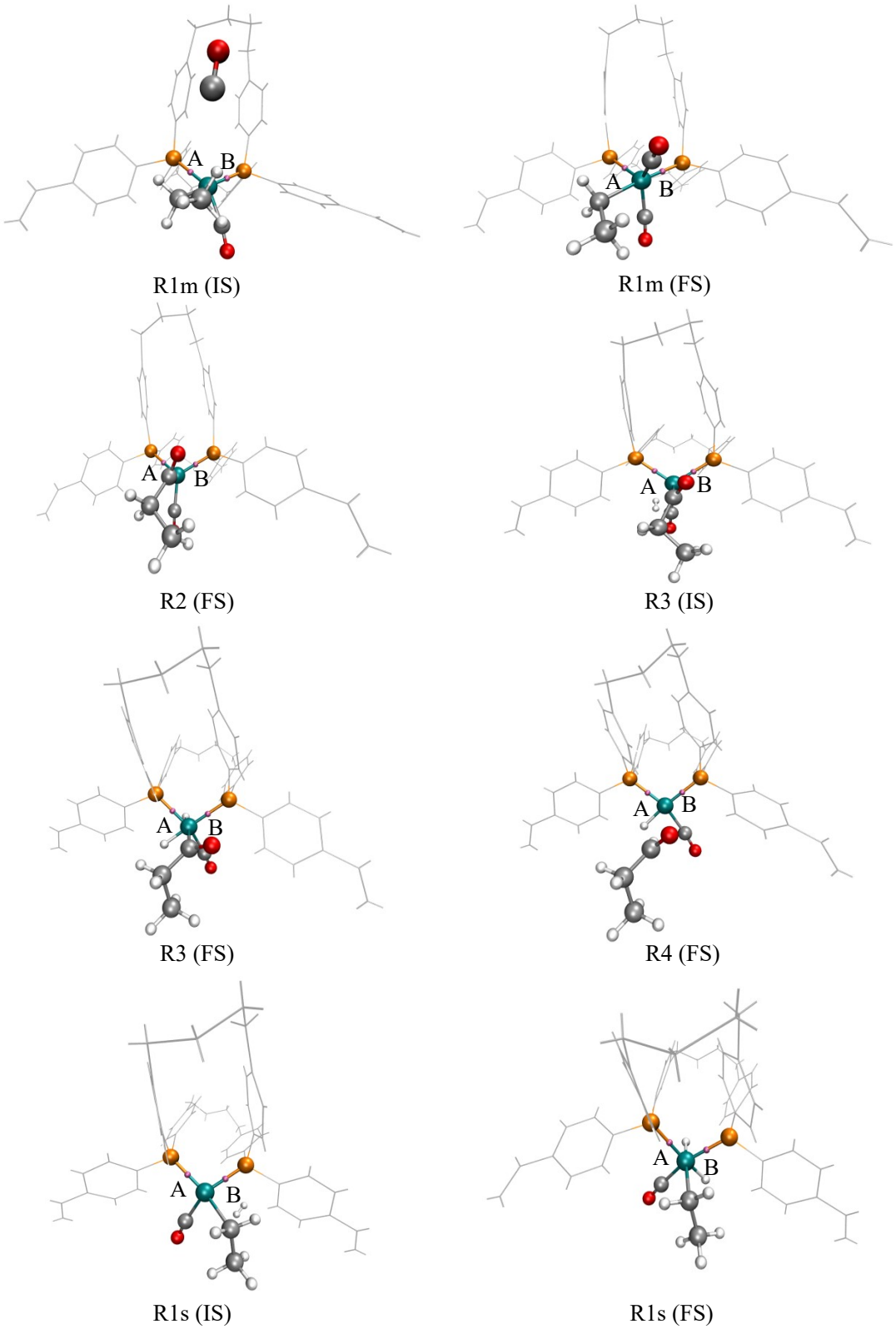


Fig. S3. AIM analysis of the stable configurations of reactants and products under the R1m-R4 and R1s path of cross-linking method 1 (Mauve balls represent the bond critical point)

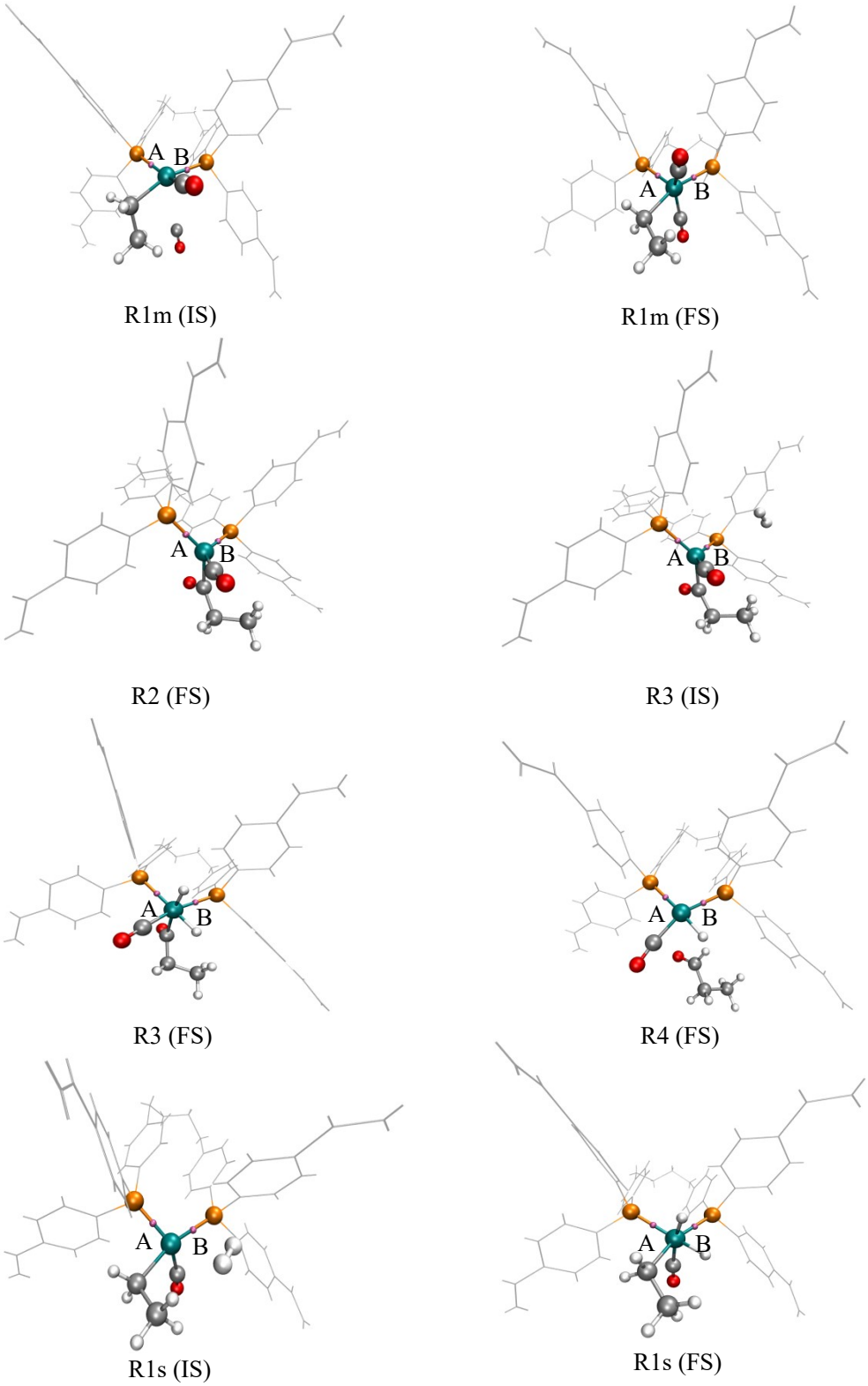


Fig. S4. AIM analysis of the stable configurations of reactants and products under the R1m-R4 and R1s path of cross-linking method 2 (Mauve balls represent the bond critical point)

Table S1. Topological parameters of the reactants and products in R1~R4 path of crosslinking method 2

Reaction /Status	BCP	ρ(r) (au)	$\nabla^2\rho$ (au)	G(r) (au)	V(r) (au)	H(r) (au)	$\lvert V(r)\rvert/G(r)$
R1m/IS	A	0.087	0.145	0.067	-0.097	-0.031	1.448
	B	0.084	0.154	0.067	-0.096	-0.029	1.433
R1m/FS	A	0.079	0.135	0.060	-0.087	-0.026	1.450
	B	0.082	0.131	0.060	-0.088	-0.027	1.467
R2/FS	A	0.077	0.123	0.056	-0.081	-0.025	1.446
	B	0.084	0.144	0.065	-0.094	-0.029	1.446
R3/IS	A	0.076	0.125	0.056	-0.081	-0.025	1.446
	B	0.082	0.143	0.063	-0.091	-0.028	1.444
R3 (FS)	A	0.070	0.135	0.054	-0.075	-0.021	1.389
	B	0.083	0.127	0.060	-0.088	-0.028	1.467
R4/FS	A	0.081	0.156	0.066	-0.092	-0.027	1.394
	B	0.089	0.143	0.068	-0.099	-0.032	1.456
R1s/IS	A	0.089	0.149	0.070	-0.102	-0.032	1.457
	B	0.085	0.151	0.067	-0.096	-0.029	1.433
R1s/FS	A	0.077	0.144	0.060	-0.084	-0.024	1.400
	B	0.084	0.138	0.064	-0.092	-0.029	1.438

The Cartesian coordinates of the reactants, intermediates and transition states:

$HRh(CO)_2$(P-frame)$_2$-1(a)

ATOM		X	Y	Z
P	1	23.7482	5.5737	14.6312
C	2	22.9021	4.6865	13.2656
C	3	24.9150	4.4421	15.4662
C	4	24.7987	6.8048	13.7679
C	5	26.1789	6.9493	13.9708
C	6	26.8505	8.0825	13.5107
C	7	26.1793	9.1127	12.8307
C	8	24.8022	8.9353	12.5817
C	9	24.1289	7.8184	13.0488
C	10	25.6082	4.9635	16.5768
C	11	26.4165	4.1516	17.3641
C	12	26.5193	2.7726	17.1159
C	13	25.8178	2.2563	16.0167
C	14	25.0358	3.0727	15.1954
C	15	21.6033	4.2149	13.5270
C	16	20.7351	3.9046	12.4809
C	17	21.1165	4.0838	11.1449
C	18	22.4516	4.4358	10.8873
C	19	23.3319	4.7300	11.9277
C	20	27.2574	1.8515	18.0595
C	21	26.9153	10.3149	12.4347
C	22	20.0922	4.0568	10.0352
C	23	26.5114	1.6768	19.4073
C	24	19.8869	5.4537	9.3965
C	25	26.4068	11.4609	11.9421
H	26	26.7312	6.1786	14.5084
H	27	27.9221	8.1808	13.6975
H	28	24.2470	9.6986	12.0363
H	29	23.0523	7.7390	12.8863
H	30	25.4952	6.0168	16.8392
H	31	26.9424	4.5982	18.2083
H	32	25.8781	1.1871	15.8026
H	33	24.5070	2.6384	14.3458
H	34	21.2401	4.1744	14.5542
H	35	19.7129	3.5987	12.7112
H	36	22.7954	4.5344	9.8556
H	37	24.3441	5.0643	11.6981
H	38	28.2772	2.2258	18.2491
H	39	27.9981	10.2547	12.5799
H	40	19.1392	3.6769	10.4327
H	41	26.6528	0.6485	19.7767
H	42	25.4343	1.7848	19.2119
H	43	19.0788	5.3897	8.6495
H	44	20.7992	5.7073	8.8341
H	45	25.3357	11.6096	11.7949
H	46	27.0571	12.2967	11.6871
P	47	22.0899	7.5037	19.6661
C	48	23.1927	6.1363	20.2263
C	49	20.8355	7.6452	21.0046
C	50	23.1414	9.0135	19.8638
C	51	22.8014	10.0846	20.6977
C	52	23.3662	11.3486	20.4982
C	53	24.2907	11.5785	19.4757
C	54	24.7416	10.4631	18.7469
C	55	24.1751	9.2078	18.9298
C	56	20.6678	6.6993	22.0234
C	57	19.5830	6.7922	22.9016
C	58	18.6616	7.8461	22.8234
C	59	18.8727	8.8193	21.8338
C	60	19.9137	8.7025	20.9209
C	61	22.9013	4.7994	19.9163
C	62	23.7268	3.7653	20.3659
C	63	24.8828	4.0319	21.1155
C	64	25.1718	5.3725	21.4117
C	65	24.3432	6.4085	20.9841
C	66	17.4285	7.8647	23.6976
C	67	24.7386	12.9677	19.0856
C	68	25.8369	2.9461	21.5587
C	69	16.1675	7.3491	22.9566
C	70	26.9412	2.6545	20.5148
C	71	24.2471	13.4008	17.6733
H	72	22.0451	9.9584	21.4710
H	73	23.0397	12.1794	21.1272
H	74	25.5018	10.5904	17.9734
H	75	24.4888	8.3848	18.2881
H	76	21.3741	5.8751	22.1250
H	77	19.4543	6.0225	23.6661
H	78	18.1894	9.6648	21.7474
H	79	20.0027	9.4289	20.1128
H	80	22.0254	4.5581	19.3146
H	81	23.4626	2.7347	20.1257
H	82	26.0641	5.6094	21.9956
H	83	24.5911	7.4374	21.2430
H	84	17.2425	8.8827	24.0769

H	85	25.8395	13.0008	19.0945
H	86	25.2858	2.0187	21.7785
H	87	15.4834	6.8870	23.6855
H	88	16.4850	6.5397	22.2850
H	89	27.8267	2.2439	21.0260
H	90	27.2622	3.6125	20.0807
H	91	24.0257	12.4971	17.0878
H	92	25.0773	13.9009	17.1530
P	93	19.2097	8.6323	16.7742
C	94	19.5342	10.4459	16.8958
C	95	17.6977	8.3418	17.7849
C	96	18.6763	8.1983	15.0602
C	97	18.4223	6.8352	14.8345
C	98	18.1959	6.3502	13.5519
C	99	18.2365	7.1931	12.4318
C	100	18.4201	8.5635	12.6652
C	101	18.6285	9.0643	13.9572
C	102	17.6814	7.2099	18.6077
C	103	16.6491	7.0030	19.5211
C	104	15.6406	7.9602	19.6940
C	105	15.6159	9.0515	18.8080
C	106	16.6098	9.2283	17.8455
C	107	19.2103	11.1098	18.0943
C	108	19.9120	12.2427	18.4923
C	109	20.9466	12.7877	17.7146
C	110	21.1712	12.2072	16.4599
C	111	20.4885	11.0523	16.0598
C	112	14.6981	7.9097	20.8735
C	113	18.2042	6.6059	11.0396
C	114	21.7347	13.9486	18.2888
C	115	15.3883	8.4210	22.1668
C	116	23.0525	14.3702	17.6261
C	117	19.6141	6.5931	10.3911
H	118	18.4322	6.1322	15.6677
H	119	18.0209	5.2825	13.4092
H	120	18.4216	9.2601	11.8242
H	121	18.7698	10.1370	14.0939
H	122	18.5242	6.5173	18.5724
H	123	16.6702	6.1125	20.1493
H	124	14.8172	9.7920	18.8907
H	125	16.5652	10.0880	17.1756
H	126	18.4617	10.6922	18.7654
H	127	19.6802	12.6935	19.4601
H	128	21.9353	12.6115	15.7952
H	129	20.7875	10.5715	15.1289
H	130	14.3203	6.8874	21.0337
H	131	17.5122	7.1694	10.3944
H	132	21.9223	13.7225	19.3511
H	133	14.6313	8.8668	22.8312
H	134	16.0588	9.2441	21.8815
H	135	23.3603	15.3141	18.1066
H	136	22.8638	14.6304	16.5717
H	137	20.3699	6.5487	11.1882
H	138	19.7763	7.5542	9.8802
H	139	17.6129	7.2347	24.5797
H	140	24.4070	13.6942	19.8434
H	141	13.8218	8.5382	20.6583
H	142	21.0722	14.8317	18.3012
H	143	27.3731	0.8729	17.5729
H	144	20.3987	3.3553	9.2431
H	145	26.3085	3.2614	22.5014
H	146	17.8104	5.5802	11.0980
C	147	20.9107	5.7564	17.0928
O	148	20.6959	4.6276	16.8830
Rh	149	21.2334	7.6264	17.4823
H	150	21.3837	9.1307	17.9726
C	151	22.5769	8.3152	16.2778
O	152	23.3430	8.9611	15.6870

$HRh(CO)_2$(P-frame)$_2$-1(b)

ATOM		X	Y	Z
P	1	24.1356	3.4092	13.3001
C	2	23.4108	3.1843	14.9797
C	3	25.5779	2.2676	13.2364
C	4	22.8471	2.6664	12.2108
C	5	22.9465	1.3926	11.6378
C	6	21.9552	0.9345	10.7622
C	7	20.8382	1.7182	10.4407
C	8	20.7389	2.9854	11.0390
C	9	21.7273	3.4554	11.8979
C	10	26.4891	2.4355	12.1794
C	11	27.6945	1.7442	12.1588
C	12	28.0674	0.8923	13.2126
C	13	27.1302	0.6818	14.2324
C	14	25.9015	1.3534	14.2495
C	15	23.7598	4.0699	16.0122
C	16	23.1580	3.9785	17.2643
C	17	22.1579	3.0245	17.5285
C	18	21.8288	2.1231	16.4957

C	19	22.4411	2.2016	15.2481
C	20	29.4339	0.2350	13.2193
C	21	19.7865	1.2162	9.4696
C	22	21.4824	3.0374	18.8295
C	23	30.6263	1.1786	12.9050
C	24	20.3269	2.4296	19.1495
H	25	23.8136	0.7656	11.8496
H	26	22.0654	-0.0499	10.3025
H	27	19.8967	3.6379	10.8055
H	28	21.6551	4.4685	12.2942
H	29	26.2620	3.1442	11.3826
H	30	28.3772	1.9082	11.3242
H	31	27.3789	0.0083	15.0558
H	32	25.2175	1.1982	15.0845
H	33	24.4688	4.8756	15.8204
H	34	23.4330	4.6970	18.0387
H	35	21.0764	1.3530	16.6688
H	36	22.1424	1.5050	14.4647
H	37	29.4222	-0.5666	12.4628
C	38	19.2448	2.2770	8.4765
H	39	21.9738	3.6454	19.5947
H	40	30.2485	2.0714	12.3859
H	41	31.2977	0.6799	12.1895
H	42	19.7510	1.8475	18.4289
H	43	19.9069	2.5194	20.1509
P	44	26.6105	6.5407	13.5269
C	45	27.9629	5.4732	14.1652
C	46	26.0815	7.6508	14.9083
C	47	27.3718	7.6504	12.2623
C	48	27.6311	9.0106	12.4834
C	49	27.7327	9.8971	11.4049
C	50	27.6149	9.4545	10.0806
C	51	27.5433	8.0668	9.8686
C	52	27.4060	7.1859	10.9355
C	53	26.1312	7.2647	16.2559
C	54	25.2986	7.8737	17.2070
C	55	24.4181	8.9024	16.8527
C	56	24.4796	9.3754	15.5317
C	57	25.2743	8.7573	14.5776
C	58	27.6226	4.4429	15.0573
C	59	28.5572	3.4863	15.4373
C	60	29.8544	3.4788	14.9077
C	61	30.2059	4.5269	14.0428
C	62	29.2812	5.5130	13.6806
C	63	23.3492	9.4424	17.7744
C	64	27.4335	10.4301	8.9357
C	65	30.7873	2.3414	15.2603
C	66	21.9167	9.0680	17.2881
C	67	31.4947	1.6314	14.0898
C	68	26.2728	10.0310	7.9875
H	69	27.6622	9.4016	13.5003
H	70	27.8434	10.9656	11.6051
H	71	27.5027	7.6728	8.8522
H	72	27.2264	6.1300	10.7325
H	73	26.7883	6.4527	16.5680
H	74	25.3183	7.5114	18.2376
H	75	23.8363	10.2033	15.2280
H	76	25.2222	9.1008	13.5454
H	77	26.6016	4.3567	15.4272
H	78	28.2547	2.6914	16.1197
H	79	31.2145	4.5716	13.6264
H	80	29.5821	6.3032	12.9919
H	81	23.4364	10.5408	17.8140
H	82	28.3653	10.5264	8.3533
H	83	30.2088	1.6021	15.8346
H	84	21.5387	8.2118	17.8702
H	85	21.9747	8.7121	16.2509
H	86	25.5600	9.4031	8.5417
H	87	26.6669	9.3933	7.1820
P	88	20.8516	7.9345	11.1073
C	89	21.7384	9.2944	10.2569
C	90	20.0468	8.6863	12.5784
C	91	19.5996	7.2333	9.9715
C	92	18.2939	6.9001	10.3758
C	93	17.5664	5.9253	9.6885
C	94	18.0916	5.2717	8.5627
C	95	19.3321	5.7158	8.0785
C	96	20.0827	6.6583	8.7778
C	97	19.5216	7.8071	13.5442
C	98	19.2848	8.2322	14.8499
C	99	19.5933	9.5376	15.2599
C	100	20.0357	10.4359	14.2763
C	101	20.2537	10.0251	12.9591
C	102	22.9401	9.6763	10.8824
C	103	23.8109	10.5797	10.2838
C	104	23.5458	11.1093	9.0108
C	105	22.3395	10.7415	8.3936
C	106	21.4421	9.8569	9.0040

C	107	19.5363	9.9289	16.7223
C	108	17.4105	4.0471	8.0019
C	109	24.5716	11.9763	8.3193
C	110	20.9177	10.2279	17.3516
C	111	25.5007	11.1980	7.3541
C	112	17.8187	2.7653	8.7717
H	113	17.8617	7.3675	11.2613
H	114	16.5753	5.6429	10.0524
H	115	19.7492	5.2717	7.1729
H	116	21.0870	6.9034	8.4278
H	117	19.3690	6.7555	13.2973
H	118	18.9230	7.5110	15.5848
H	119	20.2492	11.4723	14.5469
H	120	20.6335	10.7418	12.2306
H	121	23.2073	9.2272	11.8400
H	122	24.7381	10.8429	10.7964
H	123	22.0926	11.1510	7.4108
H	124	20.5129	9.5962	8.4947
H	125	19.0466	9.1198	17.2863
H	126	25.1778	12.4880	9.0829
H	127	20.7637	10.5410	18.3977
H	128	21.3599	11.0972	16.8366
H	129	26.2018	11.9132	6.8923
H	130	24.8838	10.7957	6.5349
H	131	23.5175	9.0857	18.8012
H	132	27.2473	11.4267	9.3642
H	133	18.9047	10.8232	16.8465
H	134	24.0668	12.7695	7.7463
H	135	29.5904	-0.2750	14.1823
H	136	31.5667	2.7037	15.9520
H	137	18.9432	0.7956	10.0456
H	138	20.2143	0.3665	8.9185
H	139	19.2644	1.8653	7.4553
H	140	19.9343	3.1334	8.4668
H	141	32.0259	0.7608	14.5092
H	142	32.2806	2.2907	13.6867
H	143	17.6496	3.9255	6.9334
H	144	16.3186	4.1666	8.0712
H	145	17.1059	1.9597	8.5297
H	146	17.7035	2.9606	9.8507
C	147	24.5691	5.3323	10.7640
O	148	24.5386	5.2470	9.6003
Rh	149	24.5240	5.6804	12.6472
H	150	24.5356	7.1908	12.1212
C	151	23.1469	6.3226	13.7956
O	152	22.3161	6.7635	14.4814

$HRh(CO)_2(P\text{-}frame)_2$-2(a)

ATOM		X	Y	Z
P	1	2.9169	1.0396	-0.7850
C	2	4.2626	-0.2186	-0.7688
C	3	3.1493	1.8563	0.8556
C	4	3.4919	2.3494	-1.9538
C	5	3.9597	3.5950	-1.5094
C	6	4.2483	4.6121	-2.4187
C	7	4.0892	4.4317	-3.8035
C	8	3.6532	3.1670	-4.2458
C	9	3.3542	2.1554	-3.3426
C	10	2.0663	2.4880	1.4841
C	11	2.2271	3.1255	2.7125
C	12	3.4745	3.1702	3.3639
C	13	4.5601	2.5392	2.7238
C	14	4.4029	1.9038	1.4968
C	15	4.2322	-1.1574	0.2764
C	16	5.1568	-2.1917	0.3380
C	17	6.1197	-2.3751	-0.6663
C	18	6.1421	-1.4412	-1.7114
C	19	5.2392	-0.3713	-1.7612
C	20	3.5829	3.8603	4.6527
C	21	4.3566	5.5531	-4.7104
C	22	7.1378	-3.4990	-0.5811
C	23	4.6984	4.0823	5.3702
C	24	4.0989	5.6098	-6.0290
H	25	4.0803	3.7865	-0.4441
H	26	4.5907	5.5795	-2.0469
H	27	3.5314	2.9748	-5.3119
H	28	2.9843	1.2043	-3.7223
H	29	1.0856	2.4663	1.0104
H	30	1.3666	3.6037	3.1844
H	31	5.5453	2.5444	3.1899
H	32	5.2641	1.4260	1.0304
H	33	3.4764	-1.0777	1.0591
H	34	5.1050	-2.8808	1.1803
H	35	6.8877	-1.5394	-2.5039
H	36	5.3029	0.3461	-2.5799
H	37	2.6348	4.2367	5.0468
H	38	4.7957	6.4323	-4.2308
H	39	4.6505	4.6133	6.3204
H	40	5.6853	3.7519	5.0440

H	41	3.6367	4.7830	-6.5696
H	42	4.3276	6.5057	-6.6053
P	43	-3.6134	1.5446	0.7325
C	44	-3.4919	3.3673	0.8554
C	45	-4.1768	0.9356	2.3653
C	46	-4.9034	1.1456	-0.5108
C	47	-6.0730	0.4111	-0.2576
C	48	-6.7317	-0.2575	-1.2981
C	49	-6.2575	-0.2040	-2.6154
C	50	-5.1794	0.6582	-2.8814
C	51	-4.5028	1.3029	-1.8549
C	52	-4.0789	1.7164	3.5292
C	53	-4.0761	1.1142	4.7901
C	54	-4.2086	-0.2735	4.9403
C	55	-4.4473	-1.0307	3.7820
C	56	-4.3933	-0.4484	2.5184
C	57	-2.2808	3.8685	1.3643
C	58	-2.0145	5.2324	1.3653
C	59	-2.9310	6.1528	0.8237
C	60	-4.1462	5.6465	0.3235
C	61	-4.4253	4.2827	0.3402
C	62	-3.9271	-0.9292	6.2700
C	63	-6.8031	-1.0804	-3.7209
C	64	-2.5710	7.5732	0.7862
C	65	-2.4545	-1.4173	6.3397
C	66	-3.2133	8.5662	0.1426
C	67	-5.7361	-1.9817	-4.4093
H	68	-6.4382	0.3066	0.7649
H	69	-7.6046	-0.8727	-1.0677
H	70	-4.8117	0.7635	-3.9038
H	71	-3.6063	1.8799	-2.0844
H	72	-3.9506	2.7962	3.4484
H	73	-3.9338	1.7346	5.6778
H	74	-4.6123	-2.1061	3.8613
H	75	-4.4789	-1.0898	1.6404
H	76	-1.5285	3.1694	1.7343
H	77	-1.0610	5.5961	1.7527
H	78	-4.8899	6.3350	-0.0788
H	79	-5.3715	3.9187	-0.0613
H	80	-4.6059	-1.7787	6.4474
H	81	-7.2487	-0.4298	-4.4909
H	82	-1.6562	7.8220	1.3328
H	83	-2.1014	-1.3843	7.3827
H	84	-1.8311	-0.7049	5.7768

H	85	-4.1145	8.3959	-0.4475
H	86	-2.8366	9.5881	0.1761
H	87	-4.7398	-1.5346	-4.2741
H	88	-5.9227	-1.9729	-5.4938
P	89	0.3177	-1.9798	-0.5869
C	90	-1.2785	-2.5953	-1.2782
C	91	0.0447	-2.3284	1.2118
C	92	1.5932	-3.2256	-1.0776
C	93	2.1093	-4.2038	-0.2147
C	94	3.2347	-4.9555	-0.5723
C	95	3.8893	-4.7435	-1.7915
C	96	3.3210	-3.8190	-2.6798
C	97	2.2039	-3.0720	-2.3327
C	98	0.5342	-1.4768	2.2096
C	99	0.2901	-1.7419	3.5621
C	100	-0.4529	-2.8590	3.9614
C	101	-0.9324	-3.7151	2.9556
C	102	-0.6950	-3.4562	1.6084
C	103	-2.4036	-1.8232	-0.9555
C	104	-3.6720	-2.2200	-1.3576
C	105	-3.8704	-3.3745	-2.1305
C	106	-2.7383	-4.1257	-2.4782
C	107	-1.4559	-3.7517	-2.0509
C	108	-0.7718	-3.1562	5.4108
C	109	5.1819	-5.4179	-2.1941
C	110	-5.2725	-3.7802	-2.5316
C	111	-2.2396	-2.8360	5.7929
C	112	-5.6902	-3.4571	-3.9824
H	113	1.6598	-4.3570	0.7659
H	114	3.6229	-5.6859	0.1393
H	115	3.8031	-3.6405	-3.6427
H	116	1.8362	-2.3259	-3.0329
H	117	1.0901	-0.5809	1.9301
H	118	0.6763	-1.0529	4.3157
H	119	-1.5115	-4.5996	3.2312
H	120	-1.0976	-4.1354	0.8562
H	121	-2.2824	-0.9035	-0.3790
H	122	-4.5327	-1.6172	-1.0731
H	123	-2.8559	-5.0349	-3.0727
H	124	-0.5968	-4.3733	-2.3079
H	125	-0.0873	-2.5994	6.0690
H	126	-5.9849	-3.3139	-1.8336
H	127	-2.5908	-3.5597	6.5451
H	128	-2.8632	-2.9938	4.9015

H	129	-6.6833	-3.9072	-4.1514
H	130	-5.0017	-3.9823	-4.6651
H	131	-4.1099	-0.2048	7.0771
H	132	-7.6286	-1.6979	-3.3331
H	133	-0.5802	-4.2245	5.5944
H	134	-5.3809	-4.8682	-2.3954
C	135	6.6286	-4.8588	-0.0539
H	136	7.9379	-3.1571	0.0973
H	137	7.6239	-3.6265	-1.5612
H	138	5.8351	-4.6842	0.6854
H	139	7.4451	-5.3402	0.5057
C	140	6.1428	-5.8879	-1.0931
H	141	5.7176	-4.7262	-2.8634
H	142	4.9446	-6.2951	-2.8210
H	143	7.0221	-6.3126	-1.6045
H	144	5.6929	-6.7324	-0.5463
C	145	0.8160	-0.1029	-3.1642
O	146	0.7732	-0.2891	-4.3128
Rh	147	0.7169	0.2703	-1.2690
H	148	0.4058	0.5632	0.2772
C	149	-0.5087	1.7103	-1.5191
O	150	-1.2077	2.6228	-1.7030

$HRh(CO)_2(P\text{-}frame)_2$-2(b)

ATOM		X	Y	Z
P	1	22.1127	4.4137	20.0617
C	2	23.7413	3.6933	19.5912
C	3	20.9315	3.0131	19.9398
C	4	22.2428	4.7326	21.8666
C	5	21.5684	4.0082	22.8605
C	6	21.6177	4.4182	24.1934
C	7	22.3515	5.5501	24.5914
C	8	23.0227	6.2760	23.5871
C	9	22.9582	5.8842	22.2564
C	10	19.6112	3.3495	19.5992
C	11	18.6368	2.3659	19.4573
C	12	18.9444	1.0040	19.6321
C	13	20.2734	0.6714	19.9666
C	14	21.2462	1.6531	20.1213
C	15	23.8683	3.1684	18.2903
C	16	25.1187	2.8837	17.7473
C	17	26.2993	3.1396	18.4651
C	18	26.1662	3.6052	19.7785
C	19	24.9137	3.8688	20.3415
C	20	17.8841	0.0085	19.4505
C	21	22.3749	5.9290	26.0082
C	22	27.6615	3.0008	17.8191
C	23	17.9991	-1.3312	19.4734
C	24	23.1009	6.9092	26.5753
H	25	20.9903	3.1230	22.5931
H	26	21.0779	3.8444	24.9494
H	27	23.5817	7.1779	23.8377
H	28	23.4451	6.4968	21.4973
H	29	19.3570	4.3966	19.4264
H	30	17.6181	2.6508	19.1888
H	31	20.5460	-0.3728	20.1209
H	32	22.2667	1.3678	20.3799
H	33	22.9752	3.0120	17.6823
H	34	25.1737	2.4989	16.7273
H	35	27.0648	3.7881	20.3722
H	36	24.8605	4.2507	21.3613
H	37	16.8926	0.4339	19.2693
H	38	21.7335	5.3216	26.6529
H	39	18.9495	-1.8403	19.6361
H	40	17.1241	-1.9626	19.3232
H	41	23.7776	7.5402	25.9976
H	42	23.0438	7.0986	27.6464
P	43	21.6474	10.6816	18.9631
C	44	20.3548	10.3233	20.2296
C	45	20.6881	10.9863	17.4224
C	46	22.3241	12.3107	19.5008
C	47	22.1131	13.5424	18.8659
C	48	22.8455	14.6736	19.2449
C	49	23.7887	14.6199	20.2767
C	50	23.9004	13.4139	20.9874
C	51	23.1946	12.2819	20.6039
C	52	19.4473	10.3709	17.2007
C	53	18.8653	10.3902	15.9292
C	54	19.4820	11.0328	14.8461
C	55	20.6862	11.7072	15.0950
C	56	21.2893	11.6631	16.3496
C	57	20.2691	9.0500	20.8091
C	58	19.2931	8.7709	21.7645
C	59	18.3739	9.7471	22.1865
C	60	18.4724	11.0294	21.6042
C	61	19.4407	11.3110	20.6473
C	62	18.9218	10.8989	13.4481
C	63	24.6825	15.7897	20.6329
C	64	17.3807	9.3879	23.2033

C	65	19.6738	9.8159	12.6247
C	66	16.4660	10.1887	23.7775
C	67	26.1938	15.4387	20.6576
H	68	21.4019	13.6222	18.0448
H	69	22.6951	15.6078	18.6995
H	70	24.5828	13.3439	21.8357
H	71	23.3479	11.3558	21.1547
H	72	18.9426	9.8512	18.0149
H	73	17.9179	9.8705	15.7741
H	74	21.1853	12.2438	14.2872
H	75	22.2476	12.1533	16.4933
H	76	20.9837	8.2810	20.5154
H	77	19.2521	7.7721	22.2028
H	78	17.7792	11.8153	21.9039
H	79	19.4919	12.3142	20.2218
H	80	18.9657	11.8639	12.9182
H	81	24.3941	16.1455	21.6351
H	82	17.4152	8.3411	23.5185
H	83	18.9642	9.3138	11.9485
H	84	20.0224	9.0472	13.3290
H	85	16.3705	11.2466	23.5297
H	86	15.7744	9.7997	24.5243
H	87	26.2986	14.3619	20.8531
H	88	26.6645	15.9443	21.5137
P	89	24.8247	9.5067	17.0500
C	90	25.4893	11.2260	17.1785
C	91	24.2125	9.3620	15.3080
C	92	26.3485	8.4498	17.0343
C	93	27.0939	8.2385	15.8614
C	94	28.1552	7.3335	15.8410
C	95	28.5110	6.6011	16.9850
C	96	27.8031	6.8605	18.1641
C	97	26.7366	7.7606	18.1910
C	98	23.2396	8.3836	15.0609
C	99	22.5974	8.2927	13.8279
C	100	22.8710	9.2087	12.8036
C	101	23.9167	10.1211	13.0149
C	102	24.5926	10.1872	14.2350
C	103	24.8625	12.3010	16.5287
C	104	25.2069	13.6165	16.8194
C	105	26.1910	13.9277	17.7676
C	106	26.8502	12.8552	18.3850
C	107	26.5068	11.5294	18.1000
C	108	21.9990	9.3148	11.5757
C	109	29.5573	5.5113	16.9336
C	110	26.4871	15.3886	18.0371
C	111	20.8585	10.3425	11.7936
C	112	27.0197	15.8098	19.4148
H	113	26.8266	8.7607	14.9428
H	114	28.6968	7.1717	14.9068
H	115	28.0545	6.3129	19.0745
H	116	26.1764	7.8957	19.1141
H	117	22.9530	7.7040	15.8598
H	118	21.8346	7.5253	13.6840
H	119	24.1951	10.8128	12.2165
H	120	25.3957	10.9140	14.3558
H	121	24.0864	12.1119	15.7917
H	122	24.6848	14.4289	16.3098
H	123	27.6406	13.0471	19.1126
H	124	27.0249	10.7216	18.6184
H	125	21.5740	8.3334	11.3134
H	126	25.5674	15.9548	17.8221
H	127	20.4890	10.6869	10.8148
H	128	21.3003	11.2251	12.2791
H	129	27.1392	16.9052	19.3822
H	130	28.0376	15.4107	19.5558
H	131	17.8584	10.6286	13.5172
H	132	24.4889	16.6315	19.9502
H	133	22.6105	9.6367	10.7193
H	134	27.2171	15.7377	17.2864
C	135	27.7533	3.7093	16.4462
H	136	27.9220	1.9356	17.6984
H	137	28.4104	3.4133	18.5115
H	138	27.0172	4.5260	16.4218
H	139	27.4495	3.0073	15.6553
C	140	29.1292	4.2875	16.0896
H	141	29.7945	5.1972	17.9609
H	142	30.4946	5.9092	16.5135
H	143	29.9092	3.5123	16.1686
H	144	29.1068	4.5898	15.0305
C	145	24.0822	9.0080	20.4261
O	146	24.6629	8.9945	21.4414
Rh	147	23.2136	8.8374	18.7310
H	148	24.0151	7.4633	18.6612
C	149	21.8139	7.7352	18.0484
O	150	20.9698	7.0562	17.6170

$HRh(CO)(P\text{-}frame)_3$-1(a)(IS)

ATOM	X	Y	Z

P1	22.9739	5.9891	15.5343
C2	22.2363	5.1733	14.0397
C3	24.2185	4.7783	16.1486
C4	24.0113	7.2553	14.6711
C5	25.4075	7.2094	14.5592
C6	26.0952	8.1882	13.8381
C7	25.4230	9.2368	13.1873
C8	24.0163	9.2694	13.2977
C9	23.3314	8.3024	14.0198
C10	25.1559	5.2052	17.1060
C11	26.0727	4.3149	17.6541
C12	26.0532	2.9507	17.3201
C13	25.1119	2.5287	16.3713
C14	24.2148	3.4262	15.7827
C15	20.8986	4.7687	14.0693
C16	20.2516	4.3562	12.9045
C17	20.8987	4.3772	11.6645
C18	22.2637	4.7112	11.6487
C19	22.9251	5.0964	12.8145
C20	26.9427	1.9508	18.0237
C21	26.1905	10.2188	12.4163
C22	20.1114	4.1537	10.3939
C23	26.4934	1.6708	19.4819
C24	20.0788	5.3780	9.4447
C25	25.7270	11.3259	11.8097
H26	25.9674	6.3992	15.0244
H27	27.1829	8.1282	13.7630
H28	23.4514	10.0535	12.7931
H29	22.2419	8.3347	14.0642
H30	25.1636	6.2439	17.4377
H31	26.7954	4.6869	18.3801
H32	25.0754	1.4754	16.0848
H33	23.5023	3.0672	15.0396
H34	20.3383	4.8447	15.0003
H35	19.1990	4.0747	12.9515
H36	22.8105	4.7108	10.7032
H37	23.9732	5.3916	12.7602
H38	27.9889	2.2970	18.0221
H39	27.2610	10.0055	12.3465
H40	19.0852	3.8688	10.6687
H41	26.7496	0.6326	19.7414
H42	25.3955	1.7273	19.5083
H43	19.3400	5.1781	8.6507
H44	21.0534	5.4519	8.9363
H45	24.6779	11.6225	11.8431
H46	26.3968	11.9782	11.2501
Rh47	21.4871	6.7892	17.1552
P48	22.2522	7.3174	19.3374
C49	23.3816	6.0768	20.1163
C50	20.9382	7.5267	20.6339
C51	23.1968	8.9064	19.4557
C52	23.0619	9.8278	20.5052
C53	23.6290	11.1037	20.4110
C54	24.3733	11.4933	19.2924
C55	24.6119	10.5225	18.3071
C56	24.0208	9.2648	18.3762
C57	20.6232	6.5308	21.5720
C58	19.5307	6.6773	22.4319
C59	18.7272	7.8266	22.4175
C60	19.0708	8.8353	21.5046
C61	20.1355	8.6801	20.6174
C62	23.0412	4.7145	20.0826
C63	23.8883	3.7514	20.6295
C64	25.1298	4.1003	21.1812
C65	25.4660	5.4617	21.2122
C66	24.6035	6.4366	20.7057
C67	17.5220	7.9304	23.3257
C68	24.8801	12.9081	19.1109
C69	26.1114	3.0551	21.6568
C70	16.2196	7.3643	22.7055
C71	27.0963	2.6102	20.5502
C72	24.3938	13.5988	17.8151
H73	22.4713	9.5761	21.3851
H74	23.4596	11.8182	21.2200
H75	25.2263	10.7663	17.4383
H76	24.1554	8.5693	17.5480
H77	21.2348	5.6321	21.6477
H78	19.3081	5.8787	23.1437
H79	18.4882	9.7586	21.4713
H80	20.3484	9.4752	19.9045
H81	22.1136	4.3937	19.6111
H82	23.5806	2.7046	20.6088
H83	26.4203	5.7694	21.6460
H84	24.8943	7.4861	20.7544
H85	17.3583	8.9790	23.6211
H86	25.9819	12.8775	19.0778
H87	25.5734	2.1761	22.0461
H88	15.5418	7.0665	23.5204

H89	16.4729	6.4339	22.1774
H90	27.9554	2.1110	21.0246
H91	27.5051	3.5154	20.0777
H92	24.4086	12.8558	17.0066
H93	25.1431	14.3501	17.5226
P94	19.6544	8.1912	16.6325
C95	20.0632	9.9793	16.9369
C96	18.1042	7.9180	17.5967
C97	19.0186	8.0950	14.8997
C98	18.1764	7.0201	14.5676
C99	17.9052	6.7067	13.2367
C100	18.4891	7.4235	12.1835
C101	19.2352	8.5631	12.5199
C102	19.4945	8.8988	13.8500
C103	18.0763	6.9056	18.5619
C104	16.9843	6.7472	19.4122
C105	15.9073	7.6406	19.3736
C106	15.8970	8.6062	18.3508
C107	16.9620	8.7285	17.4580
C108	19.4209	10.7493	17.9223
C109	19.9680	11.9539	18.3664
C110	21.1660	12.4598	17.8396
C111	21.7349	11.7547	16.7726
C112	21.2127	10.5319	16.3481
C113	14.8802	7.6717	20.4786
C114	18.4069	6.9298	10.7552
C115	21.8071	13.6655	18.4957
C116	15.4648	8.3271	21.7604
C117	23.0359	14.3334	17.8577
C118	19.8055	6.7406	10.1002
H119	17.7545	6.3981	15.3586
H120	17.2739	5.8446	13.0115
H121	19.6584	9.1836	11.7271
H122	20.0834	9.7903	14.0652
H123	18.9444	6.2609	18.6778
H124	17.0062	5.9493	20.1538
H125	15.0473	9.2872	18.2666
H126	16.9237	9.4852	16.6730
H127	18.5120	10.3820	18.3946
H128	19.4719	12.4881	19.1802
H129	22.6394	12.1233	16.2936
H130	21.7712	9.9704	15.6010
H131	14.5234	6.6567	20.7161
H132	17.8094	7.6277	10.1469
H133	22.0588	13.3768	19.5301
H134	14.6470	8.8082	22.3188
H135	16.1328	9.1415	21.4424
H136	23.1908	15.2715	18.4151
H137	22.7863	14.6429	16.8295
H138	20.5795	6.9134	10.8624
H139	19.9595	7.5184	9.3367
H140	17.7346	7.3767	24.2524
H141	24.6211	13.5152	19.9928
H142	14.0036	8.2452	20.1430
H143	21.0328	14.4439	18.5994
H144	26.9270	1.0094	17.4547
H145	20.5244	3.2994	9.8326
H146	26.6901	3.4668	22.4980
H147	17.8513	5.9798	10.7463
H148	22.2234	8.1559	16.7900
C149	20.6854	5.0766	17.5163
O150	20.2487	4.0104	17.7202
C149	27.4602	12.1349	15.1668
O150	28.2127	11.2722	15.1630

HRh(CO)(P-frame)$_3$-1(a)(TS)

ATOM	X	Y	Z
C149	27.3481	12.0681	15.4981
O150	28.2259	11.6417	16.0946
P1	23.9284	6.4135	15.2848
C2	22.8925	5.7772	13.9018
C3	24.8573	4.9468	15.8952
C4	25.2137	7.3923	14.3997
C5	26.4605	6.9020	13.9797
C6	27.3667	7.7363	13.3261
C7	27.0656	9.0837	13.0511
C8	25.8122	9.5702	13.4771
C9	24.9145	8.7446	14.1418
C10	25.8515	5.1583	16.8667
C11	26.4891	4.0881	17.4910
C12	26.1313	2.7619	17.2010
C13	25.1497	2.5567	16.2220
C14	24.5245	3.6230	15.5721
C15	21.5888	5.3733	14.2240
C16	20.7018	4.9620	13.2321
C17	21.0612	4.9829	11.8781
C18	22.3714	5.3737	11.5587
C19	23.2758	5.7610	12.5511
C20	26.6937	1.5895	17.9710

C21	28.0556	9.9158	12.3632
C22	20.0471	4.5916	10.8235
C23	25.9044	1.3161	19.2761
C24	19.9233	5.5209	9.6023
C25	27.9253	11.2010	11.9866
H26	26.7251	5.8623	14.1737
H27	28.3327	7.3367	13.0106
H28	25.5434	10.6103	13.2953
H29	23.9575	9.1495	14.4755
H30	26.1313	6.1760	17.1448
H31	27.2687	4.2921	18.2271
H32	24.8625	1.5356	15.9612
H33	23.7654	3.4227	14.8148
H34	21.2527	5.4207	15.2652
H35	19.6931	4.6612	13.5146
H36	22.6962	5.3915	10.5166
H37	24.2814	6.0724	12.2665
H38	27.7570	1.7553	18.2069
H39	28.9992	9.4080	12.1431
H40	19.0659	4.4937	11.3115
H41	25.9675	0.2451	19.5273
H42	24.8430	1.5247	19.0753
H43	19.1493	5.0986	8.9396
H44	20.8594	5.4809	9.0214
H45	27.0163	11.7767	12.1639
H46	28.7421	11.7180	11.4844
Rh47	20.8606	6.7807	17.5257
P48	21.8333	7.0293	19.6096
C49	22.7780	5.6466	20.3820
C50	20.4722	7.4162	20.8004
C51	22.9561	8.4922	19.7631
C52	22.8776	9.4416	20.7909
C53	23.5648	10.6570	20.6899
C54	24.3655	10.9524	19.5808
C55	24.5402	9.9418	18.6209
C56	23.8358	8.7455	18.6976
C57	19.9764	6.4910	21.7296
C58	18.8525	6.7974	22.5040
C59	18.1938	8.0324	22.3967
C60	18.7158	8.9626	21.4854
C61	19.8187	8.6563	20.6914
C62	22.4124	4.3251	20.0846
C63	23.1799	3.2496	20.5323
C64	24.3646	3.4597	21.2533
C65	24.7085	4.7820	21.5736
C66	23.9290	5.8611	21.1581
C67	16.9438	8.3108	23.2049
C68	25.0136	12.3090	19.3911
C69	25.3099	2.3310	21.5850
C70	15.6295	7.9174	22.4815
C71	26.3809	2.1350	20.4853
C72	24.7136	12.9905	18.0340
H73	22.2374	9.2651	21.6547
H74	23.4439	11.4036	21.4785
H75	25.1937	10.1109	17.7632
H76	23.9148	8.0215	17.8848
H77	20.4707	5.5275	21.8573
H78	18.4865	6.0579	23.2197
H79	18.2452	9.9422	21.3838
H80	20.1742	9.3913	19.9702
H81	21.5339	4.1379	19.4663
H82	22.8706	2.2335	20.2825
H83	25.6177	4.9715	22.1485
H84	24.2332	6.8762	21.4133
H85	16.9043	9.3743	23.4888
H86	26.1061	12.1806	19.4675
H87	24.7532	1.3930	21.7355
H88	14.8707	7.6648	23.2388
H89	15.8171	6.9854	21.9318
H90	27.2652	1.6448	20.9226
H91	26.7104	3.1321	20.1579
H92	24.6710	12.2160	17.2568
H93	25.5762	13.6197	17.7663
P94	19.3482	8.2619	16.5949
C95	19.9603	9.9890	16.8894
C96	17.7235	8.2032	17.4680
C97	18.8579	8.1721	14.8166
C98	18.0635	7.0831	14.4216
C99	17.8260	6.8228	13.0729
C100	18.3987	7.6142	12.0678
C101	19.1379	8.7355	12.4704
C102	19.3635	9.0176	13.8173
C103	17.5191	7.2190	18.4402
C104	16.3813	7.2192	19.2406
C105	15.4449	8.2554	19.1568
C106	15.6099	9.2007	18.1295
C107	16.7155	9.1637	17.2773
C108	19.4120	10.8215	17.8773

C109	20.1114	11.9374	18.3398
C110	21.3703	12.2904	17.8315
C111	21.8582	11.5281	16.7611
C112	21.1822	10.3895	16.3196
C113	14.3995	8.4473	20.2296
C114	18.2564	7.2841	10.5989
C115	22.1284	13.4099	18.5166
C116	15.0448	8.9907	21.5351
C117	23.4713	13.9023	17.9584
C118	19.5968	6.9982	9.8681
H119	17.6447	6.4158	15.1770
H120	17.2094	5.9648	12.7964
H121	19.5567	9.4029	11.7142
H122	19.9401	9.9027	14.0833
H123	18.2917	6.4707	18.6039
H124	16.2655	6.4299	19.9826
H125	14.8713	9.9971	18.0138
H126	16.8105	9.9123	16.4891
H127	18.4604	10.5687	18.3414
H128	19.6814	12.5261	19.1539
H129	22.8124	11.7784	16.2995
H130	21.6634	9.7573	15.5732
H131	13.8685	7.5056	20.4408
H132	17.7646	8.1347	10.1014
H133	22.2738	13.1038	19.5664
H134	14.2962	9.5789	22.0882
H135	15.8301	9.7034	21.2418
H136	23.7065	14.8261	18.5119
H137	23.3408	14.2153	16.9092
H138	20.4212	7.4582	10.4335
H139	19.5829	7.5031	8.8901
H140	17.0098	7.7434	24.1456
H141	24.7331	12.9754	20.2218
H142	13.6440	9.1626	19.8748
H143	21.4569	14.2829	18.5697
H144	26.6501	0.6948	17.3323
H145	20.2946	3.5825	10.4508
H146	25.8149	2.5536	22.5370
H147	17.5721	6.4300	10.4778
H148	21.7510	8.0795	17.2752
C149	19.8899	5.1108	17.5340
O150	19.3436	4.0847	17.4074

HRh(CO)(P-frame)$_3$-1(a)(FS)

ATOM	X	Y	Z
C149	22.5769	8.3152	16.2778
O150	23.3430	8.9611	15.6870
P1	23.7482	5.5737	14.6312
C2	22.9021	4.6865	13.2656
C3	24.9150	4.4421	15.4662
C4	24.7987	6.8048	13.7679
C5	26.1789	6.9493	13.9708
C6	26.8505	8.0825	13.5107
C7	26.1793	9.1127	12.8307
C8	24.8022	8.9353	12.5817
C9	24.1289	7.8184	13.0488
C10	25.6082	4.9635	16.5768
C11	26.4165	4.1516	17.3641
C12	26.5193	2.7726	17.1159
C13	25.8178	2.2563	16.0167
C14	25.0358	3.0727	15.1954
C15	21.6033	4.2149	13.5270
C16	20.7351	3.9046	12.4809
C17	21.1165	4.0838	11.1449
C18	22.4516	4.4358	10.8873
C19	23.3319	4.7300	11.9277
C20	27.2574	1.8515	18.0595
C21	26.9153	10.3149	12.4347
C22	20.0922	4.0568	10.0352
C23	26.5114	1.6768	19.4073
C24	19.8869	5.4537	9.3965
C25	26.4068	11.4609	11.9421
H26	26.7312	6.1786	14.5084
H27	27.9221	8.1808	13.6975
H28	24.2470	9.6986	12.0363
H29	23.0523	7.7390	12.8863
H30	25.4952	6.0168	16.8392
H31	26.9424	4.5982	18.2083
H32	25.8781	1.1871	15.8026
H33	24.5070	2.6384	14.3458
H34	21.2401	4.1744	14.5542
H35	19.7129	3.5987	12.7112
H36	22.7954	4.5344	9.8556
H37	24.3441	5.0643	11.6981
H38	28.2772	2.2258	18.2491
H39	27.9981	10.2547	12.5799
H40	19.1392	3.6769	10.4327
H41	26.6528	0.6485	19.7767
H42	25.4343	1.7848	19.2119

H43	19.0788	5.3897	8.6495
H44	20.7992	5.7073	8.8341
H45	25.3357	11.6096	11.7949
H46	27.0571	12.2967	11.6871
Rh47	21.2334	7.6264	17.4823
P48	22.0899	7.5037	19.6661
C49	23.1927	6.1363	20.2263
C50	20.8355	7.6452	21.0046
C51	23.1414	9.0135	19.8638
C52	22.8014	10.0846	20.6977
C53	23.3662	11.3486	20.4982
C54	24.2907	11.5785	19.4757
C55	24.7416	10.4631	18.7469
C56	24.1751	9.2078	18.9298
C57	20.6678	6.6993	22.0234
C58	19.5830	6.7922	22.9016
C59	18.6616	7.8461	22.8234
C60	18.8727	8.8193	21.8338
C61	19.9137	8.7025	20.9209
C62	22.9013	4.7994	19.9163
C63	23.7268	3.7653	20.3659
C64	24.8828	4.0319	21.1155
C65	25.1718	5.3725	21.4117
C66	24.3432	6.4085	20.9841
C67	17.4285	7.8647	23.6976
C68	24.7386	12.9677	19.0856
C69	25.8369	2.9461	21.5587
C70	16.1675	7.3491	22.9566
C71	26.9412	2.6545	20.5148
C72	24.2471	13.4008	17.6733
H73	22.0451	9.9584	21.4710
H74	23.0397	12.1794	21.1272
H75	25.5018	10.5904	17.9734
H76	24.4888	8.3848	18.2881
H77	21.3741	5.8751	22.1250
H78	19.4543	6.0225	23.6661
H79	18.1894	9.6648	21.7474
H80	20.0027	9.4289	20.1128
H81	22.0254	4.5581	19.3146
H82	23.4626	2.7347	20.1257
H83	26.0641	5.6094	21.9956
H84	24.5911	7.4374	21.2430
H85	17.2425	8.8827	24.0769
H86	25.8395	13.0008	19.0945
H87	25.2858	2.0187	21.7785
H88	15.4834	6.8870	23.6855
H89	16.4850	6.5397	22.2850
H90	27.8267	2.2439	21.0260
H91	27.2622	3.6125	20.0807
H92	24.0257	12.4971	17.0878
H93	25.0773	13.9009	17.1530
P94	19.2097	8.6323	16.7742
C95	19.5342	10.4459	16.8958
C96	17.6977	8.3418	17.7849
C97	18.6763	8.1983	15.0602
C98	18.4223	6.8352	14.8345
C99	18.1959	6.3502	13.5519
C100	18.2365	7.1931	12.4318
C101	18.4201	8.5635	12.6652
C102	18.6285	9.0643	13.9572
C103	17.6814	7.2099	18.6077
C104	16.6491	7.0030	19.5211
C105	15.6406	7.9602	19.6940
C106	15.6159	9.0515	18.8080
C107	16.6098	9.2283	17.8455
C108	19.2103	11.1098	18.0943
C109	19.9120	12.2427	18.4923
C110	20.9466	12.7877	17.7146
C111	21.1712	12.2072	16.4599
C112	20.4885	11.0523	16.0598
C113	14.6981	7.9097	20.8735
C114	18.2042	6.6059	11.0396
C115	21.7347	13.9486	18.2888
C116	15.3883	8.4210	22.1668
C117	23.0525	14.3702	17.6261
C118	19.6141	6.5931	10.3911
H119	18.4322	6.1322	15.6677
H120	18.0209	5.2825	13.4092
H121	18.4216	9.2601	11.8242
H122	18.7698	10.1370	14.0939
H123	18.5242	6.5173	18.5724
H124	16.6702	6.1125	20.1493
H125	14.8172	9.7920	18.8907
H126	16.5652	10.0880	17.1756
H127	18.4617	10.6922	18.7654
H128	19.6802	12.6935	19.4601
H129	21.9353	12.6115	15.7952
H130	20.7875	10.5715	15.1289

H131	14.3203	6.8874	21.0337
H132	17.5122	7.1694	10.3944
H133	21.9223	13.7225	19.3511
H134	14.6313	8.8668	22.8312
H135	16.0588	9.2441	21.8815
H136	23.3603	15.3141	18.1066
H137	22.8638	14.6304	16.5717
H138	20.3699	6.5487	11.1882
H139	19.7763	7.5542	9.8802
H140	17.6129	7.2347	24.5797
H141	24.4070	13.6942	19.8434
H142	13.8218	8.5382	20.6583
H143	21.0722	14.8317	18.3012
H144	27.3731	0.8729	17.5729
H145	20.3987	3.3553	9.2431
H146	26.3085	3.2614	22.5014
H147	17.8104	5.5802	11.0980
H148	21.3837	9.1307	17.9726
C149	20.9107	5.7564	17.0928
O150	20.6959	4.6276	16.8830

$HRh(CO)(P\text{-}frame)_3$-1(b)(IS)

ATOM	X	Y	Z
P1	23.6988	3.8171	12.8501
C2	23.0657	3.7227	14.5856
C3	25.1182	2.6118	12.8915
C4	22.3806	2.8926	11.9435
C5	22.6778	1.9466	10.9521
C6	21.6528	1.3121	10.2477
C7	20.3019	1.5867	10.5072
C8	20.0143	2.5297	11.5047
C9	21.0311	3.1828	12.1975
C10	26.1298	2.7520	11.9310
C11	27.2734	1.9614	11.9649
C12	27.4819	1.0222	12.9830
C13	26.4492	0.8463	13.9143
C14	25.2861	1.6211	13.8705
C15	23.3301	4.7769	15.4714
C16	22.9101	4.7234	16.8000
C17	22.1922	3.6192	17.2980
C18	21.9117	2.5697	16.3975
C19	22.3372	2.6181	15.0755
C20	28.7857	0.2530	13.0634
C21	19.2192	0.9295	9.6836
C22	21.7575	3.6139	18.6961
C23	30.0657	1.1105	12.8948
C24	21.1101	2.6297	19.3506
H25	23.7150	1.6906	10.7350
H26	21.9146	0.5762	9.4840
H27	18.9784	2.7644	11.7525
H28	20.7522	3.9109	12.9588
H29	26.0456	3.5248	11.1708
H30	28.0354	2.1158	11.1996
H31	26.5660	0.1121	14.7151
H32	24.5318	1.4774	14.6433
H33	23.8437	5.6680	15.1086
H34	23.1357	5.5617	17.4616
H35	21.3406	1.7041	16.7342
H36	22.0836	1.7957	14.4067
H37	28.7779	-0.5093	12.2671
C38	18.7852	1.7788	8.4646
H39	21.9989	4.5244	19.2527
H40	29.8325	1.9814	12.2665
H41	30.8082	0.5277	12.3289
H42	20.8372	1.6865	18.8756
H43	20.8390	2.7446	20.3994
Rh44	24.3114	5.9411	11.8120
P45	26.0753	6.7480	13.2482
C46	27.3420	5.5840	13.9107
C47	25.5558	7.6934	14.7577
C48	26.9993	8.0006	12.2494
C49	26.9779	9.3630	12.5707
C50	27.2239	10.3281	11.5879
C51	27.5220	9.9678	10.2694
C52	27.7218	8.6014	10.0047
C53	27.4497	7.6344	10.9667
C54	26.1023	7.5961	16.0453
C55	25.4620	8.2125	17.1310
C56	24.2929	8.9711	16.9683
C57	23.8116	9.1409	15.6602
C58	24.4134	8.4893	14.5945
C59	26.9261	4.6458	14.8703
C60	27.7827	3.6421	15.3042
C61	29.0750	3.5015	14.7806
C62	29.5066	4.4647	13.8575
C63	28.6570	5.4927	13.4306
C64	23.5041	9.4973	18.1504
C65	27.4867	10.9760	9.1409
C66	29.9187	2.3285	15.2329

C67	22.0158	9.0539	18.1253
C68	30.7645	1.5958	14.1760
C69	26.6197	10.4904	7.9442
H70	26.6737	9.6839	13.5665
H71	27.1070	11.3841	11.8417
H72	28.0074	8.2786	9.0024
H73	27.4856	6.5825	10.6822
H74	27.0051	7.0103	16.2177
H75	25.8743	8.0759	18.1336
H76	22.9154	9.7289	15.4722
H77	23.9595	8.5398	13.6082
H78	25.9138	4.6791	15.2709
H79	27.4218	2.9163	16.0342
H80	30.5174	4.4147	13.4476
H81	29.0226	6.2217	12.7073
H82	23.5599	10.5987	18.1898
H83	28.5085	11.1960	8.7892
H84	29.2453	1.6052	15.7182
H85	21.6854	8.8383	19.1535
H86	21.9600	8.0971	17.5854
H87	26.0485	9.6059	8.2617
H88	27.2786	10.1451	7.1334
P89	22.2773	7.1823	11.5538
C90	22.6709	8.7131	10.5690
C91	21.2962	7.8448	12.9853
C92	20.9743	6.3604	10.5287
C93	19.6025	6.5004	10.7893
C94	18.6589	5.8340	10.0062
C95	19.0414	5.0342	8.9188
C96	20.4113	4.9305	8.6405
C97	21.3618	5.5597	9.4438
C98	21.1385	7.0064	14.0997
C99	20.5875	7.4762	15.2916
C100	20.2000	8.8178	15.4307
C101	20.2765	9.6320	14.2893
C102	20.8007	9.1564	13.0841
C103	23.3152	9.7895	11.1995
C104	23.8583	10.8377	10.4627
C105	23.7954	10.8628	9.0635
C106	23.1062	9.8163	8.4352
C107	22.5489	8.7636	9.1711
C108	19.8208	9.4030	16.7719
C109	18.0083	4.2513	8.1446
C110	24.4951	11.9669	8.2997
C111	21.0271	10.0574	17.4944
C112	25.6253	11.4984	7.3537
C113	17.7275	2.8641	8.7691
H114	19.2678	7.1269	11.6160
H115	17.5981	5.9443	10.2437
H116	20.7484	4.3286	7.7951
H117	22.4204	5.4111	9.2352
H118	21.5002	5.9801	14.0574
H119	20.5009	6.7937	16.1388
H120	19.9361	10.6690	14.3444
H121	20.8542	9.8264	12.2263
H122	23.4254	9.8130	12.2809
H123	24.3673	11.6475	10.9881
H124	23.0088	9.8046	7.3475
H125	22.0366	7.9602	8.6427
H126	19.3870	8.6238	17.4182
H127	24.8964	12.6852	9.0301
H128	20.6492	10.7356	18.2755
H129	21.5471	10.7046	16.7715
H130	26.1529	12.3915	6.9787
H131	25.1695	11.0263	6.4689
H132	23.9802	9.1389	19.0744
H133	27.0993	11.9263	9.5365
H134	19.0402	10.1664	16.6300
H135	23.7642	12.5318	7.6982
H136	28.8253	-0.3097	14.0097
H137	30.6078	2.6644	16.0272
H138	18.3385	0.7132	10.3088
H139	19.5914	-0.0418	9.3257
H140	18.3909	1.1042	7.6892
H141	19.6870	2.2373	8.0336
H142	31.2285	0.7329	14.6811
H143	31.6053	2.2394	13.8693
H144	18.3277	4.1269	7.0979
H145	17.0688	4.8247	8.1197
H146	16.7430	2.5143	8.4225
H147	17.6285	3.0006	9.8564
H148	24.7833	7.2522	11.0851
C149	24.8003	5.2245	10.1337
O150	25.1358	4.9626	9.0405
C149	18.0718	4.8282	13.9069
O150	17.0356	5.3130	13.8989

HRh(CO)(P-frame)$_3$-1(b)(TS)

ATOM	X	Y	Z

C149	20.6535	4.9297	14.6161
O150	19.9430	4.0903	14.2989
P1	24.1800	2.7457	13.2796
C2	23.5418	2.2825	14.9389
C3	25.8719	2.0140	13.2097
C4	23.1278	1.7399	12.1429
C5	23.6211	1.2529	10.9262
C6	22.7421	0.8782	9.9061
C7	21.3509	0.9679	10.0640
C8	20.8686	1.3496	11.3256
C9	21.7368	1.7411	12.3423
C10	26.7539	2.5534	12.2584
C11	28.0954	2.1839	12.2371
C12	28.6229	1.2925	13.1838
C13	27.7324	0.7290	14.1061
C14	26.3789	1.0782	14.1211
C15	23.3889	3.2746	15.9186
C16	22.9305	2.9508	17.1949
C17	22.5920	1.6285	17.5383
C18	22.7313	0.6395	16.5423
C19	23.1905	0.9589	15.2709
C20	30.1037	0.9693	13.1920
C21	20.4253	0.7570	8.8896
C22	22.1048	1.3377	18.8892
C23	31.0437	2.1986	13.1711
C24	21.6483	0.1612	19.3611
H25	24.6968	1.2088	10.7514
H26	23.1492	0.5433	8.9499
H27	19.7937	1.3765	11.5089
H28	21.3227	2.0877	13.2879
H29	26.3860	3.3069	11.5585
H30	28.7510	2.6306	11.4881
H31	28.1057	0.0200	14.8486
H32	25.7298	0.6478	14.8832
H33	23.6157	4.3133	15.6718
H34	22.8224	3.7403	17.9411
H35	22.4759	-0.3956	16.7681
H36	23.2633	0.1758	14.5147
H37	30.3190	0.3606	12.2987
C38	19.9235	2.0820	8.2505
H39	22.1189	2.1913	19.5727
H40	30.5598	3.0069	12.6045
H41	31.9502	1.9398	12.6024
H42	21.5839	-0.7373	18.7461
H43	21.3102	0.0730	20.3931
Rh44	23.9874	5.0285	12.5988
P45	25.6175	6.3766	13.6169
C46	27.1233	5.6190	14.3520
C47	24.8982	7.4758	14.9141
C48	26.2757	7.5620	12.3622
C49	26.6089	8.8896	12.6620
C50	26.8914	9.7959	11.6351
C51	26.8676	9.4104	10.2868
C52	26.6201	8.0576	10.0054
C53	26.3152	7.1542	11.0210
C54	25.3286	7.5263	16.2471
C55	24.6184	8.2751	17.1940
C56	23.4788	9.0134	16.8444
C57	23.0844	8.9911	15.4972
C58	23.7636	8.2240	14.5564
C59	26.9688	4.6183	15.3251
C60	28.0551	3.8519	15.7314
C61	29.3299	4.0284	15.1728
C62	29.4930	5.0631	14.2429
C63	28.4081	5.8474	13.8381
C64	22.6896	9.7800	17.8907
C65	27.0094	10.4358	9.1776
C66	30.4428	3.0875	15.5812
C67	21.1556	9.7867	17.6741
C68	31.5136	2.7449	14.5308
C69	26.0838	10.1712	7.9669
H70	26.5914	9.2391	13.6951
H71	27.0945	10.8390	11.8882
H72	26.6043	7.7091	8.9721
H73	26.0319	6.1296	10.7721
H74	26.2119	6.9666	16.5574
H75	24.9596	8.2739	18.2318
H76	22.2034	9.5456	15.1742
H77	23.3879	8.1799	13.5330
H78	25.9823	4.3960	15.7331
H79	27.8999	3.0549	16.4608
H80	30.4716	5.2498	13.7977
H81	28.5581	6.6225	13.0859
H82	23.0553	10.8212	17.9292
H83	28.0572	10.4753	8.8342
H84	29.9783	2.1567	15.9419
H85	20.6485	9.6137	18.6362
H86	20.8927	8.9283	17.0392

H87	25.2156	9.5885	8.3078
H88	26.6079	9.5332	7.2388
P89	21.1857	8.3315	11.2271
C90	21.9058	9.7078	10.2526
C91	20.1827	9.1340	12.5392
C92	20.0839	7.3522	10.1407
C93	18.7983	6.9428	10.5322
C94	18.1619	5.8826	9.8830
C95	18.7696	5.2028	8.8170
C96	20.0113	5.6778	8.3703
C97	20.6683	6.7123	9.0303
C98	19.7817	8.3327	13.6246
C99	19.3482	8.9006	14.8215
C100	19.3597	10.2922	15.0055
C101	19.6782	11.0900	13.8958
C102	20.0689	10.5285	12.6788
C103	22.9551	10.3947	10.8891
C104	23.7430	11.3009	10.1905
C105	23.5593	11.5187	8.8171
C106	22.4824	10.8718	8.1929
C107	21.6555	9.9912	8.9005
C108	19.2125	10.9153	16.3739
C109	18.1331	3.9650	8.2290
C110	24.5867	12.3095	8.0425
C111	20.5938	11.0817	17.0598
C112	25.5582	11.4112	7.2288
C113	18.6305	2.6378	8.8608
H114	18.3031	7.4353	11.3697
H115	17.1749	5.5645	10.2259
H116	20.5008	5.1956	7.5231
H117	21.6712	6.9926	8.7068
H118	19.8796	7.2484	13.5596
H119	19.0695	8.2465	15.6493
H120	19.6546	12.1776	13.9969
H121	20.3399	11.1807	11.8487
H122	23.1859	10.1853	11.9347
H123	24.5625	11.8026	10.7071
H124	22.2940	11.0414	7.1300
H125	20.8306	9.4949	8.3881
H126	18.5544	10.3056	17.0118
H127	25.1597	12.9315	8.7464
H128	20.5212	11.8498	17.8466
H129	21.3004	11.4794	16.3141
H130	26.3930	12.0352	6.8686
H131	25.0300	11.0579	6.3286
H132	22.9281	9.3515	18.8752
H133	26.8035	11.4283	9.6051
H134	18.7384	11.9035	16.2788
H135	24.0983	13.0074	7.3442
H136	30.3362	0.3263	14.0551
H137	30.9616	3.5118	16.4584
H138	19.5558	0.1479	9.1875
H139	20.9610	0.1785	8.1228
H140	19.7426	1.9024	7.1776
H141	20.7260	2.8321	8.3124
H142	32.1956	2.0111	14.9919
H143	32.1338	3.6350	14.3366
H144	18.3022	3.9310	7.1403
H145	17.0438	4.0310	8.3701
H146	17.8400	1.8774	8.7441
H147	18.7560	2.7908	9.9438
H148	23.6567	6.5179	12.1111
C149	23.1209	4.6364	10.9884
O150	22.7773	4.4849	9.8840

$HRh(CO)(P\text{-}frame)_3$-1(b)(FS)

ATOM	X	Y	Z
C149	23.1469	6.3226	13.7956
O150	22.3161	6.7635	14.4814
P1	24.1356	3.4092	13.3001
C2	23.4108	3.1843	14.9797
C3	25.5779	2.2676	13.2364
C4	22.8471	2.6664	12.2108
C5	22.9465	1.3926	11.6378
C6	21.9552	0.9345	10.7622
C7	20.8382	1.7182	10.4407
C8	20.7389	2.9854	11.0390
C9	21.7273	3.4554	11.8979
C10	26.4891	2.4355	12.1794
C11	27.6945	1.7442	12.1588
C12	28.0674	0.8923	13.2126
C13	27.1302	0.6818	14.2324
C14	25.9015	1.3534	14.2495
C15	23.7598	4.0699	16.0122
C16	23.1580	3.9785	17.2643
C17	22.1579	3.0245	17.5285
C18	21.8288	2.1231	16.4957
C19	22.4411	2.2016	15.2481
C20	29.4339	0.2350	13.2193

C21	19.7865	1.2162	9.4696
C22	21.4824	3.0374	18.8295
C23	30.6263	1.1786	12.9050
C24	20.3269	2.4296	19.1495
H25	23.8136	0.7656	11.8496
H26	22.0654	-0.0499	10.3025
H27	19.8967	3.6379	10.8055
H28	21.6551	4.4685	12.2942
H29	26.2620	3.1442	11.3826
H30	28.3772	1.9082	11.3242
H31	27.3789	0.0083	15.0558
H32	25.2175	1.1982	15.0845
H33	24.4688	4.8756	15.8204
H34	23.4330	4.6970	18.0387
H35	21.0764	1.3530	16.6688
H36	22.1424	1.5050	14.4647
H37	29.4222	-0.5666	12.4628
C38	19.2448	2.2770	8.4765
H39	21.9738	3.6454	19.5947
H40	30.2485	2.0714	12.3859
H41	31.2977	0.6799	12.1895
H42	19.7510	1.8475	18.4289
H43	19.9069	2.5194	20.1509
Rh44	24.5240	5.6804	12.6472
P45	26.6105	6.5407	13.5269
C46	27.9629	5.4732	14.1652
C47	26.0815	7.6508	14.9083
C48	27.3718	7.6504	12.2623
C49	27.6311	9.0106	12.4834
C50	27.7327	9.8971	11.4049
C51	27.6149	9.4545	10.0806
C52	27.5433	8.0668	9.8686
C53	27.4060	7.1859	10.9355
C54	26.1312	7.2647	16.2559
C55	25.2986	7.8737	17.2070
C56	24.4181	8.9024	16.8527
C57	24.4796	9.3754	15.5317
C58	25.2743	8.7573	14.5776
C59	27.6226	4.4429	15.0573
C60	28.5572	3.4863	15.4373
C61	29.8544	3.4788	14.9077
C62	30.2059	4.5269	14.0428
C63	29.2812	5.5130	13.6806
C64	23.3492	9.4424	17.7744
C65	27.4335	10.4301	8.9357
C66	30.7873	2.3414	15.2603
C67	21.9167	9.0680	17.2881
C68	31.4947	1.6314	14.0898
C69	26.2728	10.0310	7.9875
H70	27.6622	9.4016	13.5003
H71	27.8434	10.9656	11.6051
H72	27.5027	7.6728	8.8522
H73	27.2264	6.1300	10.7325
H74	26.7883	6.4527	16.5680
H75	25.3183	7.5114	18.2376
H76	23.8363	10.2033	15.2280
H77	25.2222	9.1008	13.5454
H78	26.6016	4.3567	15.4272
H79	28.2547	2.6914	16.1197
H80	31.2145	4.5716	13.6264
H81	29.5821	6.3032	12.9919
H82	23.4364	10.5408	17.8140
H83	28.3653	10.5264	8.3533
H84	30.2088	1.6021	15.8346
H85	21.5387	8.2118	17.8702
H86	21.9747	8.7121	16.2509
H87	25.5600	9.4031	8.5417
H88	26.6669	9.3933	7.1820
P89	20.8516	7.9345	11.1073
C90	21.7384	9.2944	10.2569
C91	20.0468	8.6863	12.5784
C92	19.5996	7.2333	9.9715
C93	18.2939	6.9001	10.3758
C94	17.5664	5.9253	9.6885
C95	18.0916	5.2717	8.5627
C96	19.3321	5.7158	8.0785
C97	20.0827	6.6583	8.7778
C98	19.5216	7.8071	13.5442
C99	19.2848	8.2322	14.8499
C100	19.5933	9.5376	15.2599
C101	20.0357	10.4359	14.2763
C102	20.2537	10.0251	12.9591
C103	22.9401	9.6763	10.8824
C104	23.8109	10.5797	10.2838
C105	23.5458	11.1093	9.0108
C106	22.3395	10.7415	8.3936
C107	21.4421	9.8569	9.0040
C108	19.5363	9.9289	16.7223

C109	17.4105	4.0471	8.0019
C110	24.5716	11.9763	8.3193
C111	20.9177	10.2279	17.3516
C112	25.5007	11.1980	7.3541
C113	17.8187	2.7653	8.7717
H114	17.8617	7.3675	11.2613
H115	16.5753	5.6429	10.0524
H116	19.7492	5.2717	7.1729
H117	21.0870	6.9034	8.4278
H118	19.3690	6.7555	13.2973
H119	18.9230	7.5110	15.5848
H120	20.2492	11.4723	14.5469
H121	20.6335	10.7418	12.2306
H122	23.2073	9.2272	11.8400
H123	24.7381	10.8429	10.7964
H124	22.0926	11.1510	7.4108
H125	20.5129	9.5962	8.4947
H126	19.0466	9.1198	17.2863
H127	25.1778	12.4880	9.0829
H128	20.7637	10.5410	18.3977
H129	21.3599	11.0972	16.8366
H130	26.2018	11.9132	6.8923
H131	24.8838	10.7957	6.5349
H132	23.5175	9.0857	18.8012
H133	27.2473	11.4267	9.3642
H134	18.9047	10.8232	16.8465
H135	24.0668	12.7695	7.7463
H136	29.5904	-0.2750	14.1823
H137	31.5667	2.7037	15.9520
H138	18.9432	0.7956	10.0456
H139	20.2143	0.3665	8.9185
H140	19.2644	1.8653	7.4553
H141	19.9343	3.1334	8.4668
H142	32.0259	0.7608	14.5092
H143	32.2806	2.2907	13.6867
H144	17.6496	3.9255	6.9334
H145	16.3186	4.1666	8.0712
H146	17.1059	1.9597	8.5297
H147	17.7035	2.9606	9.8507
H148	24.5356	7.1908	12.1212
C149	24.5691	5.3323	10.7640
O150	24.5386	5.2470	9.6003

$HRh(CO)(P\text{-}frame)_3$-2(b)(IS)

ATOM	X	Y	Z
C1	24.4343	9.5299	21.0476
O2	25.0996	9.9455	21.9200
P3	23.0529	6.3209	19.7742
C4	24.4357	5.2366	19.1785
C5	21.5599	5.5134	19.0315
C6	22.8843	5.7442	21.5352
C7	22.1320	4.6132	21.8878
C8	22.0491	4.2010	23.2172
C9	22.7103	4.8928	24.2480
C10	23.4690	6.0218	23.8850
C11	23.5446	6.4409	22.5611
C12	20.3214	6.1544	19.1916
C13	19.1478	5.5875	18.7014
C14	19.1582	4.3601	18.0102
C15	20.4040	3.7242	17.8473
C16	21.5758	4.2796	18.3528
C17	24.6444	5.0587	17.8014
C18	25.7443	4.3477	17.3258
C19	26.7127	3.8249	18.1946
C20	26.5007	4.0050	19.5681
C21	25.3807	4.6858	20.0559
C22	17.8997	3.8064	17.5026
C23	22.5757	4.4278	25.6330
C24	27.9105	3.0413	17.6818
C25	17.7263	2.6587	16.8236
C26	23.0666	5.0147	26.7385
H27	21.6013	4.0487	21.1219
H28	21.4518	3.3212	23.4651
H29	24.0039	6.5885	24.6471
H30	24.1178	7.3338	22.3126
H31	20.2733	7.1076	19.7182
H32	18.1993	6.1055	18.8534
H33	20.4620	2.7654	17.3315
H34	22.5127	3.7393	18.2263
H35	23.9432	5.4777	17.0801
H36	25.8491	4.2252	16.2478
H37	27.2287	3.6098	20.2803
H38	25.2565	4.7973	21.1331
H39	17.0151	4.4126	17.7179
H40	21.9997	3.5059	25.7535
H41	18.5532	1.9945	16.5694
H42	16.7337	2.3463	16.5011
H43	23.6389	5.9427	26.7066
H44	22.9039	4.5744	27.7215

Rh45	23.6828	8.6241	19.5717
P46	21.7131	10.0694	19.3987
C47	20.4717	9.9053	20.7573
C48	20.6669	10.0119	17.8765
C49	22.1450	11.8689	19.5906
C50	21.9304	12.8727	18.6400
C51	22.5024	14.1407	18.7982
C52	23.2916	14.4532	19.9064
C53	23.3943	13.4828	20.9176
C54	22.8380	12.2204	20.7628
C55	19.4143	9.3790	17.8364
C56	18.7217	9.2408	16.6309
C57	19.2274	9.7466	15.4252
C58	20.4593	10.4145	15.4770
C59	21.1754	10.5138	16.6677
C60	20.6522	8.9550	21.7678
C61	19.7450	8.8611	22.8238
C62	18.6264	9.7086	22.9053
C63	18.4599	10.6729	21.8887
C64	19.3651	10.7733	20.8416
C65	18.5068	9.4908	14.1218
C66	24.0778	15.7396	20.0169
C67	17.7061	9.5716	24.0391
C68	19.0891	8.2856	13.3379
C69	16.5586	10.2422	24.2427
C70	25.6141	15.5076	20.0665
H71	21.3404	12.6763	17.7476
H72	22.3606	14.8859	18.0119
H73	23.9534	13.7029	21.8291
H74	22.9582	11.4919	21.5622
H75	18.9708	8.9863	18.7502
H76	17.7596	8.7241	16.6308
H77	20.8884	10.8400	14.5692
H78	22.1546	10.9843	16.6518
H79	21.5215	8.2966	21.7316
H80	19.9086	8.1166	23.6051
H81	17.6211	11.3675	21.9300
H82	19.2243	11.5448	20.0831
H83	18.5317	10.3893	13.4844
H84	23.7748	16.2594	20.9399
H85	18.0123	8.8330	24.7852
H86	18.2823	7.8302	12.7438
H87	19.3862	7.5227	14.0711
H88	16.1822	10.9876	23.5410
H89	15.9571	10.0598	25.1325
H90	25.7952	14.4758	20.4000
H91	26.0486	16.1546	20.8438
P92	24.7752	9.0379	17.4923
C93	25.2637	10.8178	17.2857
C94	23.9128	8.5963	15.9142
C95	26.4042	8.1530	17.3388
C96	26.8922	7.6322	16.1317
C97	28.0364	6.8298	16.1039
C98	28.7303	6.5101	17.2780
C99	28.2872	7.1039	18.4674
C100	27.1531	7.9067	18.5002
C101	22.8255	7.7179	16.0210
C102	22.0836	7.3363	14.9050
C103	22.3627	7.8670	13.6385
C104	23.4706	8.7242	13.5234
C105	24.2445	9.0715	14.6316
C106	24.6378	11.7077	16.3994
C107	24.8812	13.0790	16.4670
C108	25.7654	13.6267	17.4037
C109	26.4482	12.7297	18.2383
C110	26.1914	11.3587	18.1915
C111	21.4595	7.6192	12.4553
C112	29.8817	5.5318	17.3362
C113	25.9230	15.1320	17.4651
C114	20.2739	8.6149	12.3999
C115	26.4057	15.7772	18.7743
H116	26.3501	7.8010	15.2028
H117	28.3628	6.4161	15.1480
H118	28.8151	6.8920	19.3992
H119	26.8119	8.2955	19.4581
H120	22.5322	7.3648	17.0112
H121	21.2504	6.6448	15.0363
H122	23.7327	9.1296	12.5429
H123	25.1027	9.7297	14.4937
H124	23.9305	11.3416	15.6580
H125	24.3383	13.7439	15.7910
H126	27.1710	13.0998	18.9663
H127	26.7078	10.7066	18.8958
H128	21.0738	6.5882	12.4728
H129	24.9557	15.5767	17.1809
H130	19.9060	8.6617	11.3634
H131	20.6673	9.6183	12.6229
H132	26.4291	16.8654	18.5980

H133	27.4544	15.4924	18.9598
H134	17.4472	9.2941	14.3406
H135	23.8141	16.4155	19.1892
H136	22.0465	7.7210	11.5301
H137	26.6239	15.4457	16.6719
C138	28.5223	3.5018	16.3366
H139	27.5873	1.9922	17.5729
H140	28.6841	3.0219	18.4650
H141	27.7745	4.0771	15.7754
H142	28.7297	2.6147	15.7195
C143	29.8292	4.3132	16.3976
H144	29.9565	5.1804	18.3768
H145	30.8276	6.0658	17.1416
H146	30.6529	3.6435	16.6951
H147	30.0708	4.6286	15.3695
H148	24.9731	7.7493	19.8141
C1	18.0481	5.1615	23.1079
O2	18.4050	5.4697	24.1496

$HRh(CO)(P\text{-}frame)_3$-2(b)(TS)

ATOM	X	Y	Z
C1	19.4874	6.0641	16.6229
O2	18.5497	6.1982	17.2618
C1	24.2697	9.0459	20.9441
O2	24.8439	9.1922	21.9567
P3	22.3470	5.1299	20.1792
C4	23.9101	4.4215	19.5193
C5	21.0721	3.8544	19.8161
C6	22.5313	4.9983	22.0072
C7	21.9827	3.9738	22.7943
C8	22.0917	4.0158	24.1842
C9	22.7497	5.0707	24.8429
C10	23.3146	6.0850	24.0439
C11	23.1967	6.0533	22.6607
C12	19.7375	4.1995	20.0956
C13	18.6988	3.3137	19.8299
C14	18.9395	2.0568	19.2416
C15	20.2759	1.7230	18.9504
C16	21.3202	2.5986	19.2343
C17	24.0711	4.3804	18.1251
C18	25.2887	4.0131	17.5517
C19	26.4074	3.7206	18.3438
C20	26.2327	3.7383	19.7364
C21	25.0101	4.0727	20.3183
C22	17.8051	1.1730	18.9568
C23	22.8022	5.0843	26.3085
C24	27.7907	3.4555	17.7718
C25	17.8248	0.0017	18.2971
C26	23.3025	6.0531	27.0946
H27	21.4637	3.1411	22.3194
H28	21.6524	3.2118	24.7783
H29	23.8362	6.9225	24.5067
H30	23.6205	6.8651	22.0713
H31	19.5104	5.1772	20.5260
H32	17.6732	3.6021	20.0668
H33	20.5084	0.7552	18.5051
H34	22.3447	2.3058	19.0039
H35	23.2418	4.6589	17.4721
H36	25.3676	3.9987	16.4655
H37	27.0823	3.5064	20.3828
H38	24.9182	4.0925	21.4043
H39	16.8414	1.5378	19.3237
H40	22.3644	4.2054	26.7902
H41	18.7396	-0.4244	17.8834
H42	16.9092	-0.5683	18.1442
H43	23.7417	6.9665	26.6922
H44	23.2806	5.9572	28.1796
Rh45	23.7413	8.9578	19.1611
P46	21.9057	10.5471	19.2367
C47	20.7015	10.0950	20.5555
C48	20.8013	10.7002	17.7629
C49	22.4348	12.2535	19.6996
C50	22.1082	13.4385	19.0278
C51	22.7887	14.6287	19.3149
C52	23.7932	14.6788	20.2869
C53	24.0149	13.5180	21.0469
C54	23.3649	12.3291	20.7518
C55	19.6342	9.9216	17.6809
C56	18.8648	9.9076	16.5174
C57	19.2136	10.6730	15.3959
C58	20.3652	11.4670	15.4903
C59	21.1546	11.4657	16.6402
C60	20.6896	8.7825	21.0450
C61	19.7771	8.4027	22.0294
C62	18.8528	9.3186	22.5614
C63	18.8749	10.6378	22.0611
C64	19.7791	11.0189	21.0772
C65	18.4058	10.5778	14.1225
C66	24.6706	15.8903	20.5151

C67	17.9271	8.8743	23.6094
C68	18.9236	9.4758	13.1664
C69	17.0097	9.6131	24.2565
C70	26.1828	15.5898	20.3549
H71	21.3446	13.4405	18.2518
H72	22.5536	15.5272	18.7396
H73	24.7502	13.5277	21.8530
H74	23.6079	11.4380	21.3265
H75	19.3193	9.3195	18.5328
H76	17.9677	9.2852	16.4825
H77	20.6587	12.0970	14.6490
H78	22.0577	12.0704	16.6612
H79	21.4088	8.0558	20.6595
H80	19.7936	7.3780	22.4065
H81	18.1718	11.3763	22.4463
H82	19.7763	12.0473	20.7136
H83	18.3980	11.5473	13.5996
H84	24.4994	16.2538	21.5416
H85	18.0212	7.8188	23.8801
H86	18.1009	9.1611	12.5059
H87	19.1732	8.5946	13.7758
H88	16.8550	10.6736	24.0533
H89	16.3784	9.1680	25.0250
H90	26.3604	14.5467	20.6523
H91	26.7474	16.2030	21.0738
P92	24.7855	9.2958	17.1120
C93	25.3346	11.0639	17.1039
C94	23.8769	9.0575	15.5269
C95	26.3528	8.3321	16.8701
C96	26.8050	7.8940	15.6157
C97	27.9314	7.0743	15.5085
C98	28.6467	6.6597	16.6421
C99	28.2196	7.1452	17.8844
C100	27.0950	7.9612	17.9990
C101	22.7462	8.2283	15.5696
C102	21.9282	8.0637	14.4513
C103	22.1837	8.7640	13.2643
C104	23.3415	9.5559	13.2081
C105	24.1872	9.6886	14.3093
C106	24.6643	12.0597	16.3759
C107	24.9326	13.4077	16.5923
C108	25.8814	13.8337	17.5332
C109	26.5905	12.8374	18.2175
C110	26.3199	11.4816	18.0143
C111	21.2046	8.7804	12.1157
C112	29.7697	5.6506	16.5562
C113	26.0817	15.3235	17.7223
C114	20.1321	9.8842	12.2986
C115	26.8045	15.8474	18.9697
H116	26.2527	8.1492	14.7118
H117	28.2354	6.7255	14.5192
H118	28.7517	6.8464	18.7902
H119	26.7521	8.2621	18.9887
H120	22.4934	7.7209	16.5033
H121	21.0634	7.4036	14.5261
H122	23.5761	10.0929	12.2860
H123	25.0773	10.3130	14.2238
H124	23.9103	11.7803	15.6435
H125	24.3722	14.1555	16.0264
H126	27.3538	13.1147	18.9457
H127	26.8681	10.7428	18.5986
H128	20.7140	7.8012	12.0061
H129	25.0906	15.8001	17.6549
H130	19.7723	10.2029	11.3083
H131	20.6304	10.7615	12.7361
H132	26.9007	16.9374	18.8353
H133	27.8389	15.4673	18.9852
H134	17.3605	10.3554	14.3829
H135	24.3651	16.7111	19.8479
H136	21.7548	8.9645	11.1813
H137	26.6356	15.7026	16.8452
C138	27.9851	3.7734	16.2806
H139	28.0652	2.4044	17.9651
H140	28.4975	4.0491	18.3717
H141	27.2553	4.5333	15.9726
H142	27.7657	2.8803	15.6757
C143	29.3757	4.3014	15.8992
H144	30.1485	5.4721	17.5737
H145	30.6177	6.0740	15.9935
H146	30.1538	3.5602	16.1451
H147	29.4030	4.4136	14.8041
H148	24.7197	7.7063	19.1810

$HRh(CO)(P\text{-}frame)_3$-2(b)(FS)

ATOM	X	Y	Z
C1	21.8139	7.7352	18.0484
O2	20.9698	7.0562	17.6170
C1	24.0822	9.0080	20.4261
O2	24.6629	8.9945	21.4414

P3	22.1127	4.4137	20.0617
C4	23.7413	3.6933	19.5912
C5	20.9315	3.0131	19.9398
C6	22.2428	4.7326	21.8666
C7	21.5684	4.0082	22.8605
C8	21.6177	4.4182	24.1934
C9	22.3515	5.5501	24.5914
C10	23.0227	6.2760	23.5871
C11	22.9582	5.8842	22.2564
C12	19.6112	3.3495	19.5992
C13	18.6368	2.3659	19.4573
C14	18.9444	1.0040	19.6321
C15	20.2734	0.6714	19.9666
C16	21.2462	1.6531	20.1213
C17	23.8683	3.1684	18.2903
C18	25.1187	2.8837	17.7473
C19	26.2993	3.1396	18.4651
C20	26.1662	3.6052	19.7785
C21	24.9137	3.8688	20.3415
C22	17.8841	0.0085	19.4505
C23	22.3749	5.9290	26.0082
C24	27.6615	3.0008	17.8191
C25	17.9991	-1.3312	19.4734
C26	23.1009	6.9092	26.5753
H27	20.9903	3.1230	22.5931
H28	21.0779	3.8444	24.9494
H29	23.5817	7.1779	23.8377
H30	23.4451	6.4968	21.4973
H31	19.3570	4.3966	19.4264
H32	17.6181	2.6508	19.1888
H33	20.5460	-0.3728	20.1209
H34	22.2667	1.3678	20.3799
H35	22.9752	3.0120	17.6823
H36	25.1737	2.4989	16.7273
H37	27.0648	3.7881	20.3722
H38	24.8605	4.2507	21.3613
H39	16.8926	0.4339	19.2693
H40	21.7335	5.3216	26.6529
H41	18.9495	-1.8403	19.6361
H42	17.1241	-1.9626	19.3232
H43	23.7776	7.5402	25.9976
H44	23.0438	7.0986	27.6464
Rh45	23.2136	8.8374	18.7310
P46	21.6474	10.6816	18.9631
C47	20.3548	10.3233	20.2296
C48	20.6881	10.9863	17.4224
C49	22.3241	12.3107	19.5008
C50	22.1131	13.5424	18.8659
C51	22.8455	14.6736	19.2449
C52	23.7887	14.6199	20.2767
C53	23.9004	13.4139	20.9874
C54	23.1946	12.2819	20.6039
C55	19.4473	10.3709	17.2007
C56	18.8653	10.3902	15.9292
C57	19.4820	11.0328	14.8461
C58	20.6862	11.7072	15.0950
C59	21.2893	11.6631	16.3496
C60	20.2691	9.0500	20.8091
C61	19.2931	8.7709	21.7645
C62	18.3739	9.7471	22.1865
C63	18.4724	11.0294	21.6042
C64	19.4407	11.3110	20.6473
C65	18.9218	10.8989	13.4481
C66	24.6825	15.7897	20.6329
C67	17.3807	9.3879	23.2033
C68	19.6738	9.8159	12.6247
C69	16.4660	10.1887	23.7775
C70	26.1938	15.4387	20.6576
H71	21.4019	13.6222	18.0448
H72	22.6951	15.6078	18.6995
H73	24.5828	13.3439	21.8357
H74	23.3479	11.3558	21.1547
H75	18.9426	9.8512	18.0149
H76	17.9179	9.8705	15.7741
H77	21.1853	12.2438	14.2872
H78	22.2476	12.1533	16.4933
H79	20.9837	8.2810	20.5154
H80	19.2521	7.7721	22.2028
H81	17.7792	11.8153	21.9039
H82	19.4919	12.3142	20.2218
H83	18.9657	11.8639	12.9182
H84	24.3941	16.1455	21.6351
H85	17.4152	8.3411	23.5185
H86	18.9642	9.3138	11.9485
H87	20.0224	9.0472	13.3290
H88	16.3705	11.2466	23.5297
H89	15.7744	9.7997	24.5243
H90	26.2986	14.3619	20.8531

H91	26.6645	15.9443	21.5137
P92	24.8247	9.5067	17.0500
C93	25.4893	11.2260	17.1785
C94	24.2125	9.3620	15.3080
C95	26.3485	8.4498	17.0343
C96	27.0939	8.2385	15.8614
C97	28.1552	7.3335	15.8410
C98	28.5110	6.6011	16.9850
C99	27.8031	6.8605	18.1641
C100	26.7366	7.7606	18.1910
C101	23.2396	8.3836	15.0609
C102	22.5974	8.2927	13.8279
C103	22.8710	9.2087	12.8036
C104	23.9167	10.1211	13.0149
C105	24.5926	10.1872	14.2350
C106	24.8625	12.3010	16.5287
C107	25.2069	13.6165	16.8194
C108	26.1910	13.9277	17.7676
C109	26.8502	12.8552	18.3850
C110	26.5068	11.5294	18.1000
C111	21.9990	9.3148	11.5757
C112	29.5573	5.5113	16.9336
C113	26.4871	15.3886	18.0371
C114	20.8585	10.3425	11.7936
C115	27.0197	15.8098	19.4148
H116	26.8266	8.7607	14.9428
H117	28.6968	7.1717	14.9068
H118	28.0545	6.3129	19.0745
H119	26.1764	7.8957	19.1141
H120	22.9530	7.7040	15.8598
H121	21.8346	7.5253	13.6840
H122	24.1951	10.8128	12.2165
H123	25.3957	10.9140	14.3558
H124	24.0864	12.1119	15.7917
H125	24.6848	14.4289	16.3098
H126	27.6406	13.0471	19.1126
H127	27.0249	10.7216	18.6184
H128	21.5740	8.3334	11.3134
H129	25.5674	15.9548	17.8221
H130	20.4890	10.6869	10.8148
H131	21.3003	11.2251	12.2791
H132	27.1392	16.9052	19.3822
H133	28.0376	15.4107	19.5558
H134	17.8584	10.6286	13.5172
H135	24.4889	16.6315	19.9502
H136	22.6105	9.6367	10.7193
H137	27.2171	15.7377	17.2864
C138	27.7533	3.7093	16.4462
H139	27.9220	1.9356	17.6984
H140	28.4104	3.4133	18.5115
H141	27.0172	4.5260	16.4218
H142	27.4495	3.0073	15.6553
C143	29.1292	4.2875	16.0896
H144	29.7945	5.1972	17.9609
H145	30.4946	5.9092	16.5135
H146	29.9092	3.5123	16.1686
H147	29.1068	4.5898	15.0305
H148	24.0151	7.4633	18.6612

R1m (IS) Crosslinking mode 1

ATOM		X	Y	Z
P	1	22.1906	7.4580	19.2595
C	2	23.4197	6.3386	20.0709
C	3	20.8331	7.4615	20.5177
C	4	23.0197	9.1029	19.3401
C	5	22.9351	10.0641	20.3588
C	6	23.5078	11.3299	20.1887
C	7	24.2091	11.6666	19.0233
C	8	24.3735	10.6654	18.0562
C	9	23.7731	9.4214	18.1982
C	10	20.4642	6.2461	21.1223
C	11	19.3784	6.1774	21.9899
C	12	18.6139	7.3110	22.3063
C	13	18.9913	8.5227	21.7152
C	14	20.0720	8.5969	20.8310
C	15	23.3195	4.9493	19.8664
C	16	24.2107	4.0675	20.4659
C	17	25.2560	4.5376	21.2867
C	18	25.3632	5.9293	21.4652
C	19	24.4616	6.8156	20.8777
C	20	17.4169	7.1779	23.2183
C	21	24.7837	13.0494	18.7835
C	22	26.2327	3.6574	21.9349
C	23	16.1508	6.6838	22.4778
C	24	26.2448	2.3134	21.9415
C	25	24.4926	13.6391	17.3824
H	26	22.3929	9.8466	21.2788
H	27	23.3909	12.0774	20.9770
H	28	24.9442	10.8708	17.1512

H	29	23.8568	8.6874	17.3943
H	30	21.0359	5.3403	20.9284
H	31	19.1240	5.2165	22.4430
H	32	18.4336	9.4332	21.9434
H	33	20.3238	9.5564	20.3865
H	34	22.5518	4.5664	19.1917
H	35	24.1051	2.9991	20.2765
H	36	26.1721	6.3241	22.0831
H	37	24.5826	7.8876	21.0357
H	38	17.2066	8.1348	23.7207
H	39	25.8780	12.9830	18.9009
H	40	15.4890	6.1765	23.1968
H	41	16.4651	5.9115	21.7611
H	42	27.0366	1.7693	22.4551
H	43	25.4831	1.7144	21.4413
H	44	24.4861	12.8215	16.6489
H	45	25.3385	14.2806	17.0925
P	46	19.7161	8.3343	16.7070
C	47	20.1772	10.1092	16.9420
C	48	18.1560	8.1018	17.6510
C	49	19.1887	8.3339	14.9328
C	50	20.1033	7.9180	13.9482
C	51	19.7627	7.9318	12.5994
C	52	18.4885	8.3524	12.1754
C	53	17.5766	8.7597	13.1680
C	54	17.9175	8.7539	14.5183
C	55	17.9760	6.8442	18.2441
C	56	16.8614	6.5778	19.0385
C	57	15.9115	7.5735	19.3032
C	58	16.0720	8.8175	18.6719
C	59	17.1667	9.0796	17.8487
C	60	19.8400	10.8297	18.0986
C	61	20.3998	12.0793	18.3460
C	62	21.3134	12.6716	17.4621
C	63	21.5971	11.9831	16.2762
C	64	21.0466	10.7220	16.0243
C	65	14.8351	7.3943	20.3458
C	66	18.0673	8.3769	10.7716
C	67	21.9087	14.0073	17.8578
C	68	15.3527	7.7882	21.7526
C	69	23.2169	14.4905	17.2178
C	70	18.8047	8.0724	9.6870
H	71	21.0890	7.5625	14.2548
H	72	20.4961	7.5938	11.8676
H	73	16.5786	9.0853	12.8691
H	74	17.1764	9.0689	15.2512
H	75	18.7442	6.0806	18.1064
H	76	16.7542	5.5902	19.4886
H	77	15.3339	9.6042	18.8449
H	78	17.2614	10.0621	17.3856
H	79	19.1451	10.4075	18.8214
H	80	20.1428	12.6030	19.2698
H	81	22.2813	12.4122	15.5425
H	82	21.3094	10.2055	15.1001
H	83	14.4697	6.3561	20.3599
H	84	17.0292	8.6823	10.6134
H	85	22.0329	13.9946	18.9525
H	86	14.4979	8.0842	22.3801
H	87	15.9724	8.6905	21.6380
H	88	23.4110	15.4892	17.6427
H	89	23.0624	14.6611	16.1397
H	90	19.8470	7.7572	9.7503
H	91	18.3745	8.1306	8.6877
H	92	17.6652	6.4573	24.0126
H	93	24.4421	13.7404	19.5698
H	94	13.9741	8.0291	20.0893
H	95	21.1500	14.7879	17.6699
H	96	27.0347	4.1792	22.4649
C	97	20.7797	5.4410	16.0324
O	98	20.3000	4.4857	15.5592
Rh	99	21.5015	6.8058	17.0887
C	100	23.8532	6.1422	15.3576
C	101	23.3791	5.8010	16.7686
H	102	23.2204	5.6802	14.5855
H	103	24.8895	5.7944	15.1885
H	104	23.3011	4.7116	16.8943
H	105	24.1082	6.1491	17.5127
H	106	23.8610	7.2276	15.1678
C	107	26.2442	9.2350	14.7637
O	108	26.4997	10.3386	14.9280

R1m (TS) Crosslinking mode 1

ATOM		X	Y	Z
P	1	22.311	7.622	19.319
C	2	23.530	6.658	20.328
C	3	20.852	7.679	20.467
C	4	23.033	9.324	19.384
C	5	22.814	10.295	20.372
C	6	23.321	11.590	20.220

C	7	24.083	11.952	19.103
C	8	24.384	10.947	18.171
C	9	23.850	9.670	18.296
C	10	20.502	6.569	21.252
C	11	19.347	6.575	22.031
C	12	18.490	7.685	22.068
C	13	18.852	8.799	21.303
C	14	20.004	8.796	20.512
C	15	23.411	5.257	20.418
C	16	24.294	4.505	21.184
C	17	25.357	5.117	21.874
C	18	25.486	6.512	21.760
C	19	24.591	7.271	21.006
C	20	17.216	7.628	22.882
C	21	24.553	13.373	18.872
C	22	26.328	4.375	22.686
C	23	16.064	6.888	22.159
C	24	26.341	3.056	22.948
C	25	24.173	13.955	17.490
H	26	22.223	10.057	21.256
H	27	23.092	12.340	20.981
H	28	25.008	11.174	17.305
H	29	24.051	8.927	17.522
H	30	21.141	5.689	21.278
H	31	19.112	5.693	22.631
H	32	18.223	9.692	21.320
H	33	20.244	9.680	19.928
H	34	22.617	4.751	19.868
H	35	24.166	3.423	21.227
H	36	26.310	7.012	22.273
H	37	24.726	8.350	20.947
H	38	16.891	8.643	23.158
H	39	25.652	13.392	18.957
H	40	15.378	6.477	22.915
H	41	16.498	6.019	21.644
H	42	27.122	2.623	23.570
H	43	25.586	2.369	22.564
H	44	24.261	13.156	16.742
H	45	24.929	14.702	17.205
P	46	20.000	8.200	16.506
C	47	20.246	10.010	16.778
C	48	18.386	7.818	17.311
C	49	19.597	8.184	14.694
C	50	19.927	7.073	13.904
C	51	19.599	7.029	12.553
C	52	18.935	8.099	11.928
C	53	18.619	9.218	12.720
C	54	18.941	9.261	14.075
C	55	18.342	6.688	18.137
C	56	17.199	6.380	18.874
C	57	16.077	7.216	18.842
C	58	16.100	8.310	17.959
C	59	17.226	8.601	17.191
C	60	19.599	10.732	17.793
C	61	20.014	12.019	18.128
C	62	21.072	12.652	17.459
C	63	21.639	11.972	16.374
C	64	21.248	10.671	16.049
C	65	14.933	7.059	19.812
C	66	18.587	8.107	10.502
C	67	21.556	13.991	17.977
C	68	15.250	7.748	21.165
C	69	22.800	14.650	17.365
C	70	18.683	7.084	9.636
H	71	20.466	6.240	14.352
H	72	19.884	6.153	11.972
H	73	18.118	10.071	12.260
H	74	18.703	10.157	14.648
H	75	19.235	6.067	18.230
H	76	17.202	5.497	19.513
H	77	15.222	8.955	17.884
H	78	17.204	9.456	16.515
H	79	18.778	10.275	18.342
H	80	19.520	12.535	18.955
H	81	22.430	12.441	15.790
H	82	21.744	10.158	15.225
H	83	14.704	5.996	19.984
H	84	18.206	9.062	10.130
H	85	21.708	13.881	19.063
H	86	14.305	8.049	21.643
H	87	15.790	8.682	20.948
H	88	22.882	15.641	17.840
H	89	22.620	14.855	16.297
H	90	19.032	6.094	9.932
H	91	18.396	7.209	8.592
H	92	17.430	7.102	23.825
H	93	24.180	14.026	19.677
H	94	14.030	7.512	19.378

H	95	20.727	14.714	17.883
H	96	27.122	4.990	23.118
C	97	21.074	5.205	16.427
O	98	20.543	4.178	16.230
Rh	99	21.815	6.747	17.173
C	100	24.059	5.071	15.839
C	101	23.664	5.670	17.186
H	102	23.434	4.204	15.582
H	103	25.109	4.727	15.851
H	104	23.675	4.886	17.954
H	105	24.404	6.423	17.506
H	106	23.965	5.789	15.011
C	107	23.608	8.383	14.582
O	108	24.705	8.674	14.729

R1m (FS) Crosslinking mode 1

R2 (IS) Crosslinking mode 1

ATOM		X	Y	Z
P	1	19.8065	9.1404	19.1522
C	2	21.0307	7.9903	19.9165
C	3	18.4645	9.1844	20.4360
C	4	20.6328	10.7886	19.3191
C	5	20.4694	11.6752	20.3949
C	6	21.0026	12.9680	20.3389
C	7	21.7445	13.4052	19.2348
C	8	22.0055	12.4707	18.2210
C	9	21.4442	11.1991	18.2502
C	10	18.1514	8.0717	21.2345
C	11	17.0347	8.0800	22.0709
C	12	16.1889	9.1963	22.1644
C	13	16.5230	10.3160	21.3935
C	14	17.6285	10.3080	20.5406
C	15	20.7931	6.6012	19.8902
C	16	21.7042	5.7040	20.4340
C	17	22.9115	6.1515	21.0055
C	18	23.1487	7.5373	21.0152
C	19	22.2306	8.4413	20.4841
C	20	14.9609	9.1485	23.0456
C	21	22.2352	14.8306	19.0967
C	22	23.9179	5.2493	21.5735
C	23	13.7403	8.4736	22.3724
C	24	23.9037	3.9054	21.5791
C	25	21.7644	15.5399	17.8047
H	26	19.8926	11.3773	21.2698
H	27	20.8171	13.6534	21.1689
H	28	22.6210	12.7527	17.3650
H	29	21.6051	10.5249	17.4106
H	30	18.7877	7.1887	21.2216
H	31	16.8258	7.1958	22.6773
H	32	15.9078	11.2165	21.4563
H	33	17.8427	11.1958	19.9509
H	34	19.8849	6.2158	19.4245
H	35	21.4784	4.6385	20.4013
H	36	24.0772	7.9137	21.4481
H	37	22.4525	9.5073	20.5112
H	38	14.6860	10.1633	23.3718
H	39	23.3376	14.8143	19.0877
H	40	13.0976	8.0482	23.1583
H	41	14.1068	7.6141	21.7922
H	42	24.7179	3.3434	22.0353
H	43	23.0963	3.3237	21.1324
H	44	21.7714	14.8023	16.9906
H	45	22.5186	16.2906	17.5233
P	46	17.3140	10.0500	16.5279
C	47	17.6324	11.8233	16.9364
C	48	15.7812	9.6185	17.4550
C	49	16.7233	10.1345	14.7824
C	50	16.7984	8.9833	13.9801
C	51	16.3107	8.9858	12.6794
C	52	15.7353	10.1435	12.1203
C	53	15.6681	11.2923	12.9288
C	54	16.1522	11.2934	14.2357
C	55	15.7775	8.4743	18.2588
C	56	14.6693	8.1471	19.0375
C	57	13.5476	8.9827	19.0810
C	58	13.5295	10.0983	18.2264
C	59	14.6176	10.4047	17.4109
C	60	17.0456	12.4746	18.0334
C	61	17.5386	13.6983	18.4829
C	62	18.6117	14.3392	17.8460
C	63	19.1046	13.7490	16.6751
C	64	18.6395	12.5080	16.2374
C	65	12.4631	8.7935	20.1132
C	66	15.2117	10.1985	10.7509
C	67	19.1886	15.5889	18.4784
C	68	12.8821	9.3988	21.4791
C	69	20.4095	16.2761	17.8496
C	70	15.3555	9.2714	9.7864
H	71	17.2600	8.0829	14.3857

H	72	16.3800	8.0717	12.0895
H	73	15.2323	12.2043	12.5173
H	74	16.0926	12.2076	14.8273
H	75	16.6662	7.8470	18.2996
H	76	14.7057	7.2483	19.6535
H	77	12.6506	10.7461	18.2096
H	78	14.5619	11.2709	16.7510
H	79	16.2198	12.0052	18.5648
H	80	17.0928	14.1560	19.3688
H	81	19.9007	14.2335	16.1121
H	82	19.0973	12.0588	15.3572
H	83	12.2222	7.7266	20.2400
H	84	14.6566	11.1105	10.5120
H	85	19.4207	15.3430	19.5276
H	86	11.9748	9.6849	22.0331
H	87	13.4233	10.3361	21.2795
H	88	20.5568	17.2103	18.4152
H	89	20.1609	16.5942	16.8237
H	90	15.9136	8.3474	9.9408
H	91	14.9165	9.4199	8.8007
H	92	15.2097	8.5865	23.9587
H	93	21.9504	15.4157	19.9855
H	94	11.5434	9.2869	19.7660
H	95	18.3861	16.3433	18.5367
H	96	24.7715	5.7544	22.0343
C	97	18.3152	6.9127	16.7214
O	98	17.8946	5.8278	16.6086
Rh	99	19.2238	8.5927	16.8017
C	100	21.2249	6.6442	15.2800
C	101	21.0118	7.3049	16.6354
H	102	20.3833	5.9922	15.0059
H	103	22.1326	6.0141	15.3017
H	104	20.9210	6.5451	17.4177
H	105	21.8681	7.9394	16.9019
H	106	21.3527	7.3731	14.4679
C	107	20.1783	9.5851	15.4956
O	108	20.8191	10.0922	14.6591

R1s (IS) Crosslinking mode 1

ATOM		X	Y	Z
P	1	22.2470	7.4245	19.3584
C	2	23.4436	6.2694	20.1607
C	3	20.9018	7.5140	20.6276
C	4	23.1062	9.0521	19.4647
C	5	22.9683	9.9899	20.4980
C	6	23.5730	11.2478	20.3988
C	7	24.3447	11.6044	19.2866
C	8	24.5431	10.6313	18.2956
C	9	23.9261	9.3870	18.3735
C	10	20.5827	6.4046	21.4271
C	11	19.4443	6.4080	22.2313
C	12	18.5838	7.5150	22.2832
C	13	18.9278	8.6355	21.5170
C	14	20.0558	8.6326	20.6954
C	15	23.2771	4.8797	20.0115
C	16	24.1701	3.9811	20.5821
C	17	25.2815	4.4298	21.3227
C	18	25.4436	5.8203	21.4640
C	19	24.5436	6.7239	20.9028
C	20	17.3114	7.4413	23.0934
C	21	24.9595	12.9820	19.1410
C	22	26.2631	3.5284	21.9330
C	23	16.1602	6.7342	22.3385
C	24	26.2524	2.1843	21.9316
C	25	24.6479	13.7000	17.8079
H	26	22.3679	9.7552	21.3766
H	27	23.4275	11.9714	21.2042
H	28	25.1662	10.8552	17.4284
H	29	24.0602	8.6590	17.5682
H	30	21.2297	5.5282	21.4305
H	31	19.2226	5.5267	22.8373
H	32	18.2959	9.5254	21.5506
H	33	20.2743	9.5130	20.0942
H	34	22.4477	4.4926	19.4202
H	35	24.0098	2.9132	20.4326
H	36	26.2984	6.2001	22.0273
H	37	24.7065	7.7937	21.0333
H	38	16.9898	8.4485	23.3994
H	39	26.0537	12.8715	19.2169
H	40	15.4544	6.3264	23.0780
H	41	16.5852	5.8630	21.8178
H	42	27.0486	1.6224	22.4186
H	43	25.4639	1.6028	21.4526
H	44	24.6213	12.9467	17.0087
H	45	25.4955	14.3570	17.5607
P	46	20.1063	8.4826	16.5333
C	47	20.4074	10.2733	16.8605
C	48	18.5917	8.0370	17.4801
C	49	19.4272	8.4459	14.8178

C	50	19.2060	7.1804	14.2448
C	51	18.6533	7.0548	12.9783
C	52	18.3093	8.1918	12.2194
C	53	18.5348	9.4520	12.7998
C	54	19.0809	9.5825	14.0776
C	55	18.5796	6.8448	18.2152
C	56	17.4572	6.4767	18.9581
C	57	16.3248	7.2988	19.0102
C	58	16.3242	8.4652	18.2271
C	59	17.4301	8.8245	17.4607
C	60	19.8640	10.9445	17.9676
C	61	20.3898	12.1620	18.3941
C	62	21.4541	12.7798	17.7215
C	63	21.9127	12.1670	16.5480
C	64	21.4201	10.9268	16.1369
C	65	15.1656	7.0148	19.9342
C	66	17.7457	8.1167	10.8677
C	67	22.0621	14.0307	18.3197
C	68	15.3785	7.6250	21.3433
C	69	23.3814	14.5779	17.7565
C	70	17.4218	7.0073	10.1793
H	71	19.4775	6.2857	14.8076
H	72	18.5012	6.0581	12.5648
H	73	18.2826	10.3506	12.2328
H	74	19.2378	10.5768	14.4962
H	75	19.4705	6.2132	18.2032
H	76	17.4776	5.5427	19.5223
H	77	15.4384	9.1042	18.2194
H	78	17.3856	9.7243	16.8452
H	79	19.0460	10.4927	18.5262
H	80	19.9778	12.6322	19.2899
H	81	22.7086	12.6310	15.9660
H	82	21.8693	10.4425	15.2685
H	83	14.9964	5.9305	20.0233
H	84	17.5814	9.0851	10.3868
H	85	22.1869	13.8465	19.3998
H	86	14.3953	7.8627	21.7771
H	87	15.8920	8.5902	21.2180
H	88	23.5890	15.5062	18.3126
H	89	23.2317	14.8945	16.7110
H	90	17.5486	6.0045	10.5889
H	91	17.0102	7.0735	9.1727
H	92	17.5165	6.8844	24.0200
H	93	24.6649	13.6131	19.9943
H	94	14.2522	7.4411	19.4945
H	95	21.3168	14.8420	18.2581
H	96	27.0912	4.0336	22.4381
C	97	22.6676	5.3607	16.8999
O	98	22.9071	4.2211	16.7872
Rh	99	21.9705	7.0905	16.9818
C	100	22.6775	6.1350	13.9701
C	101	22.5662	7.3095	14.9342
H	102	23.3893	5.3748	14.3193
H	103	23.0174	6.4731	12.9755
H	104	23.5706	7.7299	15.1350
H	105	21.9603	8.0958	14.4640
H	106	21.7105	5.6333	13.8206
H	107	17.8762	4.2597	15.8687
H	108	18.4768	3.8091	15.8227

R1s (TS) Crosslinking mode 1

ATOM		X	Y	Z
P	1	21.986	7.054	19.238
C	2	23.129	5.811	19.998
C	3	20.578	7.107	20.436
C	4	22.987	8.586	19.494
C	5	23.258	9.241	20.708
C	6	23.975	10.442	20.713
C	7	24.491	10.996	19.529
C	8	24.329	10.258	18.352
C	9	23.562	9.101	18.328
C	10	19.784	5.948	20.536
C	11	18.642	5.931	21.327
C	12	18.219	7.070	22.034
C	13	19.019	8.213	21.951
C	14	20.182	8.232	21.170
C	15	24.274	5.457	19.261
C	16	25.202	4.560	19.770
C	17	25.026	3.971	21.037
C	18	23.883	4.334	21.768
C	19	22.950	5.241	21.263
C	20	16.917	7.028	22.801
C	21	25.203	12.335	19.503
C	22	25.972	3.007	21.613
C	23	15.681	6.958	21.874
C	24	27.086	2.517	21.044
C	25	24.901	13.216	18.272
H	26	22.901	8.832	21.654
H	27	24.127	10.967	21.659

H	28	24.753	10.614	17.414
H	29	23.383	8.596	17.384
H	30	20.052	5.059	19.964
H	31	18.052	5.014	21.385
H	32	18.732	9.114	22.498
H	33	20.766	9.149	21.120
H	34	24.436	5.891	18.274
H	35	26.079	4.314	19.172
H	36	23.721	3.894	22.754
H	37	22.076	5.495	21.861
H	38	16.838	7.901	23.468
H	39	26.290	12.145	19.520
H	40	14.837	6.512	22.422
H	41	15.916	6.257	21.060
H	42	27.712	1.800	21.575
H	43	27.412	2.804	20.044
H	44	24.882	12.581	17.375
H	45	25.753	13.897	18.120
P	46	19.842	8.313	16.506
C	47	20.488	9.953	17.062
C	48	18.163	8.281	17.303
C	49	19.397	8.607	14.732
C	50	19.448	7.558	13.802
C	51	19.041	7.739	12.485
C	52	18.567	8.983	12.034
C	53	18.501	10.029	12.973
C	54	18.908	9.848	14.293
C	55	17.614	7.066	17.725
C	56	16.427	7.030	18.458
C	57	15.766	8.209	18.825
C	58	16.266	9.417	18.315
C	59	17.430	9.455	17.551
C	60	20.276	10.326	18.400
C	61	20.869	11.465	18.928
C	62	21.697	12.291	18.155
C	63	21.877	11.943	16.809
C	64	21.297	10.785	16.272
C	65	14.659	8.224	19.849
C	66	18.142	9.228	10.651
C	67	22.319	13.497	18.830
C	68	15.241	8.312	21.285
C	69	23.634	14.093	18.306
C	70	18.265	8.396	9.603
H	71	19.806	6.581	14.126
H	72	19.093	6.894	11.799
H	73	18.133	11.007	12.656
H	74	18.844	10.689	14.983
H	75	18.162	6.144	17.528
H	76	16.038	6.064	18.785
H	77	15.746	10.351	18.541
H	78	17.795	10.419	17.198
H	79	19.649	9.709	19.040
H	80	20.704	11.711	19.979
H	81	22.504	12.562	16.165
H	82	21.487	10.534	15.229
H	83	14.024	7.329	19.757
H	84	17.686	10.208	10.480
H	85	22.447	13.243	19.894
H	86	14.495	8.770	21.954
H	87	16.096	9.005	21.257
H	88	23.839	14.972	18.939
H	89	23.481	14.502	17.294
H	90	18.724	7.410	9.685
H	91	17.916	8.691	8.614
H	92	16.919	6.139	23.451
H	93	24.988	12.888	20.431
H	94	14.011	9.095	19.669
H	95	21.572	14.310	18.823
H	96	25.711	2.664	22.618
C	97	22.069	4.753	16.970
O	98	22.530	3.688	16.949
Rh	99	21.235	6.432	16.970
C	100	22.976	6.524	14.260
C	101	22.859	7.214	15.620
H	102	23.130	5.439	14.361
H	103	23.824	6.921	13.672
H	104	23.812	7.089	16.158
H	105	22.726	8.297	15.467
H	106	22.073	6.665	13.650
H	107	19.988	5.726	17.747
H	108	20.566	5.873	15.653

R1s (FS) Crosslinking mode 1

ATOM		X	Y	Z
P	1	22.0869	7.3123	19.3843
C	2	23.4034	6.2640	20.1454
C	3	20.7526	7.3620	20.6613
C	4	22.9790	8.9268	19.4310
C	5	23.2114	9.7515	20.5454

C	6	23.8930	10.9638	20.3944
C	7	24.4198	11.3627	19.1539
C	8	24.2925	10.4665	18.0885
C	9	23.5564	9.2949	18.2107
C	10	20.1317	6.1382	20.9815
C	11	18.9927	6.1023	21.7762
C	12	18.4053	7.2792	22.2751
C	13	19.0438	8.4894	21.9875
C	14	20.1995	8.5331	21.1946
C	15	24.4271	5.8145	19.2932
C	16	25.5269	5.1314	19.7913
C	17	25.6507	4.8609	21.1676
C	18	24.6146	5.2997	22.0118
C	19	23.5106	5.9960	21.5163
C	20	17.1022	7.1919	23.0378
C	21	25.1111	12.7002	18.9581
C	22	26.8046	4.1599	21.7394
C	23	15.8857	6.9348	22.1124
C	24	27.8849	3.7022	21.0833
C	25	24.8983	13.3553	17.5775
H	26	22.8513	9.4654	21.5338
H	27	24.0116	11.6175	21.2618
H	28	24.7232	10.7000	17.1162
H	29	23.4029	8.6676	17.3369
H	30	20.5294	5.2081	20.5765
H	31	18.5299	5.1385	21.9989
H	32	18.6304	9.4223	22.3756
H	33	20.6553	9.4986	20.9819
H	34	24.3608	6.0116	18.2229
H	35	26.2972	4.8006	19.0956
H	36	24.6833	5.1004	23.0831
H	37	22.7346	6.3311	22.2052
H	38	16.9375	8.1079	23.6250
H	39	26.1953	12.5471	19.0958
H	40	15.1054	6.3980	22.6743
H	41	16.2111	6.2500	21.3158
H	42	28.6927	3.1980	21.6121
H	43	28.0060	3.8140	20.0047
H	44	24.9589	12.5820	16.8009
H	45	25.7514	14.0215	17.3777
P	46	19.7849	8.1981	16.6274
C	47	20.4240	9.9054	16.9264
C	48	18.1436	8.1715	17.4919
C	49	19.2518	8.2817	14.8579
C	50	19.2785	7.1451	14.0375
C	51	18.8022	7.1890	12.7310
C	52	18.2768	8.3759	12.1883
C	53	18.2492	9.5120	13.0180
C	54	18.7155	9.4676	14.3281
C	55	17.6367	6.9418	17.9310
C	56	16.4616	6.8753	18.6776
C	57	15.7686	8.0355	19.0447
C	58	16.2278	9.2553	18.5246
C	59	17.3822	9.3241	17.7453
C	60	20.2685	10.4969	18.1891
C	61	20.8755	11.7125	18.4873
C	62	21.6688	12.3955	17.5533
C	63	21.8052	11.8174	16.2841
C	64	21.2023	10.5916	15.9769
C	65	14.6748	8.0140	20.0823
C	66	17.7627	8.4804	10.8182
C	67	22.2892	13.7118	17.9776
C	68	15.2735	8.2074	21.4992
C	69	23.6182	14.1936	17.3706
C	70	17.6094	7.4865	9.9254
H	71	19.6879	6.2167	14.4341
H	72	18.8572	6.2872	12.1212
H	73	17.8449	10.4466	12.6256
H	74	18.6636	10.3686	14.9386
H	75	18.2005	6.0319	17.7300
H	76	16.1059	5.9002	19.0149
H	77	15.6822	10.1741	18.7511
H	78	17.7111	10.2956	17.3772
H	79	19.6764	9.9971	18.9533
H	80	20.7516	12.1366	19.4857
H	81	22.4064	12.3116	15.5191
H	82	21.3479	10.1663	14.9840
H	83	14.1125	7.0679	20.0376
H	84	17.4672	9.4897	10.5184
H	85	22.3920	13.6856	19.0733
H	86	14.4955	8.5919	22.1773
H	87	16.0408	8.9940	21.4325
H	88	23.7913	15.1942	17.7993
H	89	23.4954	14.3625	16.2884
H	90	17.8662	6.4511	10.1507
H	91	17.2102	7.6870	8.9317
H	92	17.1755	6.3666	23.7626
H	93	24.8100	13.3922	19.7606

H	94	13.9567	8.8223	19.8785
H	95	21.5489	14.5077	17.7807
H	96	26.7591	4.0136	22.8223
C	97	22.0657	4.7367	17.3846
O	98	22.4981	3.6590	17.3890
Rh	99	21.2295	6.4117	17.2634
C	100	22.8656	6.1043	14.5042
C	101	22.7602	7.0228	15.7186
H	102	23.1510	5.0804	14.7889
H	103	23.6234	6.4618	13.7827
H	104	23.7396	7.0569	16.2215
H	105	22.5374	8.0513	15.3939
H	106	21.9160	6.0298	13.9551
H	107	20.0500	5.8602	18.2222
H	108	20.4346	5.6753	16.1057

R2 (TS) Crosslinking mode 1

ATOM		X	Y	Z
P	1	19.744	9.342	19.374
C	2	20.987	8.328	20.295
C	3	18.332	9.374	20.573
C	4	20.462	11.045	19.459
C	5	20.204	12.008	20.446
C	6	20.661	13.323	20.296
C	7	21.419	13.71	19.186
C	8	21.782	12.709	18.271
C	9	21.288	11.417	18.387
C	10	18.021	8.251	21.358
C	11	16.869	8.224	22.144
C	12	15.98	9.31 22.189	
C	13	16.307	10.436	21.425
C	14	17.45	10.465	20.624
C	15	21.005	6.934	20.106
C	16	21.902	6.125	20.797
C	17	22.831	6.677	21.697
C	18	22.821	8.074	21.866
C	19	21.918	8.886	21.183
C	20	14.706	9.224	22.999
C	21	21.828	15.147	18.938
C	22	23.805	5.875	22.447
C	23	13.553	8.51 22.254	
C	24	23.963	4.54 22.422	
C	25	21.462	15.679	17.532
H	26	19.608	11.753	21.322
H	27	20.388	14.067	21.049
H	28	22.412	12.954	17.415
H	29	21.512	10.691	17.606
H	30	18.688	7.39 21.369	
H	31	16.66	7.334	22.742
H	32	15.655	11.311	21.448
H	33	17.653	11.353	20.03
H	34	20.301	6.483	19.403
H	35	21.88	5.049	20.627
H	36	23.537	8.528	22.553
H	37	21.942	9.964	21.338
H	38	14.38	10.23	23.304
H	39	22.922	15.218	19.05
H	40	12.838	8.126	22.998
H	41	13.973	7.623	21.758
H	42	24.728	4.058	23.029
H	43	23.347	3.888	21.802
H	44	21.602	14.865	16.808
H	45	22.195	16.449	17.247
P	46	17.467	9.766	16.463
C	47	17.678	11.58	16.726
C	48	15.89	9.361	17.335
C	49	16.989	9.659	14.685
C	50	17.219	8.462	13.986
C	51	16.806	8.318	12.667
C	52	16.158	9.366	11.988
C	53	15.954	10.569	12.688
C	54	16.359	10.715	14.013
C	55	15.884	8.322	18.271
C	56	14.747	8.034	19.023
C	57	13.591	8.814	18.908
C	58	13.575	9.811	17.916
C	59	14.695	10.073	17.127
C	60	17.005	12.276	17.741
C	61	17.375	13.576	18.079
C	62	18.417	14.241	17.417
C	63	19.02	13.577	16.34
C	64	18.674	12.265	16.009
C	65	12.451	8.691	19.889
C	66	15.702	9.261	10.597
C	67	18.834	15.604	17.933
C	68	12.787	9.385	21.236
C	69	20.066	16.311	17.35
C	70	15.719	8.169	9.811
H	71	17.739	7.646	14.488

H	72	17.005	7.379	12.151
H	73	15.47	11.406	12.18
H	74	16.199	11.666	14.521
H	75	16.795	7.75	18.436
H	76	14.786	7.218	19.744
H	77	12.669	10.403	17.769
H	78	14.642	10.851	16.365
H	79	16.198	11.792	18.288
H	80	16.862	14.077	18.903
H	81	19.808	14.067	15.769
H	82	19.21	11.762	15.205
H	83	12.201	7.634	20.072
H	84	15.296	10.186	10.179
H	85	18.961	15.51	19.024
H	86	11.851	9.734	21.699
H	87	13.367	10.293	21.01
H	88	20.086	17.313	17.808
H	89	19.913	16.487	16.273
H	90	16.092	7.203	10.155
H	91	15.348	8.211	8.787
H	92	14.916	8.671	23.927
H	93	21.404	15.799	19.718
H	94	11.554	9.156	19.454
H	95	17.978	16.289	17.809
H	96	24.463	6.459	23.096
C	97	18.579	6.74	17.149
O	98	18.303	5.617	16.972
Rh	99	19.324	8.529	17.086
C	100	21.853	6.957	15.329
C	101	21.57	7.89	16.493
H	102	21.031	6.245	15.181
H	103	22.77	6.377	15.522
H	104	21.416	7.331	17.425
H	105	22.386	8.592	16.694
H	106	21.997	7.514	14.394
C	107	20.453	9.241	15.768
O	108	20.887	9.858	14.845

R2 (FS) Crosslinking mode 1

ATOM		X	Y	Z
P	1	19.8231	9.2014	19.4089
C	2	21.1153	8.0983	20.1331
C	3	18.4794	9.1396	20.6667
C	4	20.5862	10.8717	19.5457
C	5	20.3786	11.8049	20.5722
C	6	20.9200	13.0917	20.4806
C	7	21.6897	13.4862	19.3804
C	8	21.9544	12.5212	18.3969
C	9	21.4019	11.2484	18.4660
C	10	18.2179	7.9670	21.3959
C	11	17.0806	7.8736	22.1998
C	12	16.1645	8.9308	22.3123
C	13	16.4523	10.1106	21.6108
C	14	17.5742	10.2066	20.7894
C	15	21.3274	6.8317	19.5679
C	16	22.2720	5.9567	20.0946
C	17	23.0553	6.3229	21.2052
C	18	22.8329	7.5948	21.7685
C	19	21.8838	8.4700	21.2471
C	20	14.8881	8.7545	23.1006
C	21	22.2213	14.8965	19.2281
C	22	24.0923	5.4622	21.7841
C	23	13.7074	8.2701	22.2200
C	24	24.4739	4.2443	21.3607
C	25	21.8711	15.5733	17.8818
H	26	19.7722	11.5449	21.4401
H	27	20.7151	13.8099	21.2780
H	28	22.5750	12.7741	17.5361
H	29	21.5803	10.5526	17.6487
H	30	18.9093	7.1259	21.3419
H	31	16.8984	6.9499	22.7531
H	32	15.7790	10.9656	21.6900
H	33	17.7463	11.1228	20.2280
H	34	20.7298	6.5407	18.7027
H	35	22.4066	4.9814	19.6273
H	36	23.4295	7.9019	22.6296
H	37	21.7536	9.4534	21.6995
H	38	14.6128	9.6943	23.6055
H	39	23.3196	14.8544	19.3124
H	40	13.0110	7.6879	22.8431
H	41	14.1102	7.5615	21.4823
H	42	25.2658	3.7011	21.8751
H	43	24.0131	3.7469	20.5067
H	44	21.8637	14.8030	17.0989
H	45	22.6880	16.2594	17.6108
P	46	17.3073	10.2479	16.5738
C	47	17.6644	12.0137	16.9599
C	48	15.7187	9.8825	17.4433
C	49	16.8421	10.2852	14.7887

C	50	17.0835	9.1406	14.0111
C	51	16.7009	9.0890	12.6758
C	52	16.0696	10.1845	12.0573
C	53	15.8417	11.3328	12.8413
C	54	16.2247	11.3871	14.1796
C	55	15.5878	8.6215	18.0420
C	56	14.4745	8.2974	18.8156
C	57	13.4669	9.2418	19.0500
C	58	13.5559	10.4721	18.3775
C	59	14.6556	10.7892	17.5807
C	60	17.2077	12.6215	18.1421
C	61	17.7274	13.8388	18.5713
C	62	18.7210	14.5118	17.8450
C	63	19.1279	13.9376	16.6338
C	64	18.6253	12.7069	16.2027
C	65	12.3994	9.0211	20.0952
C	66	15.6580	10.1843	10.6498
C	67	19.2856	15.7957	18.4176
C	68	12.9223	9.3903	21.5084
C	69	20.5683	16.3951	17.8251
C	70	15.6885	9.1504	9.7922
H	71	17.5874	8.2906	14.4746
H	72	16.8980	8.1818	12.1045
H	73	15.3549	12.1969	12.3856
H	74	16.0475	12.2985	14.7513
H	75	16.3838	7.8829	17.9120
H	76	14.4169	7.3101	19.2747
H	77	12.7613	11.2103	18.5079
H	78	14.6935	11.7592	17.0847
H	79	16.4560	12.1249	18.7523
H	80	17.3739	14.2643	19.5132
H	81	19.8767	14.4365	16.0186
H	82	19.0181	12.2642	15.2879
H	83	12.0517	7.9764	20.0886
H	84	15.2838	11.1449	10.2847
H	85	19.4346	15.6355	19.4982
H	86	12.0719	9.6870	22.1420
H	87	13.5503	10.2876	21.4049
H	88	20.7397	17.3435	18.3599
H	89	20.3914	16.6812	16.7753
H	90	16.0268	8.1557	10.0855
H	91	15.3718	9.2733	8.7570
H	92	15.0663	8.0154	23.8958
H	93	21.8812	15.5189	20.0709
H	94	11.5257	9.6457	19.8586
H	95	18.5035	16.5717	18.3546
H	96	24.5924	5.8840	22.6606
C	97	18.6748	6.6983	16.9256
O	98	18.3959	5.5626	16.8136
Rh	99	18.8710	8.5389	17.2982
C	100	20.7263	7.1689	14.0760
C	101	21.1866	7.6584	15.4545
H	102	19.7189	6.7350	14.1273
H	103	21.4111	6.3950	13.7038
H	104	21.1961	6.8367	16.1765
H	105	22.2048	8.0703	15.3824
H	106	20.7127	7.9953	13.3536
C	107	20.2981	8.7977	15.9532
O	108	20.4482	9.9327	15.5334

R3 (IS) Crosslinking mode 1

ATOM		X	Y	Z
P	1	19.8438	9.2056	19.4063
C	2	21.1456	8.1083	20.1204
C	3	18.4999	9.1469	20.6662
C	4	20.6038	10.8769	19.5392
C	5	20.4037	11.8072	20.5704
C	6	20.9384	13.0968	20.4757
C	7	21.6992	13.4955	19.3703
C	8	21.9586	12.5330	18.3830
C	9	21.4094	11.2585	18.4535
C	10	18.2434	7.9853	21.4140
C	11	17.1012	7.8952	22.2115
C	12	16.1796	8.9490	22.3077
C	13	16.4652	10.1212	21.5921
C	14	17.5899	10.2119	20.7737
C	15	21.1955	6.7593	19.7310
C	16	22.1429	5.8905	20.2633
C	17	23.0962	6.3464	21.1941
C	18	23.0460	7.7027	21.5688
C	19	22.0902	8.5719	21.0481
C	20	14.9003	8.7734	23.0919
C	21	22.2278	14.9066	19.2161
C	22	24.1415	5.4926	21.7672
C	23	13.7223	8.2861	22.2088
C	24	24.3505	4.1836	21.5404
C	25	21.8737	15.5820	17.8702
H	26	19.8077	11.5422	21.4438
H	27	20.7394	13.8123	21.2771

H	28	22.5706	12.7895	17.5172
H	29	21.5800	10.5671	17.6311
H	30	18.9357	7.1445	21.3718
H	31	16.9211	6.9766	22.7741
H	32	15.7896	10.9753	21.6608
H	33	17.7604	11.1226	20.2031
H	34	20.4800	6.4004	18.9894
H	35	22.1525	4.8517	19.9337
H	36	23.7787	8.0787	22.2853
H	37	22.0853	9.6163	21.3596
H	38	14.6224	9.7144	23.5932
H	39	23.3264	14.8672	19.2988
H	40	13.0278	7.6994	22.8298
H	41	14.1291	7.5812	21.4696
H	42	25.1738	3.6627	22.0280
H	43	23.7216	3.5901	20.8758
H	44	21.8661	14.8116	17.0874
H	45	22.6884	16.2698	17.5969
P	46	17.3229	10.2422	16.5763
C	47	17.6797	12.0076	16.9651
C	48	15.7226	9.8818	17.4264
C	49	16.8738	10.2929	14.7876
C	50	17.1284	9.1582	14.0004
C	51	16.7618	9.1222	12.6596
C	52	16.1261	10.2197	12.0488
C	53	15.8861	11.3586	12.8428
C	54	16.2515	11.3969	14.1866
C	55	15.5866	8.6208	18.0233
C	56	14.4741	8.3013	18.7999
C	57	13.4733	9.2513	19.0405
C	58	13.5670	10.4825	18.3700
C	59	14.6626	10.7924	17.5645
C	60	17.2129	12.6219	18.1402
C	61	17.7304	13.8409	18.5675
C	62	18.7286	14.5104	17.8437
C	63	19.1414	13.9323	16.6363
C	64	18.6414	12.6995	16.2079
C	65	12.4073	9.0328	20.0874
C	66	15.7069	10.2285	10.6433
C	67	19.2880	15.7986	18.4115
C	68	12.9325	9.4042	21.4993
C	69	20.5687	16.4003	17.8169
C	70	15.7356	9.2015	9.7767
H	71	17.6251	8.3024	14.4612
H	72	16.9799	8.2272	12.0767
H	73	15.4020	12.2265	12.3915
H	74	16.0637	12.3008	14.7669
H	75	16.3781	7.8780	17.8904
H	76	14.4108	7.3115	19.2529
H	77	12.7742	11.2228	18.5001
H	78	14.7047	11.7637	17.0712
H	79	16.4495	12.1333	18.7422
H	80	17.3667	14.2738	19.5021
H	81	19.8934	14.4290	16.0232
H	82	19.0388	12.2536	15.2964
H	83	12.0586	7.9884	20.0831
H	84	15.3268	11.1904	10.2875
H	85	19.4359	15.6436	19.4931
H	86	12.0830	9.6989	22.1352
H	87	13.5575	10.3033	21.3940
H	88	20.7385	17.3493	18.3513
H	89	20.3892	16.6860	16.7674
H	90	16.0840	8.2067	10.0580
H	91	15.3968	9.3280	8.7490
H	92	15.0762	8.0364	23.8896
H	93	21.8874	15.5284	20.0592
H	94	11.5336	9.6577	19.8515
H	95	18.5035	16.5720	18.3447
H	96	24.8200	6.0076	22.4538
C	97	18.6726	6.6765	16.9803
O	98	18.4121	5.5339	16.8941
Rh	99	18.8641	8.5222	17.3231
C	100	20.7877	7.0537	14.1995
C	101	21.2206	7.6041	15.5638
H	102	19.7854	6.6082	14.2528
H	103	21.4889	6.2752	13.8699
H	104	21.2259	6.8144	16.3209
H	105	22.2361	8.0230	15.4913
H	106	20.7743	7.8493	13.4434
C	107	20.3149	8.7545	16.0016
O	108	20.4746	9.8788	15.5564
H	109	16.9446	4.8575	19.4247
H	110	16.4793	5.0324	19.9896

R3 (TS) Crosslinking mode 1

ATOM	X	Y	Z
P 1	19.701	9.040	19.557
C 2	20.964	7.887	20.260
C 3	18.423	9.103	20.884

C	4	20.582	10.657	19.611
C	5	20.451	11.638	20.605
C	6	21.066	12.887	20.455
C	7	21.842	13.192	19.329
C	8	22.028	12.177	18.380
C	9	21.401	10.945	18.508
C	10	18.150	7.998	21.705
C	11	16.950	7.923	22.419
C	12	15.989	8.943	22.355
C	13	16.321	10.093	21.621
C	14	17.502	10.164	20.889
C	15	20.954	6.534	19.882
C	16	21.877	5.635	20.407
C	17	22.857	6.058	21.326
C	18	22.861	7.415	21.697
C	19	21.935	8.317	21.177
C	20	14.613	8.762	22.956
C	21	22.481	14.551	19.121
C	22	23.872	5.164	21.895
C	23	13.531	8.489	21.872
C	24	24.041	3.853	21.652
C	25	22.302	15.149	17.703
H	26	19.848	11.445	21.492
H	27	20.925	13.645	21.230
H	28	22.645	12.357	17.500
H	29	21.528	10.210	17.716
H	30	18.854	7.167	21.753
H	31	16.743	7.029	23.012
H	32	15.624	10.932	21.581
H	33	17.702	11.045	20.285
H	34	20.212	6.197	19.156
H	35	21.842	4.593	20.087
H	36	23.610	7.768	22.407
H	37	21.973	9.363	21.482
H	38	14.331	9.651	23.543
H	39	23.562	14.443	19.310
H	40	12.821	7.734	22.244
H	41	14.028	8.036	21.002
H	42	24.845	3.301	22.137
H	43	23.398	3.286	20.977
H	44	22.224	14.326	16.980
H	45	23.220	15.693	17.432
P	46	17.237	10.247	16.663
C	47	17.816	11.978	16.952
C	48	15.524	10.184	17.379
C	49	16.879	10.240	14.848
C	50	17.201	9.113	14.079
C	51	16.887	9.060	12.724
C	52	16.241	10.133	12.084
C	53	15.921	11.261	12.864
C	54	16.230	11.313	14.221
C	55	14.969	8.909	17.566
C	56	13.813	8.727	18.327
C	57	13.179	9.813	18.945
C	58	13.645	11.098	18.627
C	59	14.787	11.286	17.845
C	60	17.589	12.618	18.182
C	61	18.218	13.815	18.500
C	62	19.110	14.436	17.615
C	63	19.318	13.817	16.376
C	64	18.694	12.607	16.052
C	65	12.123	9.627	20.008
C	66	15.901	10.132	10.656
C	67	19.752	15.736	18.050
C	68	12.735	9.729	21.428
C	69	21.129	16.124	17.494
C	70	16.016	9.110	9.791
H	71	17.702	8.273	14.561
H	72	17.161	8.173	12.152
H	73	15.421	12.108	12.393
H	74	15.974	12.205	14.794
H	75	15.475	8.041	17.142
H	76	13.429	7.717	18.481
H	77	13.129	11.971	19.034
H	78	15.118	12.301	17.631
H	79	16.913	12.176	18.909
H	80	18.029	14.273	19.473
H	81	20.000	14.262	15.649
H	82	18.917	12.132	15.097
H	83	11.617	8.656	19.886
H	84	15.509	11.082	10.281
H	85	19.804	15.725	19.151
H	86	11.931	9.921	22.157
H	87	13.382	10.619	21.449
H	88	21.389	17.092	17.954
H	89	21.049	16.328	16.413
H	90	16.380	8.126	10.088
H	91	15.734	9.232	8.746

H	92	14.645	7.922	23.664
H	93	22.118	15.256	19.884
H	94	11.350	10.403	19.903
H	95	19.059	16.561	17.808
H	96	24.565	5.648	22.590
C	97	18.402	6.587	16.931
O	98	18.225	5.475	16.603
Rh	99	18.575	8.384	17.521
C	100	21.127	7.001	14.687
C	101	21.172	7.641	16.080
H	102	20.206	6.419	14.549
H	103	21.978	6.319	14.558
H	104	21.115	6.882	16.866
H	105	22.122	8.185	16.204
H	106	21.172	7.769	13.904
C	107	20.065	8.688	16.244
O	108	20.109	9.721	15.599
H	109	16.547	7.665	19.195
H	110	17.139	7.215	19.041

R3 (FS) Crosslinking mode 1

R4 (IS) Crosslinking mode 1

ATOM		X	Y	Z
P	P 1	19.8067	9.1932	19.2763
C	2	21.0717	8.0928	20.0692
C	3	18.4800	9.1964	20.5776
C	4	20.5971	10.8579	19.3537
C	5	20.6438	11.7105	20.4719
C	6	21.1875	12.9945	20.3588
C	7	21.7217	13.4636	19.1503
C	8	21.7707	12.5653	18.0769
C	9	21.1989	11.3030	18.1705
C	10	18.0379	7.9567	21.0716
C	11	16.9480	7.8754	21.9308
C	12	16.2378	9.0196	22.3322
C	13	16.7035	10.2546	21.8717
C	14	17.8039	10.3442	21.0097
C	15	21.0539	6.7016	19.8593
C	16	21.9487	5.8616	20.5127
C	17	22.9099	6.3739	21.4055
C	18	22.9310	7.7673	21.5987
C	19	22.0305	8.6112	20.9527
C	20	14.9924	8.8720	23.1755
C	21	22.2338	14.8793	18.9774
C	22	23.8795	5.5395	22.1193
C	23	13.7590	8.4536	22.3392
C	24	24.0065	4.2006	22.0726
C	25	21.7473	15.5894	17.6932
H	26	20.2378	11.3897	21.4305
H	27	21.1695	13.6555	21.2284
H	28	22.2134	12.8647	17.1272
H	29	21.1847	10.6665	17.2917
H	30	18.5449	7.0390	20.7758
H	31	16.6293	6.8935	22.2870
H	32	16.1973	11.1719	22.1799
H	33	18.1229	11.3256	20.6696
H	34	20.3326	6.2779	19.1604
H	35	21.8990	4.7899	20.3211
H	36	23.6729	8.1958	22.2753
H	37	22.0936	9.6839	21.1275
H	38	14.7809	9.8065	23.7174
H	39	23.3355	14.8370	18.9412
H	40	13.0515	7.9084	22.9836
H	41	14.0999	7.7297	21.5850
H	42	24.7748	3.6944	22.6555
H	43	23.3642	3.5689	21.4581
H	44	21.7243	14.8562	16.8756
H	45	22.5038	16.3314	17.3964
P	46	17.2893	10.0349	16.6143
C	47	17.7104	11.7845	17.0206
C	48	15.6831	9.7819	17.5057
C	49	16.7866	10.1481	14.8385
C	50	17.2884	9.2460	13.8903
C	51	16.8779	9.2927	12.5625
C	52	15.9487	10.2529	12.1224
C	53	15.4647	11.1708	13.0739
C	54	15.8717	11.1222	14.4039
C	55	15.4100	8.5237	18.0595
C	56	14.2909	8.3180	18.8684
C	57	13.4263	9.3728	19.1848
C	58	13.6478	10.6068	18.5532
C	59	14.7442	10.8074	17.7170
C	60	17.4054	12.2924	18.2929
C	61	17.8861	13.5286	18.7074
C	62	18.6824	14.3241	17.8714
C	63	18.9322	13.8441	16.5786
C	64	18.4695	12.5913	16.1581
C	65	12.3948	9.2598	20.2804
C	66	15.4797	10.3488	10.7359

C	67	19.2021	15.6356	18.4254
C	68	13.0194	9.6175	21.6549
C	69	20.3995	16.3313	17.7640
C	70	15.7333	9.4946	9.7282
H	71	18.0317	8.5123	14.1911
H	72	17.2998	8.5795	11.8545
H	73	14.7509	11.9341	12.7588
H	74	15.4800	11.8582	15.1049
H	75	16.1151	7.7088	17.9038
H	76	14.1238	7.3296	19.2990
H	77	12.9687	11.4393	18.7492
H	78	14.8960	11.7933	17.2797
H	79	16.7941	11.7042	18.9723
H	80	17.6501	13.8792	19.7151
H	81	19.5282	14.4385	15.8846
H	82	18.7359	12.2275	15.1665
H	83	11.9691	8.2452	20.3168
H	84	14.8508	11.2190	10.5272
H	85	19.4305	15.4694	19.4906
H	86	12.2334	9.9881	22.3315
H	87	13.7101	10.4606	21.4984
H	88	20.5535	17.2702	18.3202
H	89	20.1295	16.6421	16.7418
H	90	16.3363	8.5955	9.8601
H	91	15.3260	9.6698	8.7331
H	92	15.1778	8.1031	23.9418
H	93	21.9879	15.4781	19.8684
H	94	11.5622	9.9473	20.0697
H	95	18.3693	16.3603	18.4259
H	96	24.5657	6.0980	22.7626
C	97	18.3978	6.9597	16.0480
O	98	18.0435	6.0006	15.4945
Rh	99	19.0103	8.3345	17.1760
C	100	21.7376	7.3034	14.6776
C	101	21.8008	8.5149	15.6150
H	102	21.0401	6.5429	15.0538
H	103	22.7277	6.8359	14.5870
H	104	22.1539	8.2010	16.6071
H	105	22.4937	9.2668	15.2042
H	106	21.4085	7.6054	13.6739
C	107	20.4160	9.1716	15.7557
O	108	20.1501	10.0980	14.9960
H	109	18.0866	7.5650	18.2857
H	110	20.1478	7.2795	17.4664

R4 (TS) Crosslinking mode 1

ATOM	X	Y	Z
P1	19.639	9.125	19.353
C2	20.943	8.042	20.164
C3	18.352	9.142	20.696
C4	20.452	10.789	19.390
C5	20.587	11.668	20.482
C6	21.146	12.936	20.303
C7	21.613	13.370	19.054
C8	21.553	12.453	17.994
C9	20.962	11.209	18.156
C10	17.883	7.903	21.167
C11	16.801	7.831	22.036
C12	16.138	8.986	22.484
C13	16.637	10.219	22.053
C14	17.722	10.299	21.173
C15	20.973	6.657	19.921
C16	21.895	5.827	20.551
C17	22.851	6.346	21.446
C18	22.824	7.733	21.679
C19	21.893	8.564	21.059
C20	14.900	8.854	23.339
C21	22.176	14.761	18.830
C22	23.865	5.525	22.114
C23	13.649	8.500	22.501
C24	24.048	4.196	22.010
C25	21.687	15.471	17.547
H26	20.239	11.376	21.475
H27	21.203	13.615	21.156
H28	21.929	12.723	17.009
H29	20.853	10.551	17.291
H30	18.369	6.980	20.850
H31	16.458	6.851	22.369
H32	16.173	11.142	22.404
H33	18.071	11.282	20.861
H34	20.264	6.225	19.210
H35	21.878	4.762	20.330
H36	23.558	8.165	22.362
H37	21.927	9.635	21.268
H38	14.723	9.780	23.907
H39	23.273	14.668	18.767
H40	12.919	7.976	23.137
H41	13.957	7.775	21.734
H42	24.849	3.701	22.556

H43	23.420	3.563	21.383
H44	21.567	14.724	16.749
H45	22.483	16.145	17.196
P46	17.160	10.111	16.691
C47	17.594	11.859	17.060
C48	15.559	9.898	17.625
C49	16.654	10.183	14.893
C50	17.511	9.649	13.919
C51	17.184	9.683	12.572
C52	15.960	10.232	12.134
C53	15.110	10.773	13.118
C54	15.453	10.771	14.463
C55	15.285	8.640	18.179
C56	14.185	8.449	19.017
C57	13.343	9.516	19.357
C58	13.577	10.756	18.742
C59	14.660	10.949	17.887
C60	17.439	12.333	18.371
C61	17.937	13.573	18.748
C62	18.618	14.396	17.840
C63	18.733	13.941	16.520
C64	18.243	12.688	16.132
C65	12.318	9.406	20.460
C66	15.545	10.265	10.727
C67	19.179	15.709	18.348
C68	12.961	9.709	21.840
C69	20.405	16.318	17.652
C70	16.185	9.725	9.677
H71	18.473	9.208	14.226
H72	17.885	9.281	11.849
H73	14.168	11.220	12.815
H74	14.770	11.232	15.189
H75	15.981	7.818	17.994
H76	14.014	7.464	19.449
H77	12.917	11.596	18.961
H78	14.838	11.944	17.477
H79	16.929	11.715	19.107
H80	17.810	13.905	19.781
H81	19.229	14.559	15.771
H82	18.388	12.353	15.104
H83	11.861	8.405	20.474
H84	14.606	10.797	10.548
H85	19.407	15.573	19.418
H86	12.193	10.099	22.525
H87	13.689	10.523	21.700
H88	20.641	17.246	18.198
H89	20.130	16.641	16.635
H90	17.121	9.172	9.779
H91	15.777	9.819	8.672
H92	15.066	8.059	24.082
H93	21.979	15.383	19.716
H94	11.507	10.125	20.273
H95	18.377	16.468	18.323
H96	24.541	6.088	22.763
C97	18.118	7.130	16.005
O98	17.814	6.235	15.311
Rh99	18.889	8.340	17.164
C100	22.345	7.097	14.376
C101	22.443	8.334	15.277
H102	21.630	6.362	14.767
H103	23.328	6.617	14.304
H104	22.786	8.054	16.280
H105	23.124	9.084	14.850
H106	22.024	7.381	13.365
C107	21.092	8.972	15.444
O108	20.767	9.965	14.823
H109	18.726	7.047	18.078
H110	20.384	7.838	16.574

R4 (FS) Crosslinking mode 1

ATOM		X	Y	Z
P	1	19.6327	9.0769	19.4063
C	2	20.9394	8.0023	20.1708
C	3	18.3446	9.0873	20.7340
C	4	20.4217	10.7349	19.3546
C	5	20.6302	11.6216	20.4247
C	6	21.1919	12.8829	20.2025
C	7	21.5868	13.2950	18.9208
C	8	21.4416	12.3744	17.8738
C	9	20.8512	11.1334	18.0792
C	10	17.8493	7.8421	21.1618
C	11	16.7709	7.7644	22.0366
C	12	16.1346	8.9192	22.5241
C	13	16.6570	10.1560	22.1298
C	14	17.7430	10.2425	21.2520
C	15	20.9958	6.6311	19.8697
C	16	21.9444	5.7999	20.4565
C	17	22.8897	6.3074	21.3670
C	18	22.8281	7.6819	21.6639

C	19	21.8736	8.5141	21.0838
C	20	14.8892	8.7917	23.3701
C	21	22.1762	14.6706	18.6681
C	22	23.9337	5.4907	21.9940
C	23	13.6341	8.4902	22.5154
C	24	24.1616	4.1760	21.8243
C	25	21.6772	15.3919	17.3951
H	26	20.3311	11.3480	21.4367
H	27	21.3083	13.5672	21.0459
H	28	21.7524	12.6353	16.8625
H	29	20.6845	10.4726	17.2270
H	30	18.3016	6.9212	20.7939
H	31	16.4080	6.7808	22.3426
H	32	16.2106	11.0760	22.5121
H	33	18.1095	11.2261	20.9666
H	34	20.2944	6.2234	19.1404
H	35	21.9564	4.7439	20.1871
H	36	23.5518	8.1042	22.3640
H	37	21.8777	9.5731	21.3350
H	38	14.7287	9.7067	23.9603
H	39	23.2689	14.5489	18.5805
H	40	12.8806	7.9847	23.1397
H	41	13.9256	7.7631	21.7438
H	42	24.9827	3.6816	22.3419
H	43	23.5492	3.5518	21.1726
H	44	21.4755	14.6444	16.6150
H	45	22.4974	16.0101	16.9991
P	46	17.1896	10.1349	16.7284
C	47	17.6150	11.9036	17.0501
C	48	15.5965	9.9379	17.6312
C	49	16.7566	10.1440	14.9413
C	50	17.7990	10.0485	13.9984
C	51	17.5236	10.0500	12.6364
C	52	16.2006	10.1240	12.1574
C	53	15.1681	10.2072	13.1092
C	54	15.4375	10.2192	14.4771
C	55	15.3272	8.6839	18.2009
C	56	14.2270	8.5022	19.0393
C	57	13.3922	9.5775	19.3758
C	58	13.6284	10.8128	18.7517
C	59	14.7043	10.9925	17.8829
C	60	17.5589	12.3502	18.3792
C	61	18.0497	13.5992	18.7346
C	62	18.6204	14.4607	17.7864
C	63	18.6138	14.0425	16.4493
C	64	18.1263	12.7813	16.0838
C	65	12.3600	9.4716	20.4727
C	66	15.8623	10.1152	10.7306
C	67	19.2124	15.7704	18.2628
C	68	12.9951	9.7303	21.8636
C	69	20.4539	16.3152	17.5380
C	70	16.7053	9.9909	9.6906
H	71	18.8360	9.9764	14.3351
H	72	18.3546	9.9858	11.9343
H	73	14.1326	10.2536	12.7661
H	74	14.6120	10.2746	15.1865
H	75	16.0201	7.8596	18.0156
H	76	14.0480	7.5183	19.4746
H	77	12.9745	11.6587	18.9741
H	78	14.8765	11.9723	17.4365
H	79	17.1376	11.7018	19.1448
H	80	18.0234	13.9064	19.7821
H	81	19.0171	14.6937	15.6717
H	82	18.1629	12.4796	15.0373
H	83	11.8783	8.4814	20.4634
H	84	14.7945	10.2189	10.5161
H	85	19.4436	15.6557	19.3335
H	86	12.2302	10.1349	22.5448
H	87	13.7507	10.5227	21.7465
H	88	20.7579	17.2282	18.0769
H	89	20.1726	16.6543	16.5282
H	90	17.7828	9.8750	9.8163
H	91	16.3318	9.9973	8.6670
H	92	15.0314	7.9731	24.0924
H	93	22.0201	15.3040	19.5554
H	94	11.5665	10.2122	20.2933
H	95	18.4345	16.5520	18.2186
H	96	24.5958	6.0452	22.6658
C	97	18.1654	7.2251	15.9431
O	98	17.8640	6.4243	15.1528
Rh	99	18.7113	8.3642	17.3215
C	100	22.9615	7.0281	14.1024
C	101	23.0515	8.2947	14.9702
H	102	22.2437	6.3061	14.5161
H	103	23.9406	6.5357	14.0401
H	104	23.3923	8.0158	15.9812
H	105	23.7610	9.0193	14.5477
H	106	22.6415	7.2787	13.0819

C	107	21.7054	8.9542	15.1056
O	108	21.4215	10.0460	14.6293
H	109	19.6701	7.1069	17.5874
H	110	20.9328	8.3765	15.6795

R1m (IS) Crosslinking mode 2

ATOM		X	Y	Z
P	1	22.4785	7.8570	19.2585
C	2	23.2090	6.1924	19.5747
C	3	21.0375	7.8685	20.4164
C	4	23.6090	9.0347	20.1229
C	5	23.6585	9.1309	21.5233
C	6	24.5275	10.0313	22.1365
C	7	25.3686	10.8729	21.3836
C	8	25.3036	10.7746	19.9806
C	9	24.4390	9.8765	19.3643
C	10	20.6764	6.7692	21.2082
C	11	19.5738	6.8402	22.0604
C	12	18.7985	8.0047	22.1536
C	13	19.1731	9.1038	21.3694
C	14	20.2680	9.0379	20.5098
C	15	22.6166	5.0941	18.9215
C	16	23.1239	3.8106	19.0756
C	17	24.2630	3.5678	19.8701
C	18	24.8511	4.6702	20.5152
C	19	24.3373	5.9595	20.3723
C	20	17.6210	8.0663	23.0973
C	21	26.2518	11.8073	22.0889
C	22	24.8587	2.2381	20.0368
C	23	16.3778	7.2436	22.6905
C	24	24.5299	1.1065	19.3905
C	25	27.1096	12.6925	21.5485
H	26	23.0103	8.5068	22.1389
H	27	24.5527	10.0963	23.2259
H	28	25.9321	11.4114	19.3587
H	29	24.3821	9.8185	18.2767
H	30	21.2640	5.8524	21.1694
H	31	19.3215	5.9724	22.6740
H	32	18.5960	10.0281	21.4324
H	33	20.5262	9.9091	19.9061
H	34	21.7471	5.2511	18.2815
H	35	22.6316	2.9809	18.5679
H	36	25.7387	4.5125	21.1306
H	37	24.8282	6.7916	20.8760
H	38	17.3244	9.1155	23.2496
H	39	15.8046	7.0572	23.6106
H	40	16.7013	6.2508	22.3391
H	41	25.0584	0.1757	19.5939
H	42	23.7471	1.0690	18.6319
H	43	27.2351	12.8071	20.4709
H	44	27.7211	13.3331	22.1826
P	45	20.0877	8.9603	16.5249
C	46	19.8482	10.7685	16.2537
C	47	18.6865	8.5274	17.6423
C	48	19.4987	8.1715	14.9577
C	49	20.4308	7.7095	14.0118
C	50	20.0159	7.0970	12.8340
C	51	18.6488	6.9090	12.5525
C	52	17.7209	7.3756	13.5018
C	53	18.1333	7.9841	14.6853
C	54	18.6027	7.2053	18.1032
C	55	17.5572	6.8045	18.9332
C	56	16.5678	7.7096	19.3433
C	57	16.6565	9.0292	18.8777
C	58	17.6997	9.4389	18.0464
C	59	20.6096	11.6423	17.0452
C	60	20.4659	13.0223	16.9206
C	61	19.5781	13.5834	15.9850
C	62	18.8291	12.6997	15.1833
C	63	18.9609	11.3190	15.3142
C	64	15.4243	7.2888	20.2349
C	65	18.1574	6.2486	11.3387
C	66	19.4804	15.0438	15.8859
C	67	15.4230	7.8890	21.6577
C	68	18.8411	15.7574	14.9430
C	69	18.8875	5.6278	10.3959
H	70	21.4955	7.8297	14.2151
H	71	20.7683	6.7597	12.1213
H	72	16.6539	7.2405	13.3130
H	73	17.3847	8.3044	15.4101
H	74	19.3581	6.4781	17.8005
H	75	17.5156	5.7694	19.2774
H	76	15.8962	9.7562	19.1723
H	77	17.7360	10.4728	17.7024
H	78	21.3364	11.2312	17.7489
H	79	21.0698	13.6813	17.5466
H	80	18.1244	13.0935	14.4505
H	81	18.3667	10.6658	14.6752
H	82	15.3929	6.1906	20.3058

H	83	17.0706	6.2687	11.2180
H	84	20.0049	15.5868	16.6772
H	85	14.3947	7.8048	22.0408
H	86	15.6222	8.9706	21.5901
H	87	18.8349	16.8463	14.9770
H	88	18.3195	15.2901	14.1068
H	89	19.9740	5.5499	10.4494
H	90	18.4069	5.1687	9.5329
H	91	17.9577	7.7012	24.0809
H	92	26.1873	11.7555	23.1796
H	93	14.4832	7.5888	19.7455
H	94	25.6718	2.1947	20.7670
C	95	20.5111	4.1543	16.0541
O	96	20.3992	3.2421	15.3758
Rh	97	22.3550	8.4105	16.9627
C	98	24.2385	6.4180	15.8508
C	99	24.3556	7.5980	16.8122
H	100	23.5103	5.6702	16.1996
H	101	25.2056	5.8924	15.7472
H	102	24.7393	7.2604	17.7844
H	103	25.0757	8.3355	16.4305
H	104	23.9318	6.7352	14.8431
C	105	22.9598	9.5546	15.6113
O	106	23.4312	10.3656	14.9158

R1m (TS) Crosslinking mode 2

ATOM	X	Y	Z		
1	File	1	by	GaussView	6.0.16
1	P	1	22.466	7.805	19.312
2	C	2	23.328	6.213	19.688
3	C	3	20.958	7.662	20.372
4	C	4	23.402	9.076	20.284
5	C	5	23.290	9.177	21.680
6	C	6	23.976	10.172	22.374
7	C	7	24.794	11.105	21.710
8	C	8	24.900	10.996	20.311
9	C	9	24.217	10.005	19.615
10	C	10	20.628	6.518	21.112
11	C	11	19.474	6.488	21.897
12	C	12	18.611	7.590	21.969
13	C	13	18.951	8.733	21.233
14	C	14	20.099	8.769	20.444
15	C	15	22.972	5.094	18.914
16	C	16	23.569	3.856	19.120
17	C	17	24.565	3.686	20.101
18	C	18	24.923	4.811	20.862
19	C	19	24.319	6.054	20.664
20	C	20	17.377	7.548	22.840
21	C	21	25.482	12.136	22.497
22	C	22	25.244	2.408	20.346
23	C	23	16.244	6.601	22.388
24	C	24	25.062	1.250	19.691
25	C	25	26.249	13.137	22.034
26	H	26	22.646	8.491	22.232
27	H	27	23.869	10.237	23.459
28	H	28	25.521	11.695	19.751
29	H	29	24.289	9.947	18.529
30	H	30	21.282	5.647	21.090
31	H	31	19.250	5.588	22.473
32	H	32	18.303	9.610	21.275
33	H	33	20.328	9.674	19.879
34	H	34	22.224	5.199	18.126
35	H	35	23.266	3.014	18.499
36	H	36	25.700	4.714	21.623
37	H	37	24.631	6.903	21.270
38	H	38	16.971	8.566	22.947
39	H	39	15.625	6.409	23.278
40	H	40	16.673	5.624	22.111
41	H	41	25.634	0.361	19.956
42	H	42	24.351	1.145	18.871
43	H	43	26.440	13.290	20.971
44	H	44	26.707	13.848	22.721
45	P	45	20.174	8.855	16.512
46	C	46	19.770	10.650	16.388
47	C	47	18.760	8.199	17.497
48	C	48	19.742	8.254	14.813
49	C	49	20.582	8.587	13.732
50	C	50	20.292	8.169	12.440
51	C	51	19.155	7.384	12.162
52	C	52	18.326	7.048	13.246
53	C	53	18.607	7.476	14.544
54	C	54	18.825	6.873	17.950
55	C	55	17.785	6.324	18.701
56	C	56	16.658	7.083	19.041
57	C	57	16.597	8.406	18.581
58	C	58	17.627	8.959	17.822
59	C	59	20.368	11.543	17.289
60	C	60	20.044	12.898	17.265
61	C	61	19.131	13.418	16.330

62	C	62	18.550	12.518	15.417
63	C	63	18.862	11.163	15.446
64	C	64	15.525	6.502	19.853
65	C	65	18.808	6.909	10.819
66	C	66	18.840	14.856	16.338
67	C	67	15.309	7.100	21.262
68	C	68	18.073	15.537	15.469
69	C	69	19.494	7.099	9.680
70	H	70	21.479	9.180	13.907
71	H	71	20.966	8.457	11.633
72	H	72	17.435	6.444	13.066
73	H	73	17.930	7.201	15.352
74	H	74	19.703	6.268	17.721
75	H	75	17.857	5.290	19.043
76	H	76	15.723	9.018	18.815
77	H	77	17.549	9.992	17.483
78	H	78	21.108	11.171	18.001
79	H	79	20.519	13.576	17.977
80	H	80	17.838	12.879	14.675
81	H	81	18.396	10.491	14.724
82	H	82	15.656	5.413	19.943
83	H	83	17.877	6.338	10.766
84	H	84	19.318	15.412	17.150
85	H	85	14.276	6.856	21.550
86	H	86	15.349	8.200	21.201
87	H	87	17.933	16.612	15.576
88	H	88	17.573	15.059	14.626
89	H	89	20.435	7.651	9.641
90	H	90	19.128	6.696	8.736
91	H	91	17.687	7.236	23.850
92	H	92	25.335	12.057	23.578
93	H	93	14.593	6.650	19.284
94	H	94	25.984	2.432	21.151
95	C	95	21.408	5.339	15.425
96	O	96	21.567	5.084	14.323
97	Rh	97	22.437	8.401	17.044
98	C	98	24.671	6.691	16.008
99	C	99	24.527	7.809	17.038
100	H	100	24.069	5.808	16.269
101	H	101	25.720	6.348	15.946
102	H	102	24.861	7.459	18.025
103	H	103	25.183	8.650	16.771
104	H	104	24.370	7.015	15.002
105	C	105	23.049	9.732	15.884
106	O	106	23.514	10.665	15.352

R1m (FS) Crosslinking mode 2

R2 (IS) Crosslinking mode 2

ATOM		X	Y	Z
P	1	22.2638	7.6244	19.2708
C	2	23.4087	6.2809	19.8575
C	3	20.8361	7.4332	20.4268
C	4	23.1998	9.0789	19.9198
C	5	23.0344	9.6480	21.1914
C	6	23.9441	10.5934	21.6690
C	7	25.0591	10.9942	20.9108
C	8	25.1968	10.4445	19.6212
C	9	24.2845	9.5189	19.1364
C	10	20.4912	6.1762	20.9511
C	11	19.3669	6.0257	21.7636
C	12	18.5568	7.1166	22.1112
C	13	18.9031	8.3697	21.5837
C	14	20.0043	8.5221	20.7386
C	15	23.3695	4.9893	19.2976
C	16	24.2754	4.0052	19.6922
C	17	25.2715	4.2709	20.6529
C	18	25.2779	5.5496	21.2359
C	19	24.3743	6.5322	20.8458
C	20	17.3526	6.9072	23.0023
C	21	26.0292	11.9320	21.4852
C	22	26.3063	3.3143	21.0570
C	23	16.0416	6.6033	22.2367
C	24	26.6249	2.1479	20.4704
C	25	27.2103	12.2993	20.9576
H	26	22.2189	9.3230	21.8366
H	27	23.8058	11.0099	22.6688
H	28	26.0288	10.7435	18.9847
H	29	24.4285	9.1016	18.1414
H	30	21.1109	5.3051	20.7406
H	31	19.1276	5.0355	22.1585
H	32	18.3013	9.2466	21.8269
H	33	20.2218	9.5104	20.3322
H	34	22.6263	4.7499	18.5364
H	35	24.2150	3.0175	19.2347
H	36	26.0246	5.7876	21.9959
H	37	24.4380	7.5118	21.3139
H	38	17.2000	7.7866	23.6473
H	39	15.3882	6.0055	22.8894
H	40	16.2877	5.9513	21.3860

H	41	27.4334	1.5331	20.8654
H	42	26.1148	1.7759	19.5810
H	43	27.5684	11.9251	19.9978
H	44	27.8649	12.9916	21.4859
P	45	19.7115	8.8139	16.6097
C	46	19.8893	10.6387	16.4583
C	47	18.2767	8.5794	17.7319
C	48	18.9852	8.3101	14.9874
C	49	19.8493	8.0063	13.9198
C	50	19.3535	7.5492	12.7066
C	51	17.9718	7.3595	12.5082
C	52	17.1102	7.7085	13.5644
C	53	17.6033	8.1759	14.7823
C	54	17.9245	7.2653	18.0739
C	55	16.7913	7.0111	18.8429
C	56	15.9983	8.0610	19.3317
C	57	16.3631	9.3722	18.9934
C	58	17.4792	9.6354	18.1963
C	59	20.5849	11.3470	17.4522
C	60	20.8572	12.7030	17.2971
C	61	20.4766	13.4004	16.1344
C	62	19.7481	12.6916	15.1609
C	63	19.4589	11.3401	15.3191
C	64	14.8382	7.8134	20.2624
C	65	17.4179	6.7975	11.2727
C	66	20.8912	14.7963	15.9599
C	67	15.2597	7.8452	21.7491
C	68	20.8711	15.5048	14.8168
C	69	18.1057	6.1777	10.2966
H	70	20.9261	8.1026	14.0631
H	71	20.0533	7.3243	11.9019
H	72	16.0327	7.5878	13.4353
H	73	16.9050	8.4177	15.5830
H	74	18.5345	6.4306	17.7283
H	75	16.5255	5.9791	19.0745
H	76	15.7557	10.2060	19.3531
H	77	17.7296	10.6636	17.9348
H	78	20.9638	10.8263	18.3332
H	79	21.4174	13.2276	18.0729
H	80	19.4069	13.2005	14.2593
H	81	18.9122	10.8168	14.5354
H	82	14.3624	6.8469	20.0339
H	83	16.3317	6.8774	11.1722
H	84	21.3012	15.2730	16.8545
H	85	14.3545	7.9697	22.3628
H	86	15.8570	8.7553	21.9104
H	87	21.2296	16.5333	14.7907
H	88	20.5216	15.0846	13.8730
H	89	19.1860	6.0356	10.3468
H	90	17.5998	5.7753	9.4197
H	91	17.5686	6.0636	23.6747
H	92	25.7506	12.3390	22.4615
H	93	14.0726	8.5873	20.0967
H	94	26.8935	3.6258	21.9261
C	95	21.0524	5.9727	16.4530
O	96	20.6548	4.9073	16.1910
Rh	97	21.8097	7.6774	16.8918
C	98	23.9029	6.5641	14.8357
C	99	23.7078	6.6902	16.3419
H	100	23.0700	6.0266	14.3610
H	101	24.8292	6.0070	14.6080
H	102	23.6965	5.7007	16.8105
H	103	24.5319	7.2496	16.8045
H	104	23.9809	7.5425	14.3409
C	105	22.7182	9.1813	16.1416
O	106	23.3396	10.0526	15.6787

R1s (IS) Crosslinking mode 2

ATOM		X	Y	Z
P	1	22.3001	7.5059	19.2568
C	2	23.2662	6.0674	19.9068
C	3	20.8720	7.5641	20.4270
C	4	23.3106	8.9535	19.8213
C	5	23.1882	9.5432	21.0896
C	6	23.9666	10.6459	21.4371
C	7	24.9031	11.1981	20.5445
C	8	25.0240	10.5983	19.2754
C	9	24.2420	9.5050	18.9221
C	10	20.5247	6.4631	21.2234
C	11	19.4307	6.5268	22.0866
C	12	18.6530	7.6886	22.1974
C	13	19.0018	8.7845	21.3958
C	14	20.0801	8.7208	20.5135
C	15	23.0491	4.7999	19.3380
C	16	23.7807	3.6926	19.7502
C	17	24.7726	3.8097	20.7437
C	18	24.9743	5.0784	21.3145
C	19	24.2356	6.1900	20.9098
C	20	17.5022	7.7411	23.1740

C	21	25.6977	12.3557	20.9666
C	22	25.6113	2.6901	21.1847
C	23	16.1923	7.0690	22.7001
C	24	25.5945	1.4264	20.7268
C	25	26.6644	12.9863	20.2750
H	26	22.4685	9.1504	21.8076
H	27	23.8498	11.0941	22.4257
H	28	25.7342	10.9935	18.5495
H	29	24.3447	9.0744	17.9258
H	30	21.1245	5.5541	21.1858
H	31	19.1937	5.6591	22.7062
H	32	18.4218	9.7068	21.4639
H	33	20.3144	9.5941	19.9034
H	34	22.3174	4.7060	18.5331
H	35	23.5929	2.7301	19.2748
H	36	25.7393	5.1946	22.0850
H	37	24.4356	7.1584	21.3671
H	38	17.2899	8.7870	23.4443
H	39	15.6226	6.7953	23.6009
H	40	16.4405	6.1171	22.2046
H	41	26.2830	0.6803	21.1224
H	42	24.9053	1.0918	19.9506
H	43	26.9724	12.6785	19.2752
H	44	27.1849	13.8400	20.7076
P	45	19.8367	8.3454	16.5900
C	46	20.0565	10.1769	16.4833
C	47	18.3881	8.1192	17.7007
C	48	19.1033	7.9970	14.9306
C	49	19.9466	8.0465	13.8044
C	50	19.4503	7.8248	12.5273
C	51	18.0882	7.5276	12.3150
C	52	17.2571	7.4647	13.4462
C	53	17.7507	7.6945	14.7316
C	54	18.2021	6.8500	18.2664
C	55	17.1152	6.5958	19.1032
C	56	16.1947	7.6052	19.4162
C	57	16.3883	8.8727	18.8474
C	58	17.4646	9.1322	18.0007
C	59	21.0723	10.7970	17.2261
C	60	21.2547	12.1778	17.1762
C	61	20.4418	12.9954	16.3709
C	62	19.4321	12.3648	15.6163
C	63	19.2478	10.9881	15.6651
C	64	15.0434	7.3748	20.3630
C	65	17.5122	7.2940	10.9867
C	66	20.6720	14.4443	16.3525
C	67	15.2773	7.9228	21.7883
C	68	20.0567	15.3537	15.5774
C	69	18.1586	7.2682	9.8086
H	70	21.0089	8.2592	13.9383
H	71	20.1331	7.8854	11.6802
H	72	16.1991	7.2292	13.3148
H	73	17.0723	7.6348	15.5820
H	74	18.9248	6.0598	18.0546
H	75	16.9894	5.5996	19.5307
H	76	15.6811	9.6744	19.0730
H	77	17.5870	10.1292	17.5777
H	78	21.7327	10.1917	17.8468
H	79	22.0561	12.6309	17.7629
H	80	18.7794	12.9620	14.9798
H	81	18.4664	10.5344	15.0549
H	82	14.8103	6.3004	20.4201
H	83	16.4320	7.1237	10.9836
H	84	21.4350	14.7937	17.0537
H	85	14.2930	8.0201	22.2704
H	86	15.6730	8.9481	21.7121
H	87	20.3103	16.4108	15.6486
H	88	19.2956	15.0807	14.8454
H	89	19.2351	7.4210	9.7224
H	90	17.6157	7.0855	8.8820
H	91	17.8236	7.2438	24.1027
H	92	25.4552	12.7292	21.9660
H	93	14.1495	7.8649	19.9465
H	94	26.3362	2.9469	21.9627
C	95	21.5166	5.8329	15.7423
O	96	21.2772	4.8401	15.1743
Rh	97	21.8816	7.2038	16.9643
C	98	24.4796	7.3689	15.5402
C	99	23.9367	6.5896	16.7361
H	100	23.9841	7.0779	14.6024
H	101	25.5642	7.1964	15.4071
H	102	24.0265	5.5072	16.5685
H	103	24.5221	6.8009	17.6420
H	104	24.3482	8.4583	15.6483
H	105	24.9834	11.8484	15.8821
H	106	24.2333	11.8079	15.9265

R1s (TS) Crosslinking mode 2

ATOM	X	Y	Z

P	1	22.356	7.704	19.248
C	2	23.399	6.259	19.830
C	3	20.890	7.520	20.404
C	4	23.284	9.099	20.022
C	5	23.174	9.478	21.373
C	6	24.028	10.448	21.886
C	7	25.003	11.083	21.096
C	8	25.051	10.750	19.727
C	9	24.226	9.757	19.215
C	10	20.531	6.291	20.993
C	11	19.422	6.195	21.840
C	12	18.648	7.320	22.160
C	13	19.014	8.545	21.581
C	14	20.104	8.640	20.714
C	15	23.215	4.978	19.261
C	16	24.002	3.894	19.642
C	17	25.029	4.039	20.593
C	18	25.183	5.305	21.186
C	19	24.389	6.389	20.813
C	20	17.453	7.176	23.079
C	21	25.927	12.041	21.721
C	22	25.936	2.953	20.985
C	23	16.148	6.754	22.361
C	24	25.950	1.690	20.522
C	25	27.033	12.572	21.171
H	26	22.453	8.969	22.019
H	27	23.951	10.698	22.941
H	28	25.753	11.247	19.060
H	29	24.326	9.466	18.162
H	30	21.123	5.386	20.811
H	31	19.164	5.228	22.278
H	32	18.439	9.445	21.804
H	33	20.348	9.622	20.283
H	34	22.464	4.841	18.483
H	35	23.862	2.938	19.139
H	36	25.972	5.446	21.928
H	37	24.574	7.353	21.289
H	38	17.281	8.112	23.631
H	39	15.505	6.241	23.093
H	40	16.404	5.992	21.609
H	41	26.666	0.960	20.900
H	42	25.260	1.338	19.756
H	43	27.369	12.324	20.163
H	44	27.645	13.281	21.728

P	45	19.882	8.794	16.544
C	46	19.962	10.634	16.401
C	47	18.471	8.545	17.695
C	48	19.098	8.266	14.937
C	49	19.903	7.987	13.817
C	50	19.357	7.550	12.620
C	51	17.965	7.353	12.489
C	52	17.163	7.640	13.608
C	53	17.707	8.095	14.806
C	54	18.178	7.226	18.087
C	55	17.054	6.948	18.860
C	56	16.209	7.978	19.303
C	57	16.518	9.293	18.925
C	58	17.623	9.575	18.121
C	59	20.773	11.363	17.289
C	60	20.889	12.747	17.167
C	61	20.285	13.435	16.098
C	62	19.437	12.706	15.242
C	63	19.283	11.330	15.388
C	64	15.026	7.716	20.205
C	65	17.336	6.867	11.255
C	66	20.532	14.874	15.948
C	67	15.348	7.905	21.704
C	68	20.149	15.671	14.934
C	69	17.959	6.365	10.173
H	70	20.993	8.081	13.891
H	71	20.016	7.377	11.768
H	72	16.082	7.511	13.531
H	73	17.046	8.290	15.656
H	74	18.831	6.410	17.767
H	75	16.833	5.914	19.128
H	76	15.871	10.108	19.256
H	77	17.812	10.612	17.824
H	78	21.346	10.843	18.055
H	79	21.549	13.288	17.847
H	80	18.932	13.207	14.415
H	81	18.659	10.786	14.683
H	82	14.639	6.699	20.037
H	83	16.242	6.909	11.252
H	84	21.064	15.331	16.783
H	85	14.399	8.039	22.247
H	86	15.886	8.859	21.823
H	87	20.359	16.740	14.963
H	88	19.620	15.294	14.057

H	89	19.043	6.271	10.105
H	90	17.392	6.018	9.310
H	91	17.696	6.415	23.836
H	92	25.665	12.320	22.748
H	93	14.212	8.408	19.934
H	94	26.668	3.228	21.750
C	95	21.514	6.090	16.151
O	96	21.155	4.987	15.941
Rh	97	22.073	7.712	16.888
C	98	24.517	6.809	15.120
C	99	24.115	6.995	16.592
H	100	23.826	6.139	14.592
H	101	25.503	6.323	15.083
H	102	24.176	6.038	17.144
H	103	24.788	7.705	17.096
H	104	24.580	7.765	14.544
H	105	22.657	9.095	15.482
H	106	22.915	9.490	16.145

R1s (FS) Crosslinking mode 2

ATOM		X	Y	Z
P	1	22.3203	7.6300	19.2680
C	2	23.4016	6.2211	19.8168
C	3	20.8859	7.4735	20.4252
C	4	23.2494	9.0609	19.9853
C	5	23.1905	9.4037	21.3471
C	6	24.0609	10.3545	21.8785
C	7	25.0357	10.9877	21.0844
C	8	25.0570	10.6724	19.7126
C	9	24.1787	9.7375	19.1766
C	10	20.5093	6.2376	20.9734
C	11	19.3971	6.1405	21.8095
C	12	18.6279	7.2624	22.1467
C	13	19.0071	8.4950	21.5945
C	14	20.1026	8.5965	20.7355
C	15	23.2267	4.9502	19.2396
C	16	24.0197	3.8693	19.6113
C	17	25.0400	4.0163	20.5705
C	18	25.2109	5.2881	21.1410
C	19	24.4137	6.3708	20.7747
C	20	17.4295	7.1048	23.0532
C	21	25.9827	11.9162	21.7113
C	22	25.9371	2.9299	20.9798
C	23	16.1248	6.7360	22.3073
C	24	25.9438	1.6637	20.5307
C	25	27.1082	12.4113	21.1674
H	26	22.4757	8.9093	22.0047
H	27	24.0045	10.5950	22.9418
H	28	25.7658	11.1699	19.0504
H	29	24.2079	9.5153	18.1107
H	30	21.0986	5.3439	20.7708
H	31	19.1345	5.1664	22.2289
H	32	18.4370	9.3947	21.8324
H	33	20.3596	9.5723	20.3205
H	34	22.4644	4.8083	18.4735
H	35	23.8547	2.9058	19.1301
H	36	25.9991	5.4346	21.8823
H	37	24.5954	7.3372	21.2397
H	38	17.2687	8.0234	23.6379
H	39	15.4631	6.2044	23.0080
H	40	16.3769	6.0050	21.5240
H	41	26.6695	0.9430	20.9060
H	42	25.2374	1.3023	19.7828
H	43	27.4342	12.1509	20.1596
H	44	27.7549	13.0771	21.7378
P	45	19.8723	8.7926	16.5159
C	46	19.9829	10.6213	16.3109
C	47	18.4592	8.5733	17.6781
C	48	19.0718	8.2386	14.9341
C	49	19.8643	7.9151	13.8189
C	50	19.2995	7.4466	12.6391
C	51	17.9075	7.2709	12.5194
C	52	17.1152	7.6288	13.6234
C	53	17.6794	8.1007	14.8085
C	54	18.1365	7.2616	18.0588
C	55	17.0119	7.0009	18.8392
C	56	16.1926	8.0443	19.2956
C	57	16.5368	9.3550	18.9344
C	58	17.6472	9.6229	18.1308
C	59	20.7775	11.3646	17.1980
C	60	20.9036	12.7444	17.0538
C	61	20.2713	13.4322	16.0013
C	62	19.4691	12.6810	15.1225
C	63	19.3258	11.3040	15.2747
C	64	15.0096	7.7953	20.1985
C	65	17.2676	6.7191	11.3206
C	66	20.4926	14.8753	15.8562
C	67	15.3535	7.9305	21.6978
C	68	20.1546	15.6474	14.8081

C	69	17.8775	6.1147	10.2851
H	70	20.9466	8.0157	13.8894
H	71	19.9528	7.2087	11.8001
H	72	16.0312	7.5153	13.5582
H	73	17.0261	8.3463	15.6443
H	74	18.7647	6.4335	17.7287
H	75	16.7664	5.9694	19.0956
H	76	15.9117	10.1844	19.2735
H	77	17.8737	10.6502	17.8453
H	78	21.3202	10.8553	17.9947
H	79	21.5314	13.3025	17.7507
H	80	18.9514	13.1776	14.3018
H	81	18.7035	10.7507	14.5719
H	82	14.5885	6.7958	20.0072
H	83	16.1768	6.7983	11.3032
H	84	21.0064	15.3466	16.6987
H	85	14.4165	8.0766	22.2561
H	86	15.9288	8.8590	21.8337
H	87	20.3748	16.7141	14.8058
H	88	19.6656	15.2443	13.9204
H	89	18.9582	5.9733	10.2445
H	90	17.3017	5.7271	9.4453
H	91	17.6536	6.3099	23.7808
H	92	25.7393	12.1932	22.7408
H	93	14.2185	8.5201	19.9517
H	94	26.6802	3.2168	21.7295
C	95	21.3617	5.9329	16.4185
O	96	21.0590	4.8844	16.0164
Rh	97	21.9680	7.7132	16.8713
C	98	24.3710	6.7498	15.0745
C	99	24.0277	7.0638	16.5280
H	100	23.7100	5.9786	14.6516
H	101	25.4083	6.3767	14.9872
H	102	24.1886	6.1736	17.1498
H	103	24.6997	7.8446	16.9065
H	104	24.2842	7.6395	14.4342
H	105	22.1490	8.0925	15.3514
H	106	22.6468	9.1630	16.8781

R2 (TS) Crosslinking mode 2

ATOM		X	Y	Z
P	1	22.630	7.808	19.355
C	2	23.473	6.208	19.703
C	3	21.303	7.869	20.640
C	4	23.829	9.050	20.026
C	5	23.854	9.422	21.379
C	6	24.789	10.344	21.843
C	7	25.738	10.924	20.980
C	8	25.705	10.546	19.625
C	9	24.764	9.636	19.155
C	10	21.129	6.890	21.626
C	11	20.093	6.996	22.555
C	12	19.214	8.088	22.551
C	13	19.415	9.083	21.584
C	14	20.428	8.968	20.634
C	15	22.776	5.002	19.477
C	16	23.387	3.771	19.684
C	17	24.728	3.687	20.111
C	18	25.417	4.893	20.323
C	19	24.807	6.132	20.127
C	20	18.049	8.114	23.512
C	21	26.704	11.885	21.527
C	22	25.424	2.416	20.342
C	23	16.775	7.457	22.922
C	24	24.932	1.174	20.192
C	25	27.670	12.544	20.862
H	26	23.134	8.994	22.076
H	27	24.788	10.627	22.897
H	28	26.420	10.972	18.921
H	29	24.735	9.375	18.096
H	30	21.806	6.039	21.680
H	31	19.975	6.214	23.308
H	32	18.756	9.952	21.554
H	33	20.532	9.743	19.873
H	34	21.742	5.030	19.133
H	35	22.813	2.862	19.505
H	36	26.456	4.859	20.657
H	37	25.374	7.043	20.311
H	38	17.822	9.147	23.820
H	39	16.199	7.007	23.745
H	40	17.092	6.618	22.284
H	41	25.551	0.300	20.393
H	42	23.907	0.979	19.873
H	43	27.832	12.424	19.790
H	44	28.333	13.233	21.384
P	45	19.797	8.793	16.488
C	46	19.709	10.613	16.210
C	47	18.438	8.519	17.709
C	48	19.111	8.119	14.920

C	49	19.855	8.302	13.737
C	50	19.392	7.813	12.523
C	51	18.178	7.102	12.438
C	52	17.457	6.903	13.629
C	53	17.910	7.405	14.849
C	54	18.291	7.255	18.306
C	55	17.297	7.032	19.262
C	56	16.435	8.059	19.671
C	57	16.590	9.317	19.072
C	58	17.568	9.547	18.105
C	59	20.536	11.444	16.979
C	60	20.472	12.829	16.846
C	61	19.589	13.436	15.934
C	62	18.777	12.594	15.151
C	63	18.834	11.210	15.286
C	64	15.393	7.872	20.749
C	65	17.644	6.565	11.183
C	66	19.554	14.900	15.846
C	67	15.851	8.407	22.126
C	68	18.785	15.659	15.043
C	69	18.149	6.709	9.945
H	70	20.807	8.832	13.776
H	71	19.989	7.977	11.625
H	72	16.516	6.350	13.592
H	73	17.319	7.242	15.749
H	74	18.962	6.446	18.017
H	75	17.200	6.039	19.703
H	76	15.925	10.135	19.360
H	77	17.649	10.537	17.658
H	78	21.243	11.002	17.685
H	79	21.119	13.459	17.459
H	80	18.083	13.023	14.428
H	81	18.190	10.584	14.669
H	82	15.118	6.809	20.837
H	83	16.722	5.987	11.296
H	84	20.243	15.412	16.525
H	85	14.959	8.631	22.730
H	86	16.353	9.374	21.964
H	87	18.856	16.745	15.077
H	88	18.073	15.237	14.332
H	89	19.060	7.274	9.744
H	90	17.655	6.256	9.086
H	91	18.339	7.573	24.426
H	92	26.607	12.064	22.602
H	93	14.479	8.408	20.451
H	94	26.462	2.520	20.668
C	95	21.653	6.346	16.629
O	96	20.650	5.658	16.627
Rh	97	21.950	8.236	17.115
C	98	22.893	5.445	14.619
C	99	22.996	5.784	16.109
H	100	22.053	4.762	14.434
H	101	23.821	4.966	14.277
H	102	23.179	4.876	16.702
H	103	23.830	6.469	16.299
H	104	22.737	6.351	14.019
C	105	23.115	9.072	15.743
O	106	23.679	9.105	14.719

R2 (FS) Crosslinking mode 2

ATOM		X	Y	Z
P	1	22.4248	7.7942	19.5120
C	2	23.4532	6.3830	20.1003
C	3	21.0003	7.7903	20.6798
C	4	23.4042	9.2632	20.0437
C	5	23.0874	10.0386	21.1688
C	6	23.8663	11.1444	21.5085
C	7	24.9898	11.5163	20.7497
C	8	25.3012	10.7302	19.6222
C	9	24.5244	9.6333	19.2736
C	10	20.8162	6.7846	21.6391
C	11	19.6859	6.7849	22.4573
C	12	18.7113	7.7880	22.3621
C	13	18.9130	8.8044	21.4158
C	14	20.0269	8.7991	20.5780
C	15	23.2621	5.1218	19.5072
C	16	24.0264	4.0268	19.8894
C	17	25.0286	4.1522	20.8719
C	18	25.2087	5.4161	21.4617
C	19	24.4362	6.5154	21.0899
C	20	17.4647	7.7127	23.2138
C	21	25.7768	12.6853	21.1552
C	22	25.8930	3.0429	21.2883
C	23	16.2956	6.9740	22.5138
C	24	25.8766	1.7784	20.8328
C	25	26.8775	13.1785	20.5616
H	26	22.2294	9.7797	21.7881
H	27	23.6053	11.7311	22.3915
H	28	26.1637	10.9781	19.0040

H	29	24.7910	9.0558	18.3897
H	30	21.5568	5.9925	21.7464
H	31	19.5636	5.9858	23.1919
H	32	18.1829	9.6093	21.3216
H	33	20.1338	9.5916	19.8358
H	34	22.5105	5.0108	18.7223
H	35	23.8545	3.0678	19.4014
H	36	25.9797	5.5361	22.2255
H	37	24.6081	7.4803	21.5665
H	38	17.1389	8.7212	23.5114
H	39	15.6845	6.4785	23.2833
H	40	16.7245	6.1638	21.9050
H	41	26.5823	1.0401	21.2118
H	42	25.1712	1.4354	20.0751
H	43	27.3199	12.7311	19.6712
H	44	27.3784	14.0564	20.9685
P	45	19.9422	8.4339	16.5824
C	46	20.1139	10.2708	16.5516
C	47	18.4374	8.1295	17.6124
C	48	19.3156	8.1134	14.8787
C	49	20.0335	8.6314	13.7821
C	50	19.6211	8.3919	12.4784
C	51	18.4845	7.6029	12.2053
C	52	17.7822	7.0787	13.3052
C	53	18.1831	7.3305	14.6181
C	54	18.2847	6.8586	18.1869
C	55	17.1808	6.5686	18.9921
C	56	16.2130	7.5430	19.2704
C	57	16.3686	8.8078	18.6830
C	58	17.4580	9.1016	17.8656
C	59	21.1471	10.8891	17.2696
C	60	21.3014	12.2740	17.2499
C	61	20.4436	13.0976	16.4985
C	62	19.4145	12.4694	15.7691
C	63	19.2556	11.0895	15.7906
C	64	15.0770	7.3011	20.2342
C	65	18.0137	7.3081	10.8485
C	66	20.6577	14.5487	16.5012
C	67	15.3760	7.8613	21.6441
C	68	19.9273	15.4836	15.8690
C	69	18.6055	7.6411	9.6886
H	70	20.9261	9.2332	13.9582
H	71	20.1893	8.8292	11.6570
H	72	16.8951	6.4682	13.1269
H	73	17.6046	6.9155	15.4433
H	74	19.0388	6.0912	18.0020
H	75	17.0850	5.5709	19.4241
H	76	15.6250	9.5845	18.8794
H	77	17.5465	10.0992	17.4369
H	78	21.8492	10.2771	17.8368
H	79	22.1195	12.7274	17.8126
H	80	18.7366	13.0688	15.1614
H	81	18.4628	10.6378	15.1940
H	82	14.8525	6.2257	20.3029
H	83	17.0752	6.7476	10.8028
H	84	21.5147	14.8799	17.0944
H	85	14.4233	8.0181	22.1725
H	86	15.8183	8.8623	21.5246
H	87	20.1886	16.5386	15.9460
H	88	19.0548	15.2415	15.2610
H	89	19.5480	8.1885	9.6429
H	90	18.1564	7.3652	8.7351
H	91	17.7123	7.1788	24.1433
H	92	25.4029	13.1947	22.0484
H	93	14.1703	7.7879	19.8430
H	94	26.6334	3.3076	22.0490
C	95	21.6164	5.7385	15.9942
O	96	20.7312	5.0754	16.5288
Rh	97	21.9852	7.3350	17.1548
C	98	22.5270	6.1121	13.6217
C	99	22.4295	5.1881	14.8341
H	100	21.5534	6.2209	13.1283
H	101	23.2402	5.7047	12.8923
H	102	21.9997	4.2133	14.5584
H	103	23.4367	5.0078	15.2433
H	104	22.8724	7.1121	13.9149
C	105	23.7436	7.5078	16.5560
O	106	24.7992	7.7873	16.1281

R3 (IS) Crosslinking mode 2

ATOM		X	Y	Z
P	1	22.3728	7.7347	19.5130
C	2	23.4043	6.3409	20.1367
C	3	20.9590	7.7613	20.6941
C	4	23.3660	9.2093	20.0044
C	5	23.0570	10.0117	21.1126
C	6	23.8478	11.1153	21.4315
C	7	24.9785	11.4564	20.6685
C	8	25.2833	10.6421	19.5589

C	9	24.4938	9.5477	19.2304
C	10	20.7768	6.7649	21.6634
C	11	19.6534	6.7779	22.4909
C	12	18.6852	7.7872	22.3977
C	13	18.8865	8.7963	21.4442
C	14	19.9925	8.7771	20.5958
C	15	23.2224	5.0677	19.5682
C	16	23.9926	3.9851	19.9741
C	17	24.9895	4.1355	20.9582
C	18	25.1598	5.4115	21.5248
C	19	24.3828	6.4988	21.1270
C	20	17.4458	7.7267	23.2603
C	21	25.7787	12.6235	21.0521
C	22	25.8598	3.0387	21.3968
C	23	16.2692	6.9879	22.5730
C	24	25.8536	1.7691	20.9553
C	25	26.8881	13.0900	20.4531
H	26	22.1937	9.7760	21.7337
H	27	23.5916	11.7243	22.3006
H	28	26.1521	10.8666	18.9406
H	29	24.7560	8.9461	18.3614
H	30	21.5132	5.9691	21.7711
H	31	19.5331	5.9850	23.2324
H	32	18.1630	9.6073	21.3517
H	33	20.0955	9.5648	19.8485
H	34	22.4772	4.9397	18.7798
H	35	23.8299	3.0161	19.5034
H	36	25.9270	5.5524	22.2889
H	37	24.5470	7.4740	21.5849
H	38	17.1272	8.7394	23.5512
H	39	15.6593	6.5019	23.3494
H	40	16.6920	6.1708	21.9690
H	41	26.5637	1.0399	21.3437
H	42	25.1522	1.4136	20.1997
H	43	27.3304	12.6168	19.5758
H	44	27.4002	13.9691	20.8433
P	45	19.8765	8.3806	16.5984
C	46	20.0297	10.2195	16.5911
C	47	18.3762	8.0798	17.6386
C	48	19.2471	8.0708	14.8935
C	49	19.9747	8.5719	13.7954
C	50	19.5464	8.3546	12.4929
C	51	18.3855	7.6004	12.2221
C	52	17.6788	7.0851	13.3231
C	53	18.0946	7.3177	14.6348
C	54	18.2205	6.8144	18.2238
C	55	17.1223	6.5388	19.0423
C	56	16.1626	7.5208	19.3207
C	57	16.3202	8.7796	18.7208
C	58	17.4035	9.0592	17.8906
C	59	20.9769	10.8423	17.4162
C	60	21.0768	12.2318	17.4680
C	61	20.2510	13.0554	16.6831
C	62	19.3134	12.4230	15.8407
C	63	19.2046	11.0383	15.7954
C	64	15.0354	7.2964	20.2994
C	65	17.8915	7.3377	10.8667
C	66	20.4044	14.5120	16.7561
C	67	15.3507	7.8724	21.6996
C	68	19.7529	15.4361	16.0288
C	69	18.4693	7.6843	9.7035
H	70	20.8835	9.1496	13.9697
H	71	20.1219	8.7809	11.6709
H	72	16.7769	6.4961	13.1467
H	73	17.5115	6.9116	15.4610
H	74	18.9642	6.0390	18.0323
H	75	17.0246	5.5455	19.4841
H	76	15.5823	9.5621	18.9153
H	77	17.4928	10.0514	17.4498
H	78	21.6570	10.2326	18.0108
H	79	21.8247	12.6879	18.1190
H	80	18.6584	13.0236	15.2099
H	81	18.4758	10.5859	15.1226
H	82	14.8065	6.2230	20.3837
H	83	16.9438	6.7928	10.8254
H	84	21.1399	14.8571	17.4878
H	85	14.4040	8.0448	22.2340
H	86	15.8015	8.8673	21.5631
H	87	19.9458	16.4986	16.1740
H	88	19.0081	15.1719	15.2768
H	89	19.4167	8.2224	9.6518
H	90	17.9985	7.4355	8.7528
H	91	17.6976	7.1998	24.1927
H	92	25.4086	13.1569	21.9329
H	93	14.1273	7.7828	19.9111
H	94	26.5971	3.3193	22.1544
C	95	21.4461	5.6628	15.9796
O	96	20.5014	5.0461	16.4655

Rh	97	21.9002	7.2223	17.1732
C	98	22.5153	6.0279	13.6659
C	99	22.2598	5.0787	14.8348
H	100	21.5878	6.2401	13.1195
H	101	23.2325	5.5803	12.9641
H	102	21.7534	4.1604	14.5012
H	103	23.2217	4.7838	15.2856
H	104	22.9306	6.9828	14.0142
C	105	23.6910	7.2070	16.6527
O	106	24.7936	7.3347	16.2766
H	107	24.0966	10.5241	16.2725
H	108	23.6352	10.3477	15.7067

R3 (TS) Crosslinking mode 2

ATOM		X	Y	Z
P	1	22.604	7.814	19.243
C	2	23.499	6.204	19.375
C	3	21.363	7.638	20.606
C	4	23.814	9.011	19.961
C	5	23.667	9.581	21.233
C	6	24.599	10.503	21.710
C	7	25.716	10.882	20.947
C	8	25.860	10.300	19.672
C	9	24.927	9.394	19.186
C	10	21.326	6.535	21.471
C	11	20.315	6.413	22.425
C	12	19.322	7.391	22.570
C	13	19.391	8.518	21.737
C	14	20.378	8.627	20.758
C	15	22.851	5.032	18.930
C	16	23.462	3.789	19.043
C	17	24.753	3.654	19.591
C	18	25.392	4.827	20.029
C	19	24.780	6.077	19.927
C	20	18.180	7.161	23.531
C	21	26.669	11.851	21.501
C	22	25.444	2.368	19.723
C	23	16.949	6.516	22.845
C	24	25.020	1.165	19.294
C	25	27.768	12.347	20.908
H	26	22.821	9.303	21.861
H	27	24.461	10.938	22.701
H	28	26.713	10.560	19.046
H	29	25.052	8.975	18.186
H	30	22.088	5.760	21.405
H	31	20.298	5.534	23.072
H	32	18.642	9.306	21.822
H	33	20.371	9.486	20.087
H	34	21.849	5.091	18.507
H	35	22.920	2.907	18.700
H	36	26.390	4.758	20.465
H	37	25.305	6.957	20.298
H	38	17.882	8.104	24.015
H	39	16.424	5.888	23.581
H	40	17.316	5.825	22.071
H	41	25.624	0.272	19.453
H	42	24.071	1.026	18.775
H	43	28.073	12.062	19.901
H	44	28.402	13.066	21.425
P	45	19.676	9.034	16.679
C	46	19.385	10.858	16.602
C	47	18.350	8.494	17.855
C	48	19.009	8.459	15.055
C	49	19.837	8.536	13.921
C	50	19.394	8.099	12.680
C	51	18.109	7.545	12.517
C	52	17.288	7.472	13.656
C	53	17.726	7.921	14.902
C	54	18.334	7.156	18.281
C	55	17.380	6.708	19.197
C	56	16.429	7.584	19.740
C	57	16.444	8.916	19.301
C	58	17.379	9.368	18.369
C	59	19.775	11.656	17.691
C	60	19.583	13.035	17.674
C	61	18.993	13.679	16.570
C	62	18.615	12.876	15.479
C	63	18.801	11.497	15.495
C	64	15.451	7.162	20.810
C	65	17.608	7.044	11.233
C	66	18.809	15.134	16.601
C	67	15.938	7.512	22.235
C	68	18.166	15.894	15.698
C	69	18.263	7.006	10.060
H	70	20.848	8.935	14.028
H	71	20.066	8.178	11.825
H	72	16.287	7.046	13.564
H	73	17.062	7.841	15.761
H	74	19.078	6.462	17.890

H	75	17.388	5.661	19.505
H	76	15.701	9.618	19.689
H	77	17.347	10.407	18.042
H	78	20.238	11.197	18.563
H	79	19.892	13.631	18.535
H	80	18.165	13.334	14.598
H	81	18.490	10.908	14.633
H	82	15.248	6.082	20.741
H	83	16.584	6.659	11.261
H	84	19.250	15.630	17.470
H	85	15.064	7.586	22.900
H	86	16.372	8.523	22.203
H	87	18.093	16.974	15.826
H	88	17.691	15.472	14.812
H	89	19.287	7.365	9.947
H	90	17.787	6.598	9.169
H	91	18.530	6.495	24.333
H	92	26.430	12.191	22.513
H	93	14.492	7.673	20.631
H	94	26.415	2.423	20.223
C	95	21.869	6.637	16.238
O	96	20.818	6.039	16.408
Rh	97	22.022	8.462	16.993
C	98	22.853	6.070	13.974
C	99	23.021	5.960	15.495
H	100	21.894	5.644	13.653
H	101	23.665	5.527	13.472
H	102	22.995	4.902	15.794
H	103	23.978	6.384	15.813
H	104	22.894	7.116	13.643
C	105	23.418	8.936	15.809
O	106	24.282	9.370	15.148
H	107	22.881	10.768	17.897
H	108	22.411	11.124	17.422

R3 (FS) Crosslinking mode 2

R4 (IS) Crosslinking mode 2

ATOM		X	Y	Z
P	1	22.4241	7.6427	19.3821
C	2	23.5455	6.3116	20.0134
C	3	20.9811	7.5417	20.5238
C	4	23.3008	9.1645	19.9629
C	5	23.1103	9.7302	21.2343
C	6	23.8469	10.8461	21.6308
C	7	24.8103	11.4362	20.7906
C	8	25.0042	10.8544	19.5232
C	9	24.2648	9.7496	19.1210
C	10	20.6892	6.3737	21.2423
C	11	19.5664	6.3134	22.0673
C	12	18.7048	7.4093	22.2200
C	13	19.0061	8.5765	21.5031
C	14	20.1125	8.6386	20.6563
C	15	23.4359	5.0062	19.4980
C	16	24.2771	3.9903	19.9382
C	17	25.2698	4.2295	20.9074
C	18	25.3671	5.5345	21.4220
C	19	24.5241	6.5560	20.9883
C	20	17.4851	7.2865	23.1034
C	21	25.5505	12.6095	21.2626
C	22	26.1990	3.1992	21.3824
C	23	16.2360	6.7529	22.3618
C	24	26.2819	1.9225	20.9677
C	25	26.5209	13.2765	20.6094
H	26	22.3824	9.3025	21.9232
H	27	23.6761	11.2734	22.6208
H	28	25.7376	11.2707	18.8329
H	29	24.4210	9.3404	18.1248
H	30	21.3456	5.5079	21.1679
H	31	19.3655	5.3934	22.6205
H	32	18.3657	9.4542	21.6023
H	33	20.3033	9.5599	20.1051
H	34	22.6766	4.7791	18.7525
H	35	24.1590	2.9935	19.5135
H	36	26.1292	5.7571	22.1716
H	37	24.6434	7.5539	21.4075
H	38	17.2482	8.2563	23.5683
H	39	15.5771	6.2678	23.0980
H	40	16.5606	5.9540	21.6785
H	41	27.0217	1.2430	21.3897
H	42	25.6257	1.5129	20.1987
H	43	26.8587	12.9918	19.6121
H	44	27.0076	14.1387	21.0630
P	45	20.0451	8.6791	16.5526
C	46	20.1437	10.5246	16.5342
C	47	18.5805	8.3546	17.6252
C	48	19.3932	8.3351	14.8623
C	49	20.1740	8.6990	13.7483
C	50	19.7440	8.4298	12.4571
C	51	18.5191	7.7714	12.2188

C	52	17.7407	7.4282	13.3363
C	53	18.1639	7.7061	14.6380
C	54	18.4043	7.0723	18.1666
C	55	17.2743	6.7749	18.9308
C	56	16.3031	7.7473	19.2030
C	57	16.4919	9.0281	18.6612
C	58	17.6073	9.3341	17.8833
C	59	21.0180	11.1956	17.4012
C	60	21.0875	12.5868	17.4074
C	61	20.2957	13.3670	16.5440
C	62	19.4139	12.6863	15.6820
C	63	19.3356	11.2975	15.6796
C	64	15.1267	7.4786	20.1092
C	65	18.0395	7.4359	10.8746
C	66	20.4353	14.8269	16.5638
C	67	15.4218	7.8177	21.5887
C	68	19.7927	15.7169	15.7880
C	69	18.7109	7.5691	9.7175
H	70	21.1298	9.2019	13.8999
H	71	20.3710	8.7342	11.6194
H	72	16.7856	6.9225	13.1835
H	73	17.5318	7.4250	15.4794
H	74	19.1567	6.2996	18.0071
H	75	17.1622	5.7656	19.3302
H	76	15.7502	9.8066	18.8559
H	77	17.7156	10.3413	17.4829
H	78	21.6755	10.6226	18.0543
H	79	21.7850	13.0824	18.0855
H	80	18.7806	13.2510	14.9979
H	81	18.6498	10.8073	14.9882
H	82	14.8117	6.4264	20.0310
H	83	17.0269	7.0241	10.8404
H	84	21.1523	15.2048	17.2977
H	85	14.4631	7.9767	22.1053
H	86	15.9402	8.7884	21.6195
H	87	19.9778	16.7858	15.8900
H	88	19.0657	15.4180	15.0317
H	89	19.7304	7.9546	9.6733
H	90	18.2559	7.2821	8.7704
H	91	17.7257	6.5984	23.9276
H	92	25.2683	12.9552	22.2611
H	93	14.2741	8.0879	19.7723
H	94	26.8998	3.5371	22.1511
C	95	21.3842	5.5467	16.6869
O	96	20.6419	4.9721	17.4809
Rh	97	22.1423	7.5787	16.9240
C	98	20.9812	5.0634	14.2234
C	99	21.8322	4.7420	15.4569
H	100	19.9196	4.8546	14.4134
H	101	21.3027	4.4497	13.3704
H	102	21.7356	3.6741	15.7098
H	103	22.8868	4.9659	15.2434
H	104	21.0721	6.1191	13.9392
C	105	23.9289	7.0440	16.6734
O	106	25.0428	6.8069	16.4471
H	107	22.6992	9.1075	16.8424
H	108	22.1269	7.6539	15.3430

R4 (TS) Crosslinking mode 2

ATOM		X	Y	Z
P	1	22.606	7.826	19.064
C	2	23.823	6.484	19.437
C	3	21.355	7.607	20.407
C	4	23.527	9.327	19.633
C	5	23.380	9.883	20.912
C	6	24.117	11.007	21.285
C	7	25.040	11.609	20.411
C	8	25.191	11.038	19.133
C	9	24.444	9.930	18.751
C	10	21.327	6.484	21.245
C	11	20.338	6.349	22.218
C	12	19.353	7.327	22.405
C	13	19.398	8.460	21.580
C	14	20.368	8.590	20.587
C	15	23.494	5.151	19.124
C	16	24.376	4.110	19.386
C	17	25.639	4.351	19.962
C	18	25.964	5.683	20.265
C	19	25.077	6.730	20.014
C	20	18.280	7.121	23.448
C	21	25.787	12.786	20.868
C	22	26.607	3.289	20.258
C	23	17.038	6.352	22.931
C	24	26.475	1.972	20.020
C	25	26.752	13.450	20.206
H	26	22.685	9.442	21.625
H	27	23.981	11.428	22.283
H	28	25.895	11.467	18.420
H	29	24.574	9.523	17.750

H	30	22.090	5.712	21.159
H	31	20.344	5.466	22.861
H	32	18.657	9.252	21.702
H	33	20.356	9.476	19.951
H	34	22.527	4.920	18.679
H	35	24.077	3.093	19.133
H	36	26.933	5.905	20.716
H	37	25.368	7.745	20.278
H	38	17.959	8.090	23.862
H	39	16.595	5.811	23.780
H	40	17.380	5.580	22.226
H	41	27.269	1.277	20.291
H	42	25.587	1.541	19.556
H	43	27.085	13.161	19.208
H	44	27.243	14.312	20.656
P	45	19.682	8.737	16.663
C	46	19.492	10.579	16.695
C	47	18.410	8.204	17.894
C	48	18.875	8.326	15.053
C	49	19.575	8.617	13.867
C	50	19.007	8.372	12.623
C	51	17.723	7.801	12.509
C	52	17.037	7.504	13.699
C	53	17.599	7.761	14.951
C	54	18.406	6.860	18.300
C	55	17.463	6.404	19.224
C	56	16.517	7.273	19.785
C	57	16.528	8.612	19.368
C	58	17.456	9.077	18.438
C	59	20.334	11.369	17.486
C	60	20.159	12.750	17.558
C	61	19.142	13.400	16.835
C	62	18.305	12.602	16.034
C	63	18.471	11.222	15.971
C	64	15.535	6.821	20.839
C	65	17.081	7.504	11.224
C	66	19.015	14.859	16.929
C	67	15.938	7.222	22.276
C	68	18.133	15.644	16.289
C	69	17.594	7.673	9.993
H	70	20.579	9.039	13.929
H	71	19.575	8.617	11.726
H	72	16.042	7.058	13.641
H	73	17.034	7.525	15.853
H	74	19.145	6.168	17.894
H	75	17.475	5.354	19.522
H	76	15.792	9.309	19.776
H	77	17.433	10.124	18.139
H	78	21.160	10.905	18.027
H	79	20.830	13.344	18.180
H	80	17.507	13.062	15.452
H	81	17.806	10.634	15.338
H	82	15.400	5.730	20.787
H	83	16.071	7.093	11.305
H	84	19.730	15.334	17.607
H	85	15.035	7.186	22.904
H	86	16.251	8.278	22.263
H	87	18.135	16.722	16.442
H	88	17.391	15.253	15.591
H	89	18.595	8.073	9.822
H	90	17.014	7.417	9.107
H	91	18.721	6.558	24.284
H	92	25.514	13.135	21.868
H	93	14.554	7.269	20.617
H	94	27.534	3.636	20.722
C	95	21.647	5.746	16.440
O	96	20.677	5.120	16.845
Rh	97	21.922	7.958	16.717
C	98	22.607	4.957	14.249
C	99	22.798	4.995	15.771
H	100	21.679	4.430	13.986
H	101	23.449	4.435	13.774
H	102	22.800	3.969	16.168
H	103	23.755	5.472	16.021
H	104	22.559	5.969	13.823
C	105	23.532	8.162	15.759
O	106	24.511	8.327	15.147
H	107	22.199	9.543	16.859
H	108	21.367	7.027	15.507

R4 (FS) Crosslinking mode 2

ATOM		X	Y	Z
P	1	22.4414	7.7680	19.3956
C	2	23.4656	6.3530	19.9802
C	3	20.9987	7.7208	20.5454
C	4	23.3739	9.2485	19.9859
C	5	23.2105	9.8237	21.2553
C	6	23.9505	10.9465	21.6219
C	7	24.8846	11.5340	20.7478

C	8	25.0459	10.9470	19.4772
C	9	24.3029	9.8335	19.1037
C	10	20.6908	6.5872	21.3114
C	11	19.5545	6.5648	22.1198
C	12	18.6918	7.6667	22.2032
C	13	19.0098	8.8009	21.4434
C	14	20.1343	8.8252	20.6190
C	15	23.2916	5.0994	19.3644
C	16	24.0531	4.0030	19.7530
C	17	25.0329	4.1201	20.7581
C	18	25.2014	5.3793	21.3616
C	19	24.4319	6.4788	20.9872
C	20	17.4662	7.5989	23.0836
C	21	25.6288	12.7150	21.1959
C	22	25.8906	3.0092	21.1856
C	23	16.2702	6.8348	22.4663
C	24	25.8751	1.7438	20.7336
C	25	26.5923	13.3784	20.5302
H	26	22.4943	9.4017	21.9605
H	27	23.8055	11.3832	22.6119
H	28	25.7558	11.3686	18.7654
H	29	24.4217	9.4081	18.1051
H	30	21.3489	5.7191	21.2876
H	31	19.3446	5.6711	22.7116
H	32	18.3653	9.6804	21.4917
H	33	20.3389	9.7226	20.0337
H	34	22.5697	4.9830	18.5531
H	35	23.8963	3.0535	19.2426
H	36	25.9595	5.4948	22.1390
H	37	24.5963	7.4393	21.4745
H	38	17.1447	8.6133	23.3648
H	39	15.6477	6.4661	23.2954
H	40	16.6555	5.9355	21.9604
H	41	26.5764	1.0053	21.1208
H	42	25.1743	1.4011	19.9716
H	43	26.9312	13.0820	19.5368
H	44	27.0797	14.2446	20.9760
P	45	20.1321	8.7493	16.5345
C	46	20.1479	10.5898	16.5177
C	47	18.7009	8.3195	17.6077
C	48	19.4818	8.3298	14.8560
C	49	20.2654	8.6310	13.7258
C	50	19.8199	8.3359	12.4459
C	51	18.5745	7.7069	12.2336
C	52	17.8017	7.4033	13.3667
C	53	18.2385	7.7163	14.6560
C	54	18.6208	7.0176	18.1247
C	55	17.5253	6.6269	18.8967
C	56	16.4906	7.5247	19.1927
C	57	16.5856	8.8280	18.6810
C	58	17.6689	9.2233	17.8990
C	59	21.0325	11.2524	17.3833
C	60	21.0606	12.6431	17.4459
C	61	20.2198	13.4289	16.6364
C	62	19.3530	12.7558	15.7512
C	63	19.3168	11.3667	15.6905
C	64	15.3049	7.1391	20.0441
C	65	18.0684	7.3618	10.9015
C	66	20.2834	14.8902	16.7423
C	67	15.3706	7.6472	21.5021
C	68	19.5298	15.7888	16.0855
C	69	18.6916	7.5351	9.7223
H	70	21.2417	9.0977	13.8593
H	71	20.4510	8.5940	11.5959
H	72	16.8350	6.9138	13.2355
H	73	17.6045	7.4751	15.5081
H	74	19.4261	6.3078	17.9239
H	75	17.4832	5.6062	19.2811
H	76	15.7911	9.5466	18.8955
H	77	17.7074	10.2431	17.5160
H	78	21.7145	10.6689	18.0033
H	79	21.7574	13.1332	18.1286
H	80	18.6988	13.3307	15.0957
H	81	18.6408	10.8791	14.9866
H	82	15.1813	6.0455	20.0448
H	83	17.0704	6.9140	10.8949
H	84	21.0279	15.2615	17.4519
H	85	14.3437	7.6497	21.8967
H	86	15.6873	8.7020	21.4908
H	87	19.6631	16.8578	16.2503
H	88	18.7634	15.4979	15.3660
H	89	19.6883	7.9708	9.6435
H	90	18.2130	7.2398	8.7893
H	91	17.7462	7.0937	24.0213
H	92	25.3530	13.0714	22.1928
H	93	14.3983	7.5547	19.5775
H	94	26.6237	3.2740	21.9534
C	95	21.4744	4.2226	15.3978

O	96	21.7336	3.6403	16.4400
Rh	97	22.2489	7.8328	17.0112
C	98	20.3644	3.3142	13.3366
C	99	21.6996	3.6479	14.0226
H	100	19.8444	2.5053	13.8677
H	101	20.5371	2.9846	12.3032
H	102	22.3329	2.7550	14.1120
H	103	22.2352	4.4042	13.4256
H	104	19.6975	4.1878	13.3007
C	105	23.8717	6.9644	16.6520
O	106	24.8424	6.4259	16.3020
H	107	22.2974	7.9726	15.4130
H	108	21.0248	5.2461	15.4193