Supporting Information

for

A Crossed Beam and *Ab Initio* Investigation on the Formation of Boronyldiacetylene ($HCCCC^{11}BO$; $X^1\Sigma^+$) via the Reaction of the Boron Monoxide Radical (^{11}BO; $X^2\Sigma^+$) with Diacetylene (C_4H_2; $X^1\Sigma_g^+$)

by

Dorian S. N. Parker[1], Nadia Balucani[2], Domenico Stranges[3], Ralf. I. Kaiser[1]*

[1]Department of Chemistry, University of Hawaii at Manoa, Honolulu, HI 96822, USA

[2] Permanent Address: Dipartimento di Chimica, University of Perugia, Perugia, Italy

[3] Permanent Address Dipartimento di Chimica, Università La Sapienza, Rome, Italy

Alexander Mebel*

Department of Chemistry and Biochemistry, Florida International University, Miami, USA

Table S1. Optimized Cartesian coordinates, rotational constants, and vibrational frequencies of various intermediates and products involved in the reactions.

Species	Rotational Constants, GHz	Cartesian Coordinates, Å				Vibrational Frequencies, cm^{-1}		
		Atom	x	y	z			
i1	16.57233	6	-1.124022	0.087290	0.000000	40.6	515.5	1250.0
	1.54418	6	0.000000	0.770285	0.000000	224.6	542.3	1781.5
	1.41256	6	1.166190	1.373584	0.000000	225.3	676.6	2006.0
		6	2.247699	1.963648	0.000000	282.4	715.5	2028.9
		5	-1.132622	-1.429929	0.000000	374.2	804.1	3059.4
		8	-1.148415	-2.635169	0.000000	379.4	965.5	3461.3
		1	-2.082082	0.613037	0.000000			
		1	3.193312	2.449111	0.000000			
i2	6.84711	6	-0.315347	1.789591	0.000000	114.2	605.7	1138.5
	2.55610	6	0.000000	0.501435	0.000000	209.0	674.9	1595.1
	1.86127	6	1.333557	-0.009401	0.000000	225.0	694.8	2028.8
		6	2.433633	-0.495280	0.000000	364.3	711.6	2211.7
		5	-1.174560	-0.484448	0.000000	456.6	714.2	3238.1
		8	-2.127846	-1.219336	0.000000	549.1	835.9	3474.4
		1	-1.227322	2.369692	0.000000			
		1	3.411835	-0.910830	0.000000			
i2t	6.78302	6	-0.121724	1.815243	0.000000	115.0	601.8	1131.8
	2.55307	6	0.000000	0.494830	0.000000	206.5	667.3	1588.2
	1.85490	6	1.271790	-0.164339	0.000000	220.8	678.9	2039.4
		6	2.326806	-0.742728	0.000000	359.8	692.5	2202.6
		5	-1.276974	-0.351540	0.000000	448.2	735.4	3232.1
		8	-2.282828	-1.011464	0.000000	550.9	853.6	3471.9
		1	0.525535	2.681478	0.000000			
		1	3.260729	-1.250108	0.000000			
i3	13.16882	6	-0.033161	1.538913	0.000000	8.1	687.8	1127.7
	2.82997	6	0.000000	0.199894	0.000000	172.5	706.4	1200.9
	2.32939	6	0.954724	-0.833032	0.000000	267.8	767.5	1610.5
		6	1.766244	-1.722709	0.000000	520.2	781.8	2205.5
		5	-1.588790	1.244887	0.000000	574.2	834.6	3289.6
		8	-1.426236	-0.137758	0.000000	648.4	1000.1	3471.1
		1	0.741156	2.284703	0.000000			
		1	2.485838	-2.505480	0.000000			
i4	22.55722	6	0.000000	0.634391	0.000000	39.3	509.5	1280.9
	1.41133	6	-1.062221	-0.140460	0.000000	179.7	688.7	1736.0
	1.32822	6	-1.033485	-1.561530	0.000000	232.8	689.2	2017.8
		6	-1.049918	-2.765104	0.000000	329.5	758.3	2204.3
		5	1.115327	1.563496	0.000000	406.4	829.8	3037.7
		8	2.050484	2.336055	0.000000	497.7	1011.6	3471.8
		1	-2.056689	0.318480	0.000000			
		1	-1.050074	-3.828174	0.000000			

i5	21.91036	6	0.924297	0.771583	0.014791	167.7	629.1	1136.3
	2.25161	6	-0.088599	-0.107611	-0.100741	179.1	676.4	1266.0
	2.04913	6	-1.479024	-0.035343	-0.022049	215.2	732.6	1624.9
		6	-2.684333	-0.012991	0.015428	482.8	832.1	2201.1
		8	2.105502	-0.034730	-0.056420	512.7	892.1	3155.7
		5	1.165739	-1.048786	0.131402	595.1	1085.4	3476.7
		1	1.038765	1.815426	0.295088			
		1	-3.745521	0.012511	0.054690			
i6	8.64423	6	-0.171516	1.676698	0.000000	47.2	608.5	1112.0
	2.81405	6	0.000000	0.374020	0.000000	116.3	647.7	1432.4
	2.12294	6	-1.055957	-0.574798	0.000000	188.9	660.5	1638.5
		6	-1.970793	-1.356520	0.000000	279.7	715.3	2206.9
		5	2.540568	0.110324	0.000000	426.7	730.4	3293.6
		8	1.282015	-0.198109	0.000000	533.3	803.1	3472.4
		1	-0.995043	2.369374	0.000000			
		1	-2.774325	-2.052518	0.000000			
i7	52.35541	6	0.000000	0.593691	0.000000	96.6	541.2	1259.3
	1.27884	6	0.317548	-0.576288	0.000000	120.4	619.5	1633.8
	1.24835	6	0.735086	-1.932175	0.000000	250.4	686.2	2018.5
		6	-0.083672	-2.965785	0.000000	361.1	843.0	2306.6
		5	-0.391484	2.008722	0.000000	487.9	862.1	3035.6
		8	-0.709868	3.172684	0.000000	517.5	1124.9	3251.8
		1	1.817539	-2.100094	0.000000			
		1	0.005053	-4.041640	0.000000			
i7t	39.42412	6	0.000000	0.569487	0.000000	96.2	539.3	1261.6
	1.31587	6	0.424360	-0.566939	0.000000	121.5	632.5	1615.3
	1.27337	6	0.932032	-1.894557	0.000000	239.3	719.0	2017.3
		6	0.150978	-2.958011	0.000000	371.4	869.8	2298.3
		5	-0.518539	1.942862	0.000000	478.5	885.9	3103.3
		8	-0.945217	3.071622	0.000000	519.1	1118.7	3246.7
		1	2.016244	-2.007152	0.000000			
		1	-0.906037	-3.180011	0.000000			
i8	15.62276	6	-1.163916	0.001913	0.000000	23.7	501.1	1304.6
	1.81701	6	0.000000	0.586325	0.000000	85.9	510.8	1474.4
	1.62770	6	1.172949	1.184613	0.000000	125.5	627.4	1812.9
		6	2.264686	1.749823	0.000000	215.8	789.1	2017.9
		8	-1.341661	-1.384377	0.000000	366.2	832.8	3185.5
		5	-0.800353	-2.560387	0.000000	433.5	994.6	3462.5
		1	-2.119950	0.510600	0.000000			
		1	3.212691	2.230305	0.000000			
i9	51.18626	6	-0.370259	-0.605409	0.000000	113.8	492.3	1163.8
	1.45812	6	0.000000	0.541076	0.000000	154.5	546.3	1352.4
	1.41773	6	0.432980	1.834445	0.000000	223.0	647.3	2183.4
		6	0.816583	2.978672	0.000000	339.4	648.0	2387.4
		8	-0.849268	-1.821166	0.000000	448.4	672.8	2596.0
		5	-0.137952	-2.977720	0.000000	491.8	982.8	3478.0

		1	1.153717	3.985922	0.000000			
		1	1.054357	-3.020694	0.000000			
i10	291.86720	8	0.000000	-3.338049	0.000000	83.9	499.1	1432.6
	1.17819	5	0.000000	-2.128128	0.000000	96.6	567.7	1825.1
	1.17345	6	0.000000	-0.669639	0.000000	180.8	585.2	2002.8
		6	0.000000	0.574669	0.000000	265.7	902.0	2086.9
		6	0.000000	1.880573	0.000000	405.7	972.8	3082.6
		6	0.000000	3.186132	0.000000	477.8	1090.6	3152.0
		1	0.926848	3.757309	0.000000			
		1	-0.926848	3.757309	0.000000			
i11	53.50657	6	0.000000	0.585486	0.000000	89.3	565.4	1098.6
	1.28395	6	-0.339489	-0.581664	0.000000	122.6	640.2	1415.1
	1.25386	6	-0.716124	-1.889211	0.000000	212.2	647.3	2152.0
		6	-1.050885	-3.049358	0.000000	297.4	689.9	2304.9
		5	0.374127	2.051977	0.000000	383.0	763.0	2391.9
		8	1.573782	2.562297	0.000000	494.9	879.5	3472.3
		1	-1.344733	-4.070714	0.000000			
		1	-0.477173	2.920934	0.000000			
i12	161.38946	6	0.000000	0.502436	0.000000	94.0	539.8	1083.7
	1.21161	6	-0.128231	-0.722962	0.000000	114.1	556.8	1507.5
	1.20258	6	-0.238250	-2.068598	0.000000	225.5	592.8	2070.0
		6	-0.338611	-3.277172	0.000000	288.2	602.3	2166.5
		5	-0.153349	1.951025	0.000000	408.6	693.0	3474.2
		8	0.652802	3.014508	0.000000	504.2	1012.5	3847.3
		1	-0.423551	-4.336078	0.000000			
		1	0.198430	3.862662	0.000000			
HC_4BO	1588.4259	1	0.000000	-0.465523	-4.246796	97.9	587.8	2177.6
p1	1.22743	6	0.000000	0.000000	0.572790	270.1	588.2	2320.5
B3LYP	1.22648	6	0.000000	-0.169457	-0.630875	270.4	688.6	3470.2
		6	0.000000	-0.314182	-1.981271	495.5	688.6	
		6	0.000000	-0.402229	-3.185325	495.9	1113.7	
		5	0.000000	0.287314	2.012703	570.4	2008.3	
		8	0.000000	0.543020	3.191421			
HC_4BO	0.000000	1	0.000000	0.000000	-4.317197	97.0	535.9	1948.1
p1	1.199626	6	0.000000	0.000000	-3.249556	97.0	535.9	2086.2
CCSD(T)	1.199626	6	0.000000	0.000000	-2.029724	257.3	556.8	2223.8
		6	0.000000	0.000000	-0.652525	257.3	649.4	3491.9
		6	0.000000	0.000000	0.574087	474.9	649.4	
		5	0.000000	0.000000	2.059396	474.9	1091.1	
		8	0.000000	0.000000	3.270815			
HC_4OB	0.000000	6	0.000000	0.000000	0.707008	49.0	502.8	1550.5
p2	1.392570	6	0.000000	0.000000	-0.497187	49.0	502.8	2191.4
	1.392570	6	0.000000	0.000000	-1.859510	157.0	624.9	2399.4
		6	0.000000	0.000000	-3.066006	157.0	662.8	3474.4
		8	0.000000	0.000000	1.991518	351.5	662.8	
		5	0.000000	0.000000	3.298124	351.5	1136.2	

		1	0.000000	0.000000	-4.128591			
HC_2BO	0.000000	1	0.000000	0.000000	-3.012324	205.0	748.4	2236.4
	3.982542	6	0.000000	0.000000	-1.947619	205.0	748.4	3460.8
	3.982542	6	0.000000	0.000000	-0.742487	520.0	769.1	
		5	0.000000	0.000000	0.732118	520.0	2000.1	
		8	0.000000	0.000000	1.936545			
HBO	0.0000000	8	0.000000	0.000000	0.596963	789.1	2901.6	
	39.522725	5	0.000000	0.000000	-0.601607	789.1		
	39.522725	1	0.000000	0.000000	-1.767669	1874.0		
TS	95.22809	6	0.000000	0.548654	0.000000	541.3*i*	469.1	690.1
i1-p1	1.22510	6	0.116276	-0.668374	0.000000	100.0	494.8	1115.6
	1.20954	6	0.293715	-2.010358	0.000000	107.8	546.5	1995.5
		6	0.448649	-3.209353	0.000000	214.2	582.7	2159.6
		5	-0.378861	1.970897	0.000000	274.4	584.5	2262.2
		8	-0.719378	3.128397	0.000000	308.6	670.2	3468.8
		1	1.912677	1.418965	0.000000			
		1	0.584817	-4.264045	0.000000			
TS	7.32217	6	-1.148852	1.235741	0.000000	347.1*i*	447.4	899.1
i1-i2	2.03870	6	0.000000	0.820642	0.000000	86.8	524.5	1878.5
	1.59469	6	1.370631	0.730406	0.000000	96.02	635.2	2042.4
		6	2.572131	0.646211	0.000000	162.7	673.4	2255.6
		5	-0.762210	-1.356511	0.000000	243.8	684.9	3452.1
		8	-1.798722	-1.977818	0.000000	309.2	688.4	3470.8
		1	-2.195642	1.429880	0.000000			
		1	3.633007	0.577221	0.000000			
TS	10.05512	6	1.175079	1.130066	-0.050758	912.0*i*	554.8	974.3
i1-i3	2.95291	6	0.086196	0.425084	-0.120050	169.2	627.5	1386.0
	2.31410	6	-1.247425	0.136766	-0.000901	176.9	651.9	1682.7
		6	-2.433966	-0.081450	0.059291	361.5	717.8	2171.6
		5	1.749970	-0.296100	0.304945	407.7	721.2	3296.9
		8	0.976274	-1.259889	-0.119495	522.4	917.5	3468.8
		1	1.438192	2.171369	-0.017923			
		1	-3.477533	-0.274554	0.123673			
TS	82.25876	6	0.000000	0.659993	0.000000	1963*i*	451.8	1072.4
i1-i4	1.23407	6	-0.562819	-0.506301	0.000000	80.6	468.9	1860.9
	1.21583	6	-0.746990	-1.849748	0.000000	154.8	507.9	2047.4
		6	-1.061196	-3.024949	0.000000	246.0	528.2	2141.0
		5	0.896292	1.818634	0.000000	264.4	576.1	2324.5
		8	1.541299	2.844986	0.000000	426.4	711.5	3466.3
		1	-1.295868	0.535906	0.000000			
		1	-1.289955	-4.062939	0.000000			
TS	251.63445	6	0.000000	0.547139	0.000000	938.8*i*	519.2	1113.9
i1-i11	1.21079	6	-0.173802	-0.681588	0.000000	98.4	531.5	1328.9
	1.20499	6	-0.389104	-2.006928	0.000000	107.4	580.1	1836.6
		6	-0.582665	-3.205648	0.000000	270.6	600.2	2070.0
		5	0.422048	1.956864	0.000000	312.0	607.0	2143.1

		8	0.498962	3.184862	0.000000	477.8	693.9	3465.1
		1	-0.756244	-4.254738	0.000000			
		1	1.527738	1.073671	0.000000			
TS	6.70397	6	-0.252770	1.785065	0.000000	715.5*i*	549.3	1069.7
i2-i2t	2.55351	6	0.000000	0.494444	0.000000	113.0	602.2	1595.1
	1.84917	6	1.316425	-0.077419	0.000000	204.4	672.6	2026.5
		6	2.398075	-0.603573	0.000000	223.3	679.4	2204.1
		5	-1.217038	-0.444112	0.000000	363.8	690.5	3418.9
		8	-2.197386	-1.142937	0.000000	464.3	703.5	3473.3
		1	-0.465260	2.830278	0.000000			
		1	3.359164	-1.057323	0.000000			
TS	7.23434	6	-1.025515	1.478784	0.000000	254.0*i*	476.7	865.7
i2-HBO	2.95248	6	0.000000	0.727209	0.000000	66.9	558.2	1459.2
	2.09675	6	1.296731	0.260353	0.000000	126.1	616.0	1883.3
		6	2.429580	-0.147208	0.000000	220.4	646.1	2227.1
		5	-1.443566	-0.268871	0.000000	271.9	669.7	2319.5
		8	-1.226427	-1.521311	0.000000	472.4	714.0	3471.2
		1	-2.607552	0.101993	0.000000			
		1	3.432029	-0.501980	0.000000			
TS	20.54599	6	0.845854	0.921042	0.023561	720.2*i*	529.3	942.5
i2t-i5	2.09289	6	-0.161817	0.140816	0.000236	158.3	570.9	1432.7
	1.90976	6	-1.541267	0.003229	-0.012283	173.1	633.4	1808.9
		6	-2.734503	-0.160910	-0.030814	286.1	643.9	2213.5
		8	2.275890	-0.324418	-0.126130	448.1	713.1	3330.3
		5	1.138595	-0.867057	0.195321	492.6	906.8	3474.2
		1	1.439296	1.797830	0.192733			
		1	-3.788996	-0.292260	-0.044501			
TS	10.26512	6	-0.111490	1.608013	0.000000	272.0*i*	606.6	1067.8
i3-i6	2.80765	6	0.000000	0.298676	0.000000	64.1	657.0	1369.1
	2.20465	6	-1.023101	-0.679037	0.000000	173.4	670.6	1647.2
		6	-1.915420	-1.486450	0.000000	285.0	715.4	2209.6
		5	2.251539	0.679974	0.000000	468.8	757.1	3277.0
		8	1.333146	-0.245223	0.000000	531.6	800.7	3473.8
		1	-0.922098	2.317483	0.000000			
		1	-2.700700	-2.202786	0.000000			
TS	91.39519	6	0.000000	0.586143	0.000000	832.6*i*	490.6	691.9
i4-p1	1.22830	6	0.164547	-0.629889	0.000000	96.6	491.5	1104.4
	1.21201	6	-0.011962	-1.985591	0.000000	109.6	541.6	1990.2
		6	-0.168937	-3.181612	0.000000	271.7	557.1	2150.9
		5	-0.081593	2.050046	0.000000	276.2	610.3	2261.1
		8	-0.158293	3.254388	0.000000	447.3	679.3	3469.2
		1	2.086212	-0.784572	0.000000			
		1	-0.313784	-4.235069	0.000000			
TS	253.64364	6	-0.006574	-0.623290	0.000000	1574*i*	462.9	1112.4
i4-i7	1.20418	6	0.000000	0.620025	0.000000	83.7	496.9	1315.7
	1.19849	6	-0.109098	1.979862	0.000000	103.7	555.3	1887.5

		6	-0.372374	3.191264	0.000000	285.4	573.3	2038.3
		5	0.100550	-2.076001	0.000000	287.2	632.2	2198.9
		8	0.182702	-3.283662	0.000000	422.3	719.5	3422.2
		1	1.176155	1.397105	0.000000			
		1	-0.212243	4.245040	0.000000			
TS	18.88482	6	0.910657	-0.694261	0.000000	339.8*i*	532.9	1190.5
i5-i8	1.98867	6	0.000000	0.248198	0.000000	132.2	562.2	1372.6
	1.79921	6	-0.296254	1.562762	0.000000	143.2	632.7	1764.7
		6	-0.667709	2.724058	0.000000	177.9	772.1	2066.5
		8	0.451009	-2.047440	0.000000	444.7	884.1	3178.8
		5	-0.861910	-1.955174	0.000000	496.4	992.3	3468.2
		1	1.992476	-0.631467	0.000000			
		1	-0.971166	3.742314	0.000000			
TS	7.33071	6	-0.510683	1.698395	0.000000	736.8*i*	495.6	900.0
r-i6	2.77278	6	0.000000	0.540714	0.000000	26.3	546.1	1444.8
	2.01182	6	1.261553	-0.050069	0.000000	97.3	552.6	1816.2
		6	2.355533	-0.551739	0.000000	185.6	662.2	2221.7
		5	-2.345807	-1.022285	0.000000	258.6	671.5	3389.9
		8	-1.113551	-0.764041	0.000000	327.9	703.3	3474.0
		1	-1.324285	2.391193	0.000000			
		1	3.323308	-0.991244	0.000000			
TS	98.39886	6	0.055917	-0.612558	0.000000	861.2*i*	495.1	689.0
i7-p1	1.21793	6	0.000000	0.600388	0.000000	98.8	495.4	1103.7
	1.20304	6	-0.061227	1.968002	0.000000	104.8	556.5	1995.6
		6	-0.495726	3.108761	0.000000	285.2	564.5	2094.4
		5	0.116088	-2.080123	0.000000	288.5	575.5	2310.2
		8	0.164982	-3.285081	0.000000	449.9	645.7	3454.8
		1	1.823082	2.144104	0.000000			
		1	-0.717163	4.149609	0.000000			
TS	44.19989	6	0.000000	0.587430	0.000000	702.2*i*	521.2	1263.7
i7-i7t	1.29331	6	0.376957	-0.565121	0.000000	95.3	540.8	1626.0
	1.25655	6	0.848696	-1.910698	0.000000	121.8	673.7	2016.0
		6	0.060413	-2.954783	0.000000	246.6	673.8	2301.6
		5	-0.464669	1.979815	0.000000	373.1	802.4	3011.2
		8	-0.845338	3.125056	0.000000	491.7	1102.8	3429.1
		1	1.939063	-2.026235	0.000000			
		1	-0.569418	-3.814254	0.000000			
TS	213.00332	6	0.644288	-0.000437	0.000000	2071*i*	463.8	1072.6
i7t-i10	1.19251	6	-0.580022	-0.021203	0.000000	92.3	506.0	1857.9
	1.18587	6	-1.931549	0.125776	0.000000	98.0	512.1	2018.2
		6	-3.202712	-0.098454	0.000000	235.9	564.3	2224.2
		5	2.107582	-0.016821	0.000000	252.6	589.0	2333.5
		8	3.316046	-0.027578	0.000000	313.6	794.0	3122.0
		1	-2.671371	1.133996	0.000000			
		1	-3.974942	-0.863360	0.000000			
TS	10.87567	6	-1.194378	0.416169	0.000000	695.6*i*	496.4	1033.6

r-i8	1.87682	6	0.000000	0.789554	0.000000	40.0	536.5	1493.8
	1.60060	6	1.323520	1.000861	0.000000	80.7	582.3	1923.5
		6	2.519984	1.222974	0.000000	131.7	660.9	2123.2
		8	-1.542710	-1.317718	0.000000	237.4	687.4	3362.4
		5	-0.981756	-2.438357	0.000000	360.9	921.9	3467.3
		1	-2.210913	0.748103	0.000000			
		1	3.566612	1.408078	0.000000			
TS	39.89325	6	0.252796	-0.762609	0.000000	1319*i*	500.4	1091.5
i8-i9	1.62544	6	0.000000	0.468894	0.000000	110.2	532.7	1259.5
	1.56180	6	-0.615375	1.660758	0.000000	148.6	553.9	1961.9
		6	-1.127458	2.765654	0.000000	302.3	637.4	2022.7
		8	1.248283	-1.693259	0.000000	384.9	794.9	2097.9
		5	0.261022	-2.648498	0.000000	469.2	805.9	3471.9
		1	-0.767135	-1.732460	0.000000			
		1	-1.584011	3.724843	0.000000			
TS	80.62540	6	0.627884	-0.451934	0.000000	703.0*i*	467.1	955.2
i9-HBO	1.35141	6	0.000000	0.618928	0.000000	45.9	507.4	1493.5
	1.32913	6	-0.427065	1.903236	0.000000	103.8	612.8	1960.2
		6	-0.830902	3.046476	0.000000	208.7	626.5	2165.8
		8	0.063220	-1.944264	0.000000	217.0	699.4	2798.4
		5	0.593887	-3.071837	0.000000	330.2	709.5	3475.9
		1	-1.177782	4.050220	0.000000			
		1	1.483081	-3.837159	0.000000			
TS	110.42248	8	-0.422945	-3.309808	0.000000	457.4*i*	492.8	729.4
i10-p1	1.18267	5	-0.291093	-2.110904	0.000000	92.8	495.5	1115.1
	1.17013	6	-0.131552	-0.651286	0.000000	99.3	567.4	2003.6
		6	0.000000	0.558338	0.000000	213.1	571.2	2146.1
		6	0.143258	1.905294	0.000000	272.3	583.0	2295.8
		6	0.322307	3.104750	0.000000	322.6	670.8	3461.0
		1	2.514161	3.362053	0.000000			
		1	0.320797	4.168360	0.000000			
TS	108.42030	6	0.000000	0.513866	0.000000	456.3*i*	491.9	690.7
i11-p1	1.21207	6	-0.051256	-0.701319	0.000000	99.0	500.9	1109.2
	1.19867	6	-0.113485	-2.057612	0.000000	100.1	570.3	1963.6
		6	-0.167736	-3.263931	0.000000	234.4	585.0	2170.0
		5	0.072934	1.985045	0.000000	274. 3	594.1	2312.3
		8	-0.035709	3.192515	0.000000	287.0	684.3	3470.2
		1	-0.216413	-4.326172	0.000000			
		1	2.132267	1.914799	0.000000			
TS	194.13229	6	0.000000	0.492213	0.000000	1875*i*	474.4	1086.5
i11-i12	1.19818	6	0.005840	-0.730997	0.000000	96.0	541.2	1515.6
	1.19083	6	-0.014232	-2.085835	0.000000	100.3	599.9	2105.2
		6	-0.029782	-3.295316	0.000000	257.2	618.6	2157.9
		5	0.246842	1.944475	0.000000	278.9	628.6	2239.2
		8	-0.243473	3.161104	0.000000	446.5	695.2	3472.7
		1	-0.046881	-4.358016	0.000000			

		1	0.989500	3.066418	0.000000			
TS	302.11320	6	0.000000	0.469325	0.000000	1474*i*	513.9	696.8
i12-p1	1.18083	6	-0.053962	-0.751970	0.000000	96.8	545.0	1115.7
	1.17624	6	-0.110931	-2.104199	0.000000	97.4	567.4	1858.6
		6	-0.160808	-3.312855	0.000000	255.8	592.7	2143.5
		5	-0.018382	1.919139	0.000000	272.2	640.9	2248.7
		8	0.104958	3.146005	0.000000	399.8	647.2	3469.5
		1	-0.204663	-4.375108	0.000000			
		1	1.411112	3.809562	0.000000			
TS	11.78019	6	-1.186706	0.595989	0.000000	693.2*i*	471.3	930.6
H abstr	1.19178	6	0.000000	0.996960	0.000000	37.4	502.9	1182.7
	1.08229	6	1.157514	1.688103	0.000000	168.4	621.0	1897.0
		6	2.212717	2.288697	0.000000	169.2	692.7	2018.3
		1	3.135263	2.817781	0.000000	225.0	741.7	2122.7
		8	-0.996750	-3.172975	0.000000	284.1	857.1	3464.5
		5	-1.324733	-2.018463	0.000000			
		1	-1.638749	-0.760153	0.000000			