

Supplementary Information

A Combined Spectroscopic and Computational Investigation on the Oxidation of *exo*-Tetrahydrodicyclopentadiene (JP-10; C₁₀H₁₆) Doped with Titanium-Aluminum-Boron Reactive Metal Nanopowder

SUPPLEMENTARY INFORMATION

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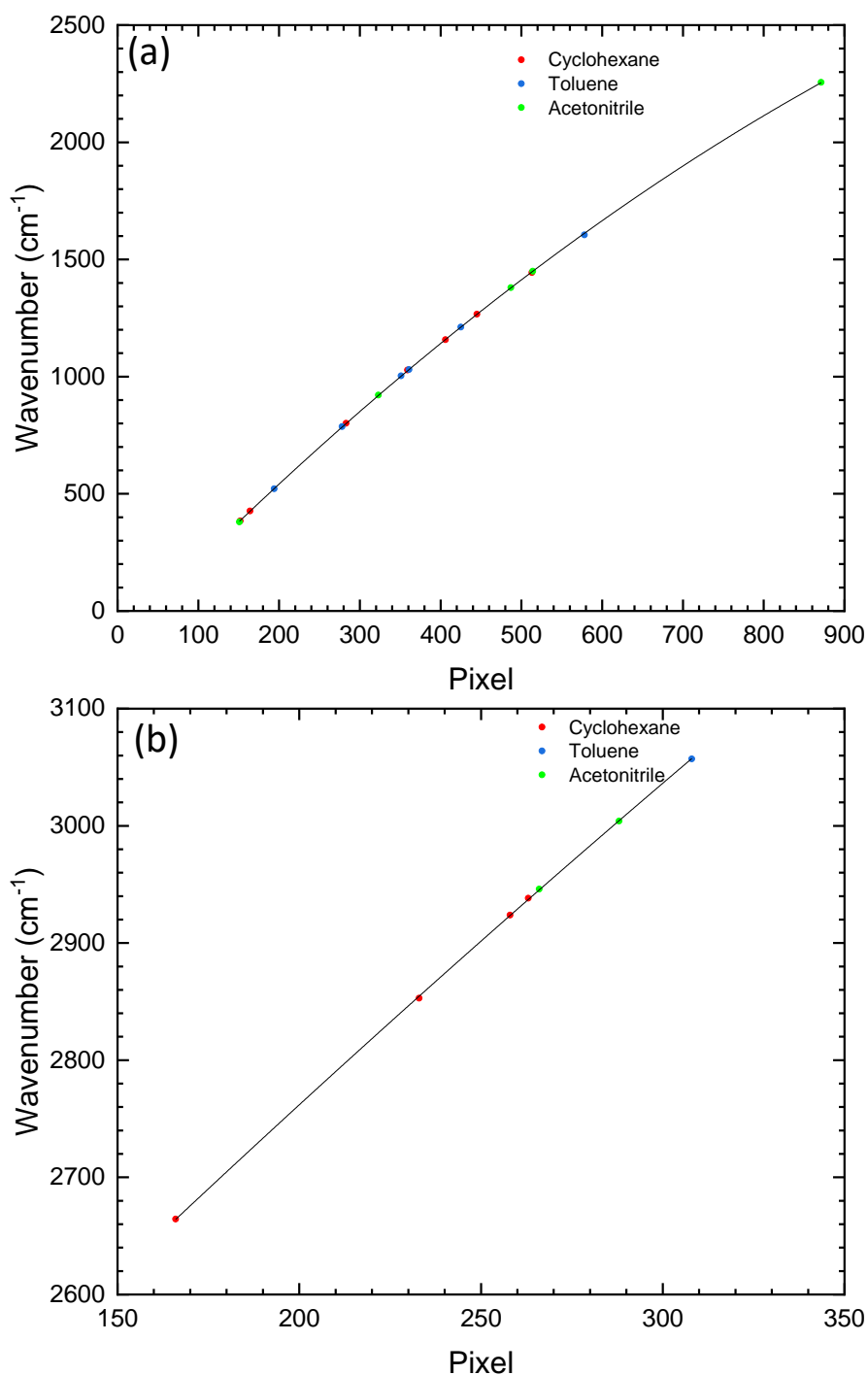


Figure S1: Calibration curves used to calibrate the (a) low energy region of Raman data (100 cm⁻¹ – 2400 cm⁻¹) and (b) high energy region of Raman data (2200 cm⁻¹ – 4000 cm⁻¹). Each region was calibrated with cyclohexane (red), toluene (blue) and acetonitrile (green) respectively. The graphs were fit with the following second order polynomials: (a) $y = -0.001x^2 + 3.5711x - 134.65$ and (b) $y = -0.001x^2 + 3.236x + 2154.1$.

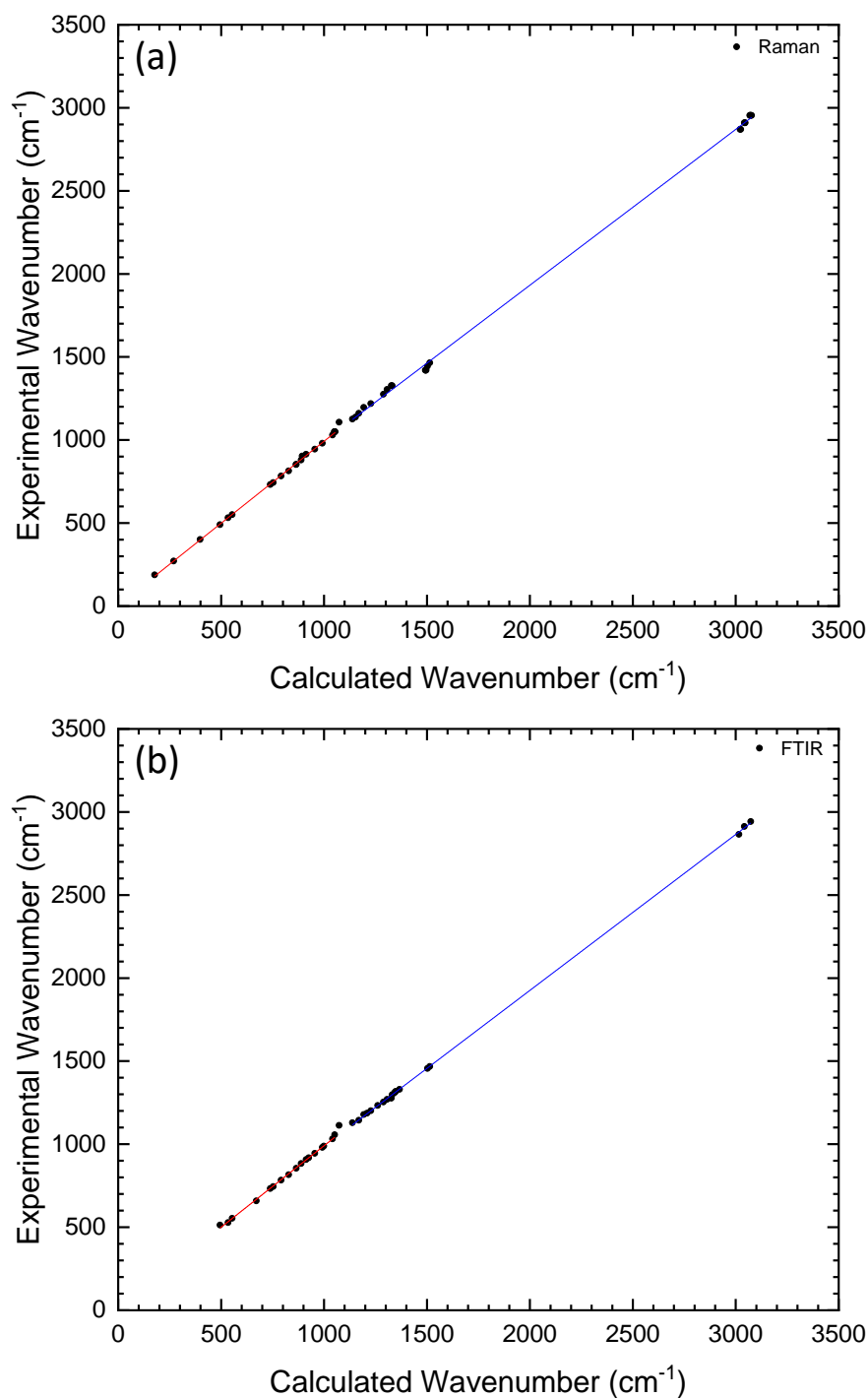


Figure S2: Comparison between the calculated vibrational wavenumber and (a) the experimental Raman wavenumber and (b) the experimental FTIR wavenumber of the normal modes of *exo*-tetrahydrodicyclopentadiene. Both the lower energy (red; 100 – 1100 cm^{-1}) and high energy region (blue; 1120 – 3100 cm^{-1}) of each plot were linearly fit to obtain a scaling factor for each region of 0.99 and 0.94 for Raman and 0.98 and 0.94 for FTIR, respectively.

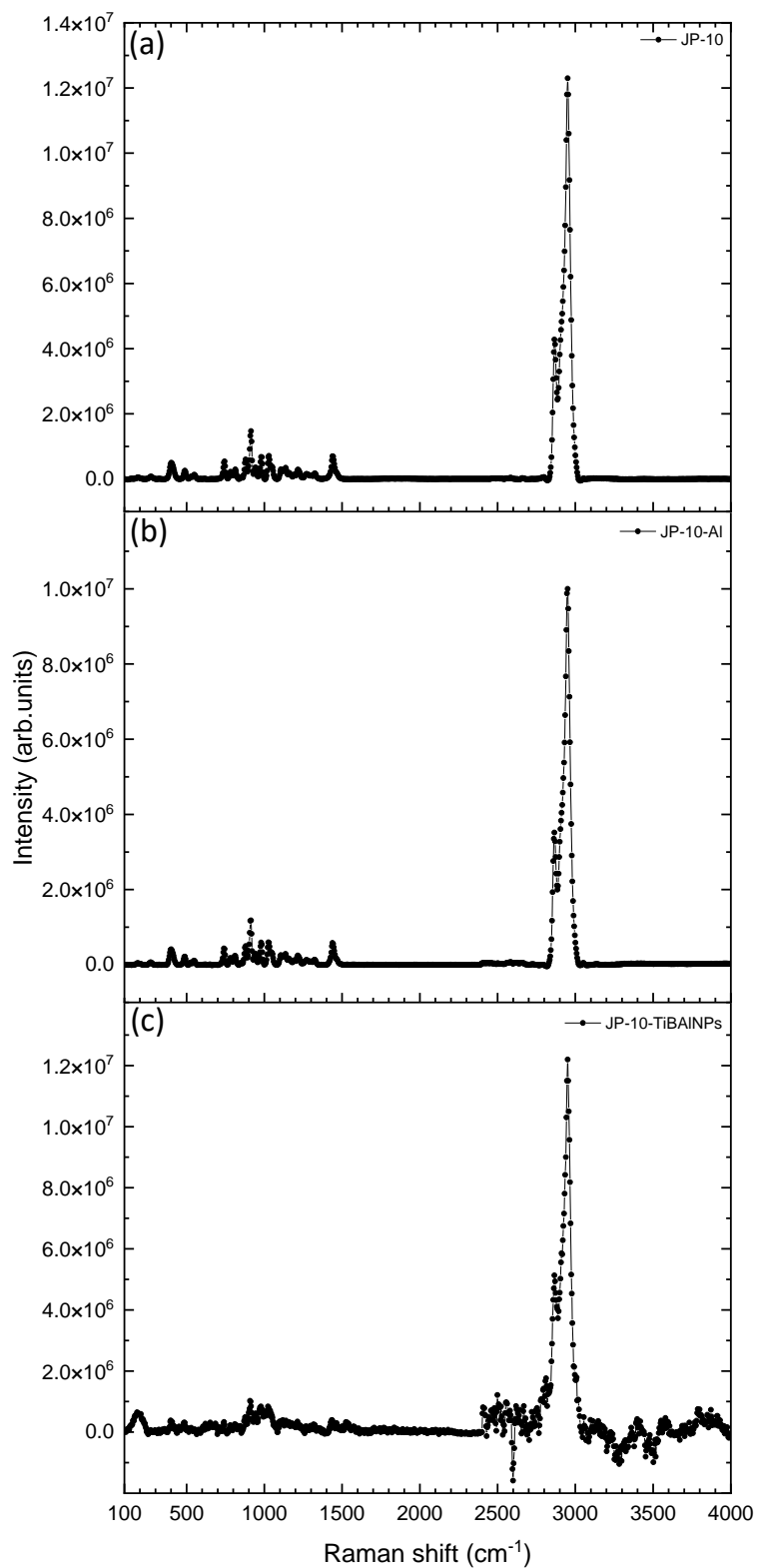


Figure S3: Overview Raman spectra of (a) JP-10, (b) JP-10-Al, and (c) JP-10-Ti-Al-B NPs (RMNPs) in the 100 – 4,000 cm⁻¹ region.

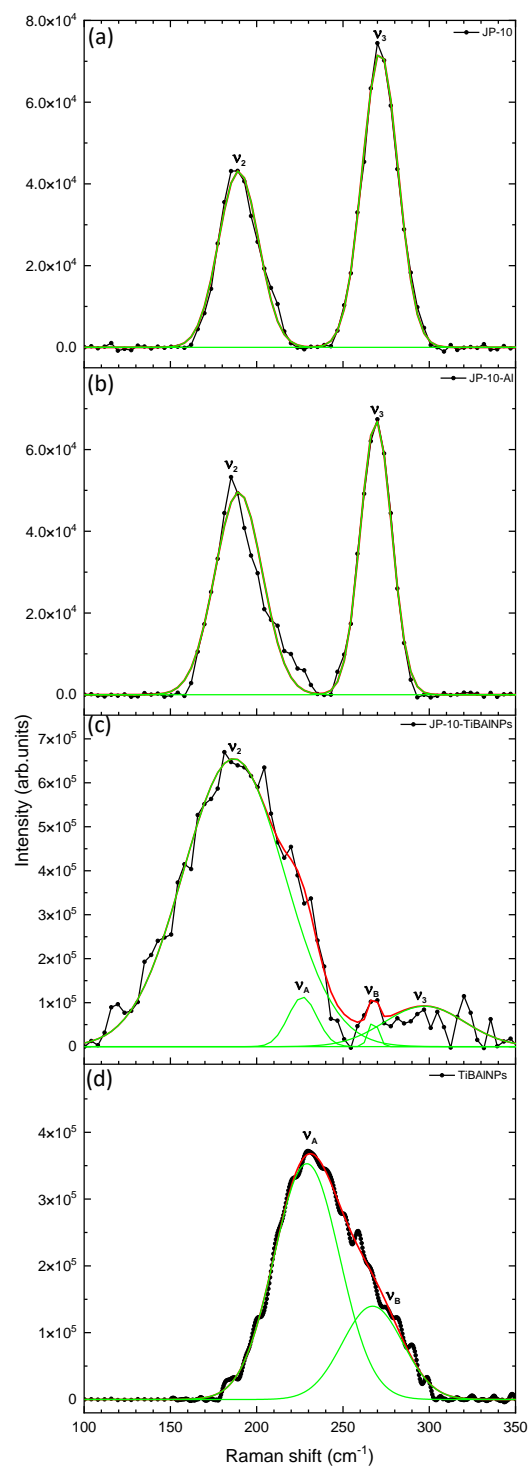


Figure S4: Raman spectra of (a) pure JP-10, (b) JP-10-Al, (c) JP-10-Ti-Al-B NPs (RMNPs), and (d) Ti-Al-BNPs (RMNPs) in the 100 – 350 cm^{-1} region. The total fit and individual peak fits are shown in red and green, respectively. Peak assignments are compiled in Table S1.

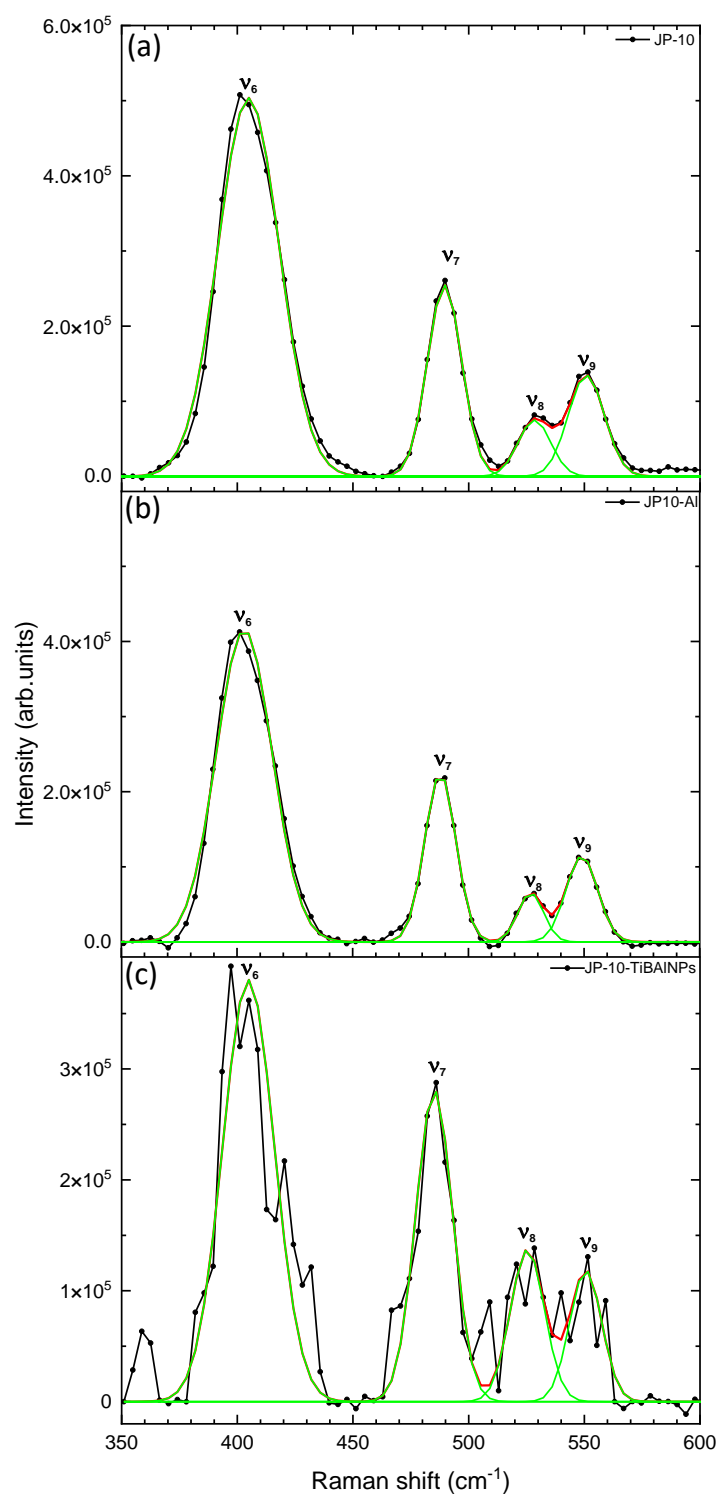


Figure S5: Raman spectra of (a) pure JP-10, (b) JP-10-Al, and (c) JP-10-Ti-Al-B NPs (RMNPs) in the 350 – 600 cm^{-1} region. The total fit and individual peak fits are shown in red and green, respectively. Peak assignments are compiled in Table S1.

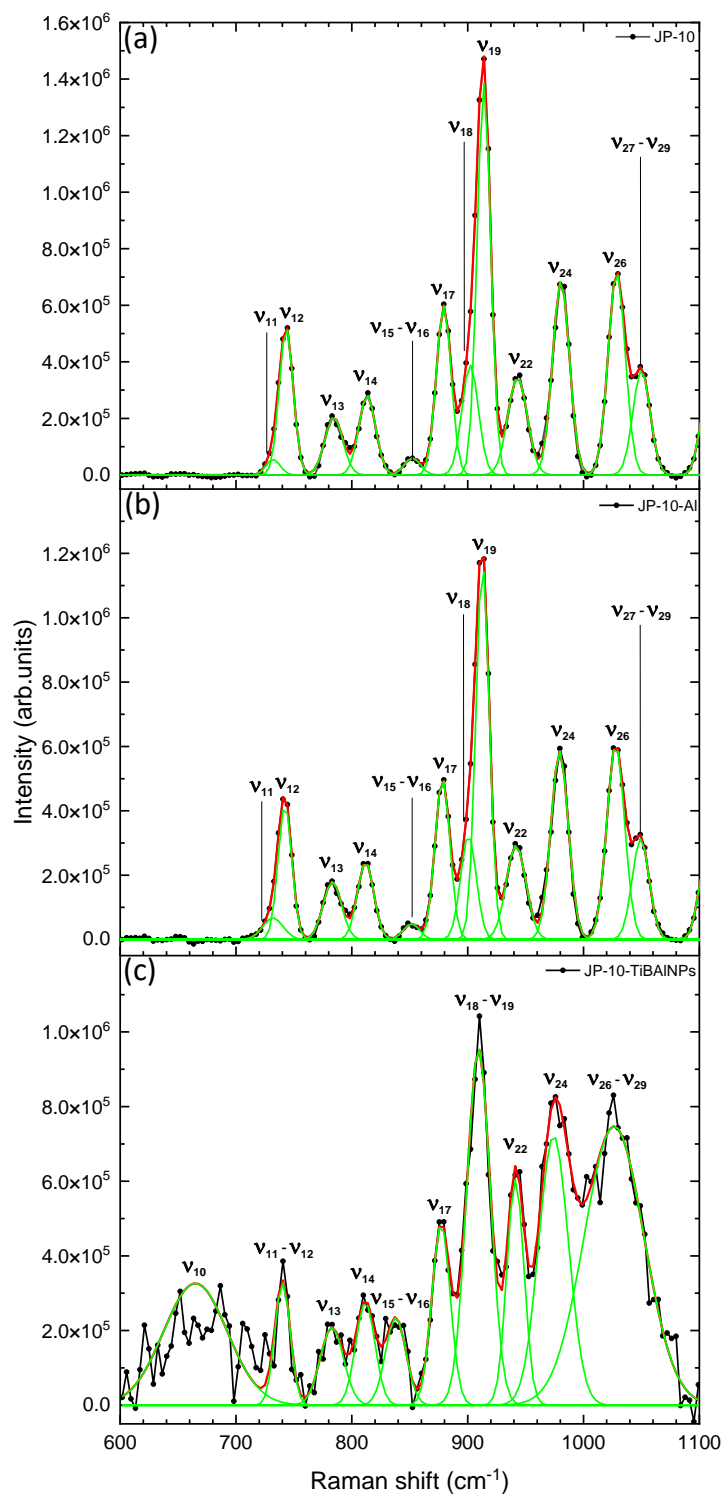


Figure S6: Raman spectra of (a) pure JP-10, (b) JP-10-Al, and (c) JP-10-Ti-Al-B NPs (RMNPs) in the 600 – 1,100 cm⁻¹ region. The total fit and individual peak fits are shown in red and green, respectively. Peak assignments are compiled in Table S1.

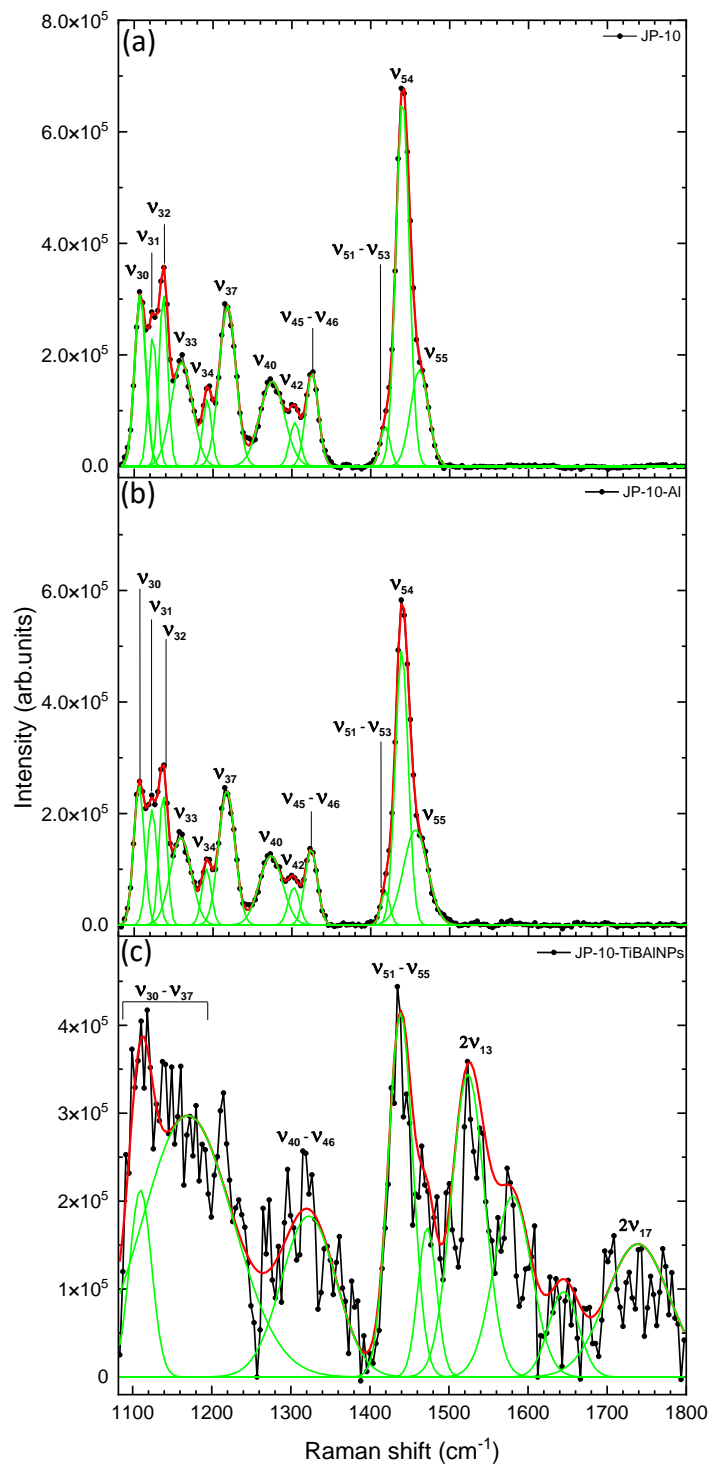


Figure S7: Raman spectra of (a) pure JP-10, (b) JP-10-Al, and (c) JP-10-Ti-Al-B NPs (RMNPs) in the 1,100 – 1,800 cm^{-1} region. The total fit and individual peak fits are shown in red and green, respectively. Peak assignments are compiled in Table S1.

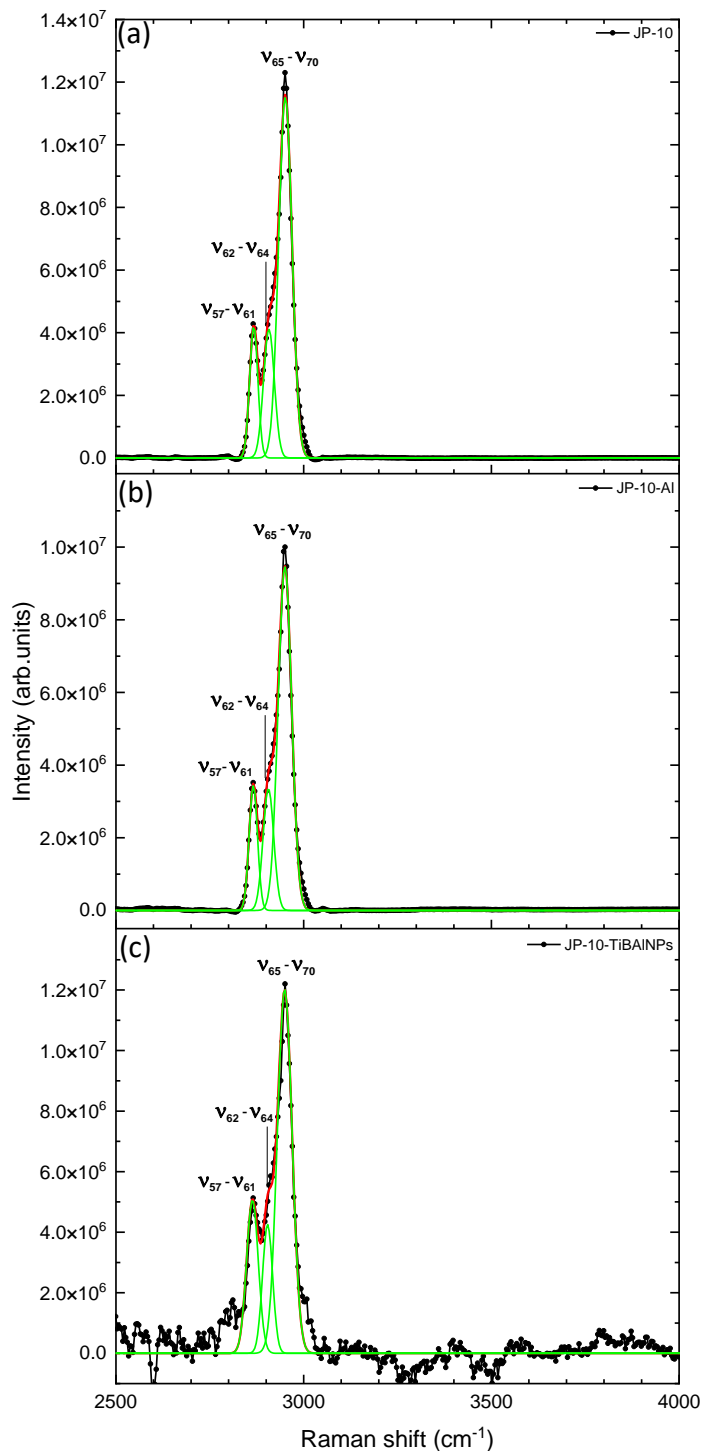


Figure S8: Raman spectra of (a) pure JP-10, (b) JP-10-Al, and (c) JP-10-Ti-Al-B NPs (RMNPs) in the 2,500 – 4,000 cm^{-1} region. The total fit and individual peak fits are shown in red and green, respectively. Peak assignments are compiled in Table S1.

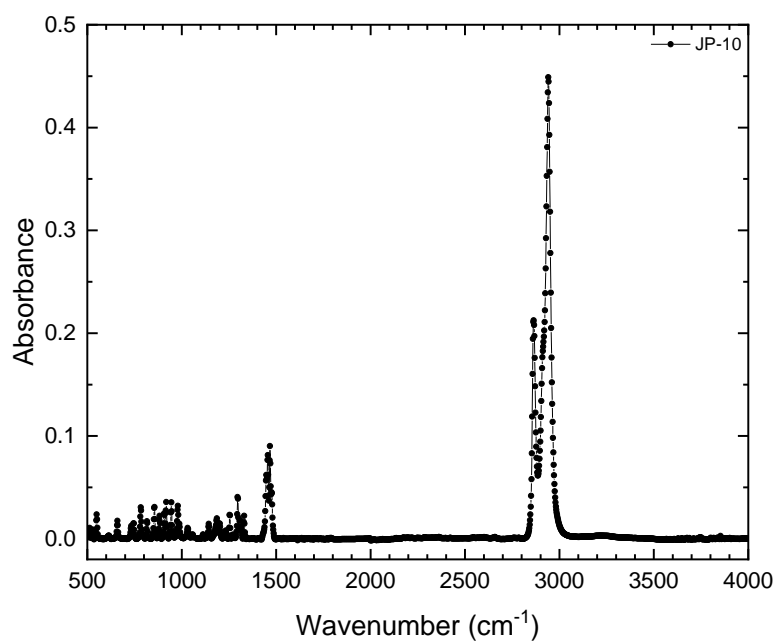


Figure S9: FTIR spectra of pure JP-10 in the 500 – 4,000 cm⁻¹ region

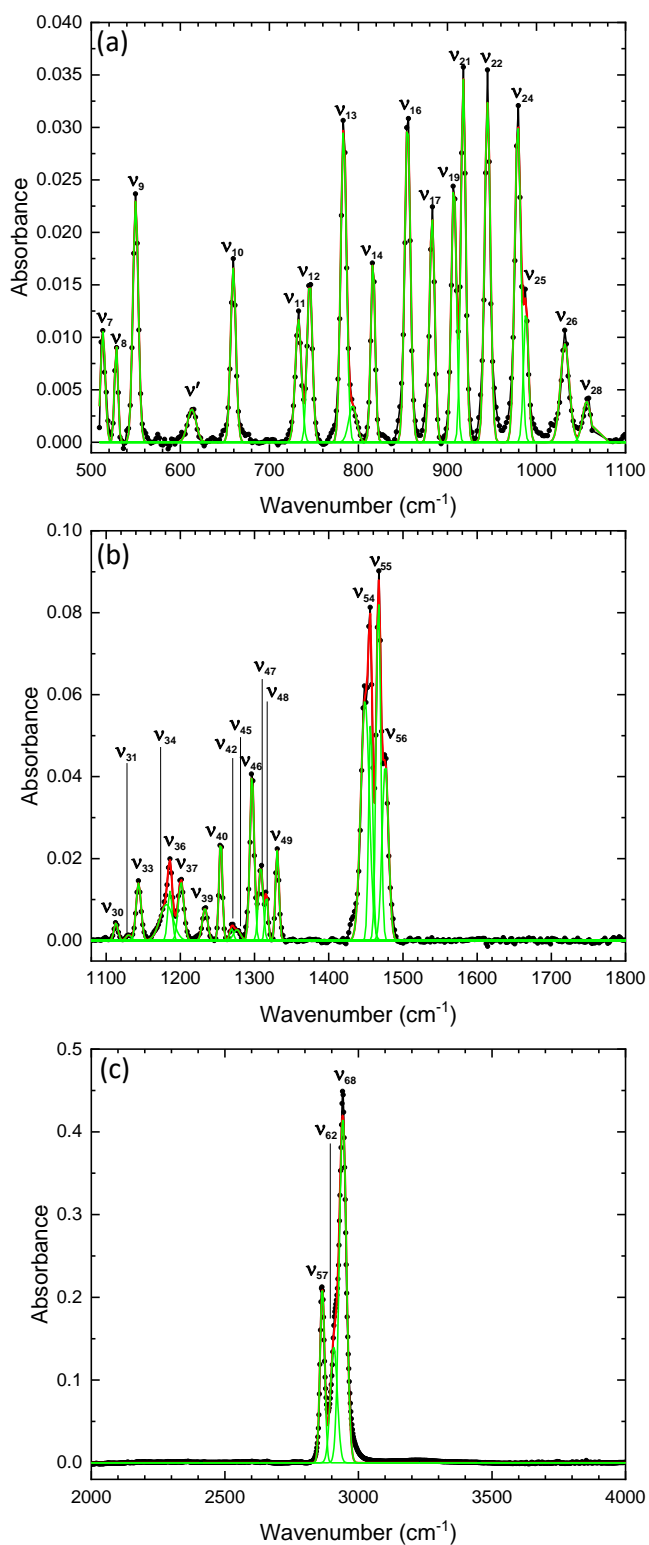


Figure S10: FTIR spectra of JP-10 in the (a) 500–1,100 cm^{-1} (b) 1,100–1,800 cm^{-1} , and (c) 2,000–4,000 cm^{-1} region. The overall fit and individual peak fits in each region are shown in red and green, respectively. Peak assignments are compiled in Table S1.

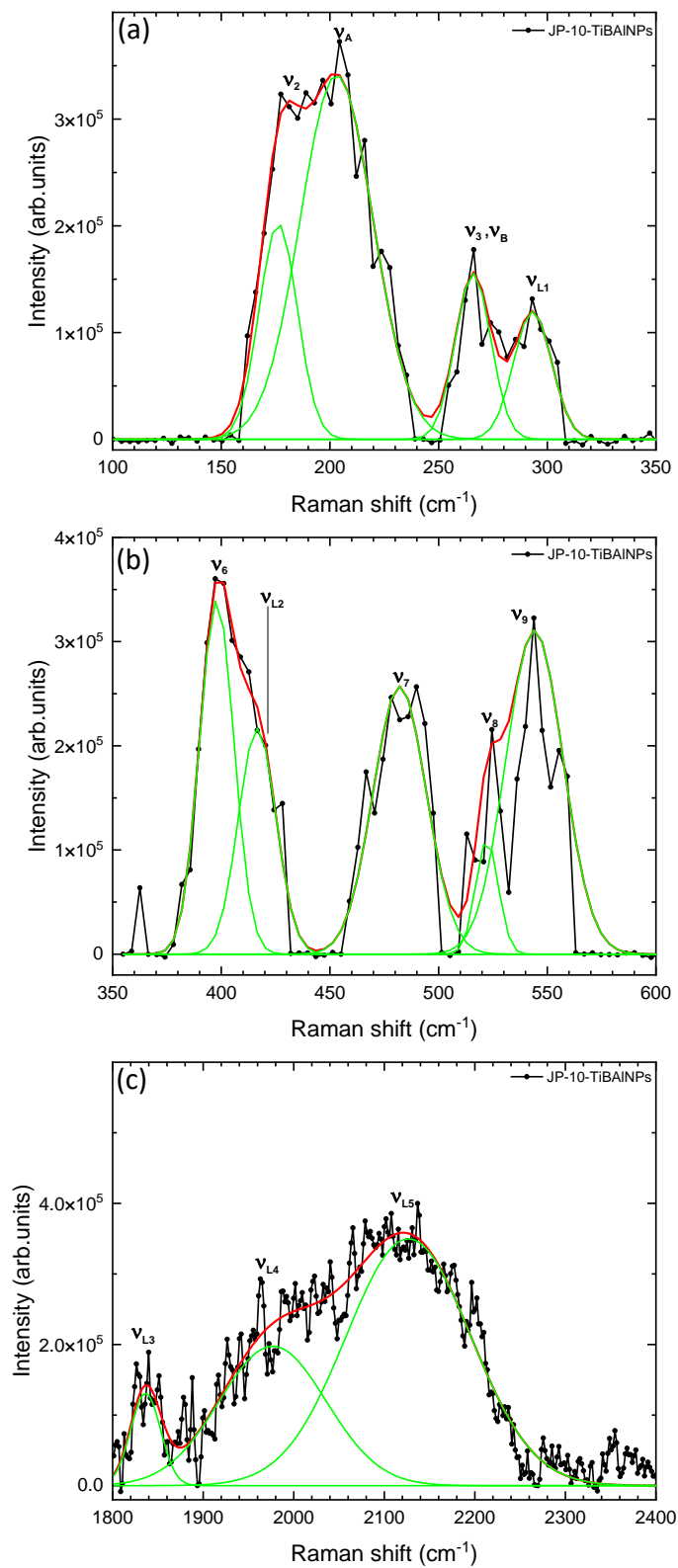


Figure S11: Raman spectra of new peaks resulting from photochemically activated JP-10-Ti-Al-B NPs (RMNPs) by a tightly focused 532 nm laser beam (45 – 50 μm) at 1 kHz

Table S1: Vibrational Mode Assignments for the Observed Peaks in the Raman Spectra of JP-10, JP-10-Al, and JP-10-Ti-Al-B NPs (RMNPs), Ti-Al-B NPs (RMNPs), and the FTIR Spectra of JP-10.

Normal Mode	Raman Wavenumber (cm ⁻¹) JP-10	Raman Wavenumber (cm ⁻¹) JP-10 Al	Raman Wavenumber (cm ⁻¹) JP-10 Ti-Al-B NPs	Raman Wavenumber (cm ⁻¹) Ti-Al-B NPs	FTIR Wavenumber (cm ⁻¹) JP-10	Calculated Wavenumber (cm ⁻¹) JP-10	Calculated FTIR Intensity JP-10	Vibrational Mode Assignment*
v ₁	-	-	-	-	-	140	0.009	Ring twist
v ₂	188	188	192		-	177	0.003	CCC bend
v _A	-	-	227	231	-	-	-	Al-B stretch
v _B	-	-	267	267	-	-	-	Ti-B stretch
v ₃	271	270	297	-	-	270	0.068	CCC bend
v ₄	-	-	-	-	-	317	0.028	CH ₂ rock
v ₅	-	-	-	-	-	319	0.046	Ring twist
v ₆	401	401	401	-	-	398	0.043	CCC bend
v ₇	490	490	482	-	513	495	0.237	CCC bend
v ₈	532	531	525	-	528	534	0.180	Ring twist
v ₉	551	551	544	-	554	554	0.661	CCC bend
v ₁₀	-	-	660*	-	659	671	0.678	Ring rock
v ₁₁	732	732	740	-	733	739	0.369	Ring rock
v ₁₂	744	743		-	745	753	0.356	CC stretch
v ₁₃	783	783		-	783	792	1.292	CC stretch
v ₁₄	814	813	813	-	816	828	0.643	CH ₂ rock
v ₁₅	853	852	845	-	-	864	0.067	CCC bend
v ₁₆				-	855	865	1.181	CCC bend
v ₁₇	879	879	879	-	883	889	0.626	CCC rock
v ₁₈	903	903	910	-	-	894	0.116	CC stretch
v ₁₉	914	914		-	907	913	0.882	Ring stretch
v ₂₀	-	-	-	-	-	918	0.041	CH ₂ bend/rock
v ₂₁	-	-	-	-	918	926	1.102	CCC rock
v ₂₂	945	944	941	-	945	955	2.044	Ring breathing

V23	-	-	-	-	-	963	0.045	CC stretch
V24	980	980	976	-	980	992	1.882	CC stretch
V25	-	-	-	-	988	999	0.806	CH ₂ bend
V26	1030	1030	1040	-	1032	1041	0.206	CH ₂ twist
V27	1050	1049		-	-	1050	0.488	CH ₂ bend
V28				-	1057	1052	0.083	CH ₂ rock
V29				-	-	1054	0.001	CH ₂ bend
V30	1107	1106	1157	-	1113	1073	0.780	CH ₂ twist/rock
V31	1126	1124		-	1129	1138	0.097	CH ₂ wag
V32	1138	1138		-	-	1153	0.026	CH ₂ twist
V33	1161	1160		-	1144	1169	1.210	CH ₂ twist
V34	1196	1196		-	1179	1193	0.188	CH ₂ wag
V35	-	-		-	-	1204	0.068	CH ₂ rock
V36	-	-		-	1186	1209	1.777	CH ₂ bend
V37	1219	1219		-	1201	1227	1.564	CH ₂ bend
V38	-	-	-	-	-	1251	0.018	CH ₂ twist
V39	-	-	-	-	1233	1261	0.807	CH ₂ twist
V40	1276	1275	1315	-	1254	1289	1.3410	CH ₂ wag
V41	-	-		-	-	1301	0.0411	CH wag
V42	1304	1303		-	1270	1306	0.1915	CH ₂ wag
V43	-	-		-	-	1312	0.372	CH ₂ wag
V44	-	-		-	-	1317	0.002	CH ₂ wag
V45	1327	1328		-	1277	1327	0.051	CH ₂ wag
V46				-	1297	1331	1.908	CH ₂ wag
V47	-	-	-	-	1310	1343	0.680	CH wag
V48	-	-	-	-	1318	1349	0.982	CH ₂ wag
V49	-	-	-	-	1330	1367	1.003	CH ₂ wag
V50	-	-	-	-	-	1372	0.514	CH ₂ twist
V51	1420	1420	1431	-	-	1492	0.776	CH wag
V52				-	-	1494	2.166	CH ₂ rock
V53				-	-	1496	1.794	CH ₂ rock
V54				1444	1442	-	1456	1503

v ₅₅	1465	1463		-	1468	1514	11.009	CH ₂ scissor
v ₅₆	-	-	-	-	1475	1526	4.457	CH ₂ rock
2v ₁₃	-	-	1560	-	-	-	-	overtone
2v ₁₇	-	-	1728	-	-	-	-	overtone
v ₅₇	2870	2869	2866	-	2865	3016	20.073	CH stretch
v ₅₈				-	-	3021	30.463	CH stretch
v ₅₉				-	-	3024	22.102	CH stretch
v ₆₀				-	-	3030	1.097	CH ₂ stretch
v ₆₁				-	-	3034	25.961	CH ₂ stretch
v ₆₂	2910	2910	2915	-	2913	3042	58.93	CH ₂ stretch
v ₆₃				-	-	3044	12.198	CH ₂ stretch
v ₆₄				-	-	3046	66.233	CH ₂ stretch
v ₆₅	2954	2953	2951	-	-	3065	6.172	CH ₂ stretch
v ₆₆				-	-	3068	46.085	CH stretch
v ₆₇				-	-	3071	38.453	CH stretch
v ₆₈				-	2942	3073	104.144	CH stretch
v ₆₉				-	-	3077	49.579	CH stretch
v ₇₀				-	-	3080	9.511	CH stretch
v ₇₁	-	-	-	-	-	3087	85.784	CH ₂ stretch
v ₇₂	-	-	-	-	-	3088	61.510	CH ₂ stretch

Table S2: Total reaction energies (ΔE) and zero point energy corrected reaction energies ($\Delta E + \Delta ZPE$) for the hydrogen abstraction channels of aluminum, boron, and titanium leading to the mono hydrides plus the corresponding JP-10 radical R1 to R6 refer (Figure 2). The Cartesian coordinates and vibrational modes are compiled in Table S6

reactants	ΔE B3LYP/def2-TZVP	$\Delta E + \Delta ZPE$ B3LYP/ def2-TZVP	ΔE MP2/6-311g*	$\Delta E + \Delta ZPE$ MP2/6-311g*
	products			
JP-10 + Al	R1 + AlH 129	R1 + AlH 91	R1 + AlH 159	R1 + AlH 131
	R2 + AlH 162	R2 + AlH 129	R2 + AlH 192	R2 + AlH 169
	R3 + AlH 151	R3 + AlH 113	R3 + AlH 180	R3 + AlH 153
	R4 + AlH 131	R4 + AlH 93	R4 + AlH 164	R4 + AlH 138
	R5 + AlH 124	R5 + AlH 84	R5 + AlH 156	R5 + AlH 127
	R6 + AlH 126	R6 + AlH 85	R6 + AlH 159	R6 + AlH 130
JP-10 + B	R1 + BH 160	R1 + BH 135	R1 + BH 111	R1 + BH 88
	R2 + BH 193	R2 + BH 173	R2 + BH 145	R2 + BH 125
	R3 + BH 182	R3 + BH 158	R3 + BH 132	R3 + BH 109
	R4 + BH 162	R4 + BH 139	R4 + BH 116	R4 + BH 94
	R5 + BH 155	R5 + BH 129	R5 + BH 108	R5 + BH 84
	R6 + BH 157	R6 + BH 131	R6 + BH 111	R6 + BH 86
JP-10 + Ti	R1 + TiH 253	R1 + TiH 223	R1 + TiH 272	R1 + TiH 243
	R2 + TiH 287	R2 + TiH 262	R2 + TiH 305	R2 + TiH 281
	R3 + TiH 274	R3 + TiH 245	R3 + TiH 293	R3 + TiH 265
	R4 + TiH 255	R4 + TiH 228	R4 + TiH 277	R4 + TiH 251
	R5 + TiH 247	R5 + TiH 217	R5 + TiH 269	R5 + TiH 240
	R6 + TiH 250	R6 + TiH 220	R6 + TiH 272	R6 + TiH 242

Table S3: Total energies (ΔE) and zero point energy corrected total energies ($\Delta E + \Delta ZPE$) computed with MP2/6-311g* for the initial van-der-Waals (vdW) complexes (vdW I), transition states (TS), final van-der-Waals (vdW II) complexes, and products during the reaction of aluminum monoxide (AlO) and boron monoxide (BO) with JP-10. R1 to R6 refer to distinct JP-10 radicals whose structures are shown in Figure 2. The Cartesian coordinates and vibrational modes of the stationary points are compiled in Table S6.

reactants	ΔE	$\Delta E + \Delta ZPE$	ΔE	$\Delta E + \Delta ZPE$	ΔE	$\Delta E + \Delta ZPE$	ΔE	$\Delta E + \Delta ZPE$
	vdW I		TS		vdW II		products	
JP-10 + BO	-9	-8	23	8	-37	-46	-29	R1 + HBO -41
	-7	-6	35	21	-5	-11	4	R2 + HBO -3
	-11	-10	42	28	-15	-24	-8	R3 + HBO -19
	-10	-9	15	1	-33	-42	-24	R4 + HBO -34
	-9	-7	28	14	-38	-49	-322	R5 + HBO -45
	-11	-10	23	8	-43	-54	-29	R6 + HBO -42
JP-10 + AlO	42	3	58	6	-60	-106	-36	R1 + AlOH -90
	42	3	55	8	-28	-71	-3	R2 + AlOH -52
	-33	-48	53	4	-40	-85	-15	R3 + AlOH -68
	-33	-8	45	8	-59	-104	-39	R4 + AlOH -82
	-33	-8	61	8	-58	-106	-39	R5 + AlOH -93
	-33	-8	65	20	-61	-109	-39	R6 + AlOH -91

Table S4: Total energies (ΔE) and zero point energy corrected total energies ($\Delta E + \Delta ZPE$) for the transition states, final van-der-Waals (vdW) complexes (vdW II), and products during the reaction of boron dioxide (BO_2) with JP-10. R1 to R6 refer to distinct JP-10 radicals whose structures are shown in Figure 2. The Cartesian coordinates and vibrational modes of the stationary points are compiled in Table S6.

reactants	ΔE	$\Delta E + \Delta ZPE$	ΔE	$\Delta E + \Delta ZPE$	ΔE	$\Delta E + \Delta ZPE$
	TS		vdW II		products	
JP-10 + BO_2	10	17	-97	-85	-62	R1 + BO_2H -56
	9	19	-69	-56	-29	R2 + BO_2H -35
	14	13	-73	-62	-41	R3 + BO_2H -35
	5	5	-99	-87	-57	R4 + BO_2H -49
	15	23	-100	-89	-65	R5 + BO_2H -60
	30	29	-93	-83	-62	R6 + BO_2H -58

Table S5: Total energies (ΔE) and zero point energy corrected total energies ($\Delta E + \Delta ZPE$) for van-der-Waals (vdW) complexes in the exit channel (vdW II), transition state to insertion (TS), the intermediates, and products accessed during the reaction of atomic and molecular oxygen with JP-10. R1 to R6 refer to distinct JP-10 radicals whose structures are shown in Figure 2. The Cartesian coordinates and vibrational modes of the stationary points are compiled in Table S7.

reactants	ΔE	$\Delta E + \Delta ZPE$	ΔE	$\Delta E + \Delta ZPE$	ΔE	$\Delta E + \Delta ZPE$
	TS		vdW II complex		products	
JP-10 + O	49	34	-4	-13	R1 + OH 14	R1 + OH -2
	60	43	26	20	R2 + OH 46	R2 + OH 34
	59	43	18	8	R3 + OH 35	R3 + OH 19
	42	28	-4	-12	R4 + OH 18	R4 + OH 3
	49	33	-6	-17	R5 + OH 11	R5 + OH -6
	50	34	-4	-15	R6 + OH 14	R6 + OH -4
reactants	ΔE	$\Delta E + \Delta ZPE$	ΔE	$\Delta E + \Delta ZPE$	ΔE	$\Delta E + \Delta ZPE$
	TS		VdW complex		products	
JP-10 + O ₂	210	196	197	191	R1 + O ₂ H 217	R1 + O ₂ H 206
	230	224*	222	227	R2 + O ₂ H 249	R2 + O ₂ H 242
	218	209	215	208	R3 + O ₂ H 237	R3 + O ₂ H 227
	205	199	193	197	R4 + O ₂ H 220	R4 + O ₂ H 211
	205	190	190	183	R5 + O ₂ H 213	R5 + O ₂ H 202
	202	188	192	184	R6 + O ₂ H 217	R6 + O ₂ H 204

* This transition state could not be located at the B3LYP/cc-pVTZ level of theory. MP2/cc-pVDZ does locate the transition state; however, with zero-point energy correction (either with harmonic or anharmonic frequencies), the energy is found lower than the corresponding R2-OOH van-der-Waals complex and likewise for CCSD/cc-pVTZ energy.

Table S6: Cartesian coordinates and vibrational frequencies of van-der-Waals complexes, transition states and products of the reactions of BO, AlO, and BO₂ with JP-10. Calculations are performed at the MP2/6-311g* level unless otherwise indicated.

Atom	X	Y	Z	
JP-10				
C	-0.362754	-0.785814	-0.514719	
C	-0.362754	0.785811	-0.514726	
C	0.879767	-1.131868	0.324589	
C	0.879774	1.131874	0.32457	
C	0.888333	0.000014	1.367226	
C	2.128868	-0.779704	-0.505758	
C	2.128874	0.779688	-0.505769	
C	-1.718206	-1.199374	0.088531	
C	-1.7182	1.199373	0.088531	
C	-2.63457	0.000002	-0.18068	
H	-0.269974	-1.189074	-1.531257	
H	-0.269983	1.189061	-1.531269	
H	0.877652	-2.154287	0.718985	
H	0.877666	2.154302	0.718943	
H	0.017186	0.000022	2.028639	
H	1.793214	0.000017	1.985804	
H	2.080761	-1.204432	-1.513657	
H	3.03321	-1.171596	-0.028391	
H	3.033218	1.171577	-0.028402	
H	2.080776	1.204402	-1.513674	
H	-1.619754	-1.353279	1.170221	
H	-2.091151	-2.135852	-0.33893	
H	-2.091143	2.135854	-0.338926	
H	-1.619744	1.353272	1.170222	
H	-2.945458	0	-1.232529	
H	-3.541266	0.000002	0.433452	

Atom	X	Y	Z	Atom	X	Y	Z
R1				R2			
C	0.354	0.792227	-0.528413	C	-0.368548	-0.850808	-0.463545
C	0.302153	-0.778172	-0.515397	C	-0.33928	0.734012	-0.552709
C	-0.89737	1.179636	0.306674	C	0.8699	-1.101186	0.369201
C	-0.948358	-1.087524	0.331605	C	0.908734	1.108559	0.276113
C	-0.919575	0.055	1.363006	C	0.88935	0.028682	1.387578
C	-2.093616	0.799885	-0.519299	C	2.136753	-0.880453	-0.434369
C	-2.193808	-0.70807	-0.499451	C	2.166287	0.689611	-0.518723
C	1.716735	1.171174	0.082399	C	-1.72899	-1.198294	0.167924
C	1.644532	-1.229103	0.090346	C	-1.690504	1.19882	0.019876
C	2.597116	-0.057416	-0.178149	C	-2.623542	-0.001658	-0.17772
H	0.276556	1.189579	-1.5475	H	-0.282434	-1.307976	-1.456254
H	0.195433	-1.184508	-1.529229	H	-0.23396	1.07083	-1.591798
H	-0.884381	2.209211	0.678687	H	0.918882	2.152385	0.610805
H	-0.969804	-2.104778	0.737439	H	0.010929	0.075407	2.034986
H	-0.038942	0.04115	2.011143	H	1.791889	0.041717	2.00679
H	-1.817305	0.086288	1.989169	H	2.097222	-1.35714	-1.41764
H	-2.515721	1.42909	-1.296802	H	3.018605	-1.260235	0.090984
H	-3.114517	-1.050831	-0.00374	H	3.071978	1.088375	-0.050091
H	-2.18461	-1.160241	-1.499772	H	2.139277	1.053781	-1.550665
H	1.617999	1.334378	1.162481	H	-1.629882	-1.289217	1.255495
H	2.119161	2.093162	-0.349509	H	-2.117367	-2.15221	-0.201788
H	1.991754	-2.17615	-0.335407	H	-2.049267	2.111606	-0.467007
H	1.540128	-1.379575	1.171964	H	-1.59262	1.41917	1.089928
H	2.91244	-0.069828	-1.228573	H	-2.933159	-0.061076	-1.228294
H	3.500956	-0.082762	0.439729	H	-3.531043	0.050878	0.432792

Atom	X	Y	Z	Atom	X	Y	Z
R3				R4			
C	-0.356909	-0.786935	-0.498841	C	0.381883	0.748353	-0.387131
C	-0.356909	0.786936	-0.498842	C	0.369798	-0.777621	-0.467491
C	0.876342	-1.136847	0.35768	C	-0.880694	1.149551	0.328404
C	0.876343	1.136848	0.357677	C	-0.918476	-1.124633	0.308762
C	0.876694	0.000002	1.352077	C	-0.97415	-0.001501	1.363299
C	2.13995	-0.780727	-0.469251	C	-2.082728	0.817626	-0.585587
C	2.139951	0.780725	-0.469253	C	-2.113107	-0.74153	-0.588011
C	-1.709529	-1.195627	0.111241	C	1.76383	1.237324	-0.037018
C	-1.709529	1.195626	0.111242	C	1.72343	-1.174362	0.150477
C	-2.627118	0	-0.165467	C	2.648676	-0.008845	-0.234208
H	-0.258293	-1.19347	-1.513472	H	0.316545	-1.152851	-1.501128
H	-0.258294	1.19347	-1.513473	H	-0.88407	2.166961	0.731442
H	0.872829	-2.154934	0.75836	H	-0.954319	-2.150872	0.690278
H	0.872831	2.154936	0.758356	H	-0.138431	-0.013533	2.070142
H	1.434973	0.000003	2.285304	H	-1.914155	0.006032	1.92833
H	2.095146	-1.207038	-1.477212	H	-1.954054	1.24021	-1.585569
H	3.040009	-1.171933	0.015217	H	-3.005986	1.229976	-0.164757
H	3.040011	1.171933	0.015212	H	-3.0493	-1.115851	-0.160616
H	2.095144	1.207033	-1.477215	H	-2.01955	-1.163956	-1.593385
H	-1.597351	-1.325376	1.194786	H	1.791759	1.566204	1.01458
H	-2.08258	-2.139695	-0.29953	H	2.085287	2.094544	-0.640614
H	-2.082581	2.139695	-0.299529	H	2.081115	-2.146893	-0.203274
H	-1.59735	1.325375	1.194787	H	1.633563	-1.230963	1.242334
H	-2.935434	0	-1.218295	H	2.929194	-0.097293	-1.28999
H	-3.534778	0	0.447119	H	3.571625	0.022113	0.353247

Atom	X	Y	Z	Atom	X	Y	Z
R5				R6			
C	-0.350357	-0.825491	-0.525469	C	-0.379506	-0.786675	-0.582736
C	-0.398433	0.743945	-0.566562	C	-0.379505	0.786675	-0.582735
C	0.872848	-1.1191	0.375624	C	0.81636	-1.130205	0.32341
C	0.822013	1.141064	0.282966	C	0.816357	1.130202	0.323417
C	0.81772	0.050663	1.36992	C	0.75241	-0.000005	1.365748
C	2.139627	-0.775111	-0.428686	C	2.113179	-0.779169	-0.428733
C	2.098416	0.781631	-0.502048	C	2.113178	0.779175	-0.428727
C	-1.684982	-1.228276	0.015957	C	-1.752008	-1.235208	-0.03154
C	-1.758062	1.153083	0.042654	C	-1.752008	1.23521	-0.031542
C	-2.65761	-0.09339	-0.054774	C	-2.595004	0.000001	-0.015902
H	-0.186253	-1.261127	-1.525257	H	-0.231031	-1.186871	-1.592632
H	-0.308853	1.125432	-1.59119	H	-0.231026	1.186872	-1.59263
H	0.869925	-2.125335	0.807725	H	0.790243	-2.153346	0.714703
H	0.792444	2.178	0.636177	H	0.790237	2.153341	0.714714
H	-0.082924	0.043228	1.990933	H	-0.169064	-0.000008	1.957326
H	1.697528	0.098727	2.021859	H	1.608153	-0.000006	2.050599
H	2.1393	-1.247328	-1.416463	H	2.126341	-1.204578	-1.437405
H	3.03548	-1.119696	0.098488	H	2.986138	-1.171974	0.103155
H	2.980972	1.220757	-0.025225	H	2.986133	1.171975	0.103172
H	2.061376	1.157243	-1.529822	H	2.126348	1.204593	-1.437394
H	-1.979126	-2.266367	0.143577	H	-1.635935	-1.651408	0.983883
H	-2.183917	2.02365	-0.466065	H	-2.192206	-2.039101	-0.634444
H	-1.625182	1.428331	1.094529	H	-2.192205	2.039101	-0.634449
H	-3.19027	-0.100958	-1.020897	H	-1.635937	1.651412	0.98388
H	-3.427575	-0.128666	0.724137	H	-3.646908	0.000001	0.253554

Atom	X	Y	Z	Atom	X	Y	Z
JP-10 B3LYP/def2-TZVP							
C	-0.36439	-0.787455	-0.51267				
C	-0.36439	0.787456	-0.512666				
C	0.883784	-1.131549	0.325555				
C	0.88378	1.131545	0.325568				
C	0.894691	-0.000008	1.370829				
C	2.135266	-0.781168	-0.507259				
C	2.135262	0.781178	-0.507253				
C	-1.724307	-1.203612	0.081085				
C	-1.724308	1.203613	0.081085				
C	-2.641653	0	-0.171254				
H	-0.268338	-1.185699	-1.524931				
H	-0.268335	1.185705	-1.524925				
H	0.882773	-2.149132	0.717323				
H	0.882766	2.149124	0.717344				
H	0.025842	-0.000015	2.029763				
H	1.793692	-0.000011	1.990989				
H	2.087322	-1.20194	-1.513055				
H	3.037011	-1.172474	-0.032878				
H	3.037006	1.172487	-0.032873				
H	2.087309	1.201957	-1.513046				
H	-1.631147	-1.372976	1.158043				
H	-2.103167	-2.129512	-0.354984				
H	-2.103167	2.129513	-0.354984				
H	-1.631152	1.372975	1.158043				
H	-2.975415	-0.000001	-1.213824				
H	-3.535404	0	0.455864				

Atom	X	Y	Z	Atom	X	Y	Z
R1 B3LYP/def2-TZVP				R2 B3LYP/def2-TZVP			
C	0.355894	0.792306	-0.53033	C	-0.368517	-0.854347	-0.460858
C	0.306604	-0.780814	-0.513364	C	-0.341361	0.738596	-0.550968
C	-0.907096	1.178281	0.301743	C	0.872674	-1.095538	0.366195
C	-0.949187	-1.088092	0.333403	C	0.913538	1.110369	0.276599
C	-0.92523	0.055858	1.365895	C	0.895574	0.026729	1.390655
C	-2.097596	0.792575	-0.522272	C	2.140003	-0.885496	-0.433762
C	-2.197766	-0.708812	-0.501063	C	2.173488	0.691194	-0.520366
C	1.721116	1.177706	0.073957	C	-1.734572	-1.202953	0.161449
C	1.653931	-1.231267	0.084292	C	-1.696414	1.202312	0.013522
C	2.605284	-0.053424	-0.166787	C	-2.629862	-0.001454	-0.16922
H	0.276334	1.184366	-1.545156	H	-0.279869	-1.305579	-1.450371
H	0.196708	-1.185292	-1.521567	H	-0.233917	1.069099	-1.585907
H	-0.89429	2.205176	0.666205	H	0.92566	2.149076	0.61005
H	-0.973161	-2.100444	0.736414	H	0.019796	0.076304	2.036094
H	-0.045505	0.046901	2.00987	H	1.793027	0.041003	2.010753
H	-1.815755	0.084477	1.99575	H	2.10369	-1.358247	-1.4156
H	-2.587128	1.435708	-1.240225	H	3.020351	-1.262102	0.089867
H	-3.116732	-1.054329	-0.007842	H	3.077083	1.087424	-0.054309
H	-2.192411	-1.161513	-1.498986	H	2.146395	1.049679	-1.55054
H	1.624834	1.356524	1.148774	H	-1.640726	-1.306851	1.245394
H	2.127653	2.089546	-0.366432	H	-2.128498	-2.147549	-0.216089
H	2.009667	-2.167152	-0.349756	H	-2.061705	2.105201	-0.479058
H	1.553791	-1.397251	1.161095	H	-1.602869	1.434633	1.078381
H	2.945529	-0.066824	-1.207068	H	-2.960412	-0.059782	-1.211171
H	3.494744	-0.075796	0.466089	H	-3.525309	0.051214	0.453034

Atom	X	Y	Z	Atom	X	Y	Z
R3 B3LYP/def2-TZVP				R4 B3LYP/def2-TZVP			
C	-0.358103	-0.788763	-0.494995	C	0.385824	0.745625	-0.365345
C	-0.358103	0.788764	-0.494995	C	0.372843	-0.773608	-0.464913
C	0.882363	-1.135664	0.362626	C	-0.880309	1.146474	0.336827
C	0.882365	1.135667	0.362621	C	-0.926054	-1.128023	0.300251
C	0.887008	0.000004	1.350522	C	-0.987893	-0.014985	1.368513
C	2.148681	-0.782213	-0.471695	C	-2.085515	0.825678	-0.583361
C	2.148682	0.782208	-0.471699	C	-2.117932	-0.735877	-0.600806
C	-1.716346	-1.199953	0.102585	C	1.76521	1.242531	-0.049022
C	-1.716345	1.199953	0.102587	C	1.73113	-1.180532	0.141465
C	-2.633868	0	-0.161136	C	2.657751	-0.006354	-0.221753
H	-0.254746	-1.189646	-1.505502	H	0.319488	-1.135781	-1.498856
H	-0.254749	1.189645	-1.505503	H	-0.883555	2.156134	0.745546
H	0.881376	-2.148915	0.761614	H	-0.964676	-2.153518	0.667466
H	0.88138	2.14892	0.761605	H	-0.159321	-0.035145	2.077982
H	1.35877	0.000005	2.323897	H	-1.926855	-0.008136	1.927694
H	2.101446	-1.205294	-1.477385	H	-1.958705	1.255107	-1.576961
H	3.046368	-1.17361	0.008706	H	-3.005279	1.23368	-0.15967
H	3.046371	1.173607	0.008696	H	-3.054104	-1.112089	-0.184484
H	2.101444	1.205284	-1.477392	H	-2.020476	-1.145441	-1.607364
H	-1.612759	-1.344406	1.182348	H	1.805892	1.603381	0.989833
H	-2.094332	-2.133664	-0.3176	H	2.087032	2.082398	-0.672779
H	-2.094332	2.133664	-0.317596	H	2.092798	-2.14166	-0.228297
H	-1.612757	1.344403	1.18235	H	1.64549	-1.259663	1.229452
H	-2.959549	0	-1.206498	H	2.968664	-0.094355	-1.266524
H	-3.531949	0	0.459732	H	3.563279	0.029505	0.385822

Atom	X	Y	Z	Atom	X	Y	Z
R5 B3LYP/def2-TZVP				R6 B3LYP/def2-TZVP			
C	-0.355427	-0.823585	-0.529747	C	-0.380728	-0.78775	-0.583878
C	-0.39841	0.748529	-0.567637	C	-0.380728	0.787747	-0.583882
C	0.8734	-1.119914	0.373906	C	0.818025	-1.129842	0.325012
C	0.825336	1.139828	0.287563	C	0.818027	1.129846	0.325005
C	0.820626	0.047198	1.374375	C	0.756104	0.000006	1.370958
C	2.144451	-0.776252	-0.428893	C	2.118718	-0.780583	-0.426884
C	2.106506	0.783674	-0.496387	C	2.118725	0.780575	-0.426879
C	-1.689329	-1.230022	-0.013332	C	-1.761282	-1.23654	-0.049169
C	-1.767002	1.158835	0.025443	C	-1.761282	1.23654	-0.049176
C	-2.658486	-0.099741	-0.030847	C	-2.585004	0	0.032446
H	-0.178314	-1.25631	-1.524508	H	-0.225482	-1.186497	-1.587341
H	-0.298134	1.128373	-1.585926	H	-0.225483	1.186489	-1.587347
H	0.868701	-2.123212	0.798886	H	0.792548	-2.148399	0.713103
H	0.79613	2.170965	0.640977	H	0.792553	2.148405	0.713089
H	-0.077847	0.041974	1.992873	H	-0.162351	0.000011	1.960684
H	1.694091	0.091691	2.028377	H	1.606275	0.000008	2.056361
H	2.144442	-1.241662	-1.416099	H	2.13352	-1.202238	-1.433342
H	3.036369	-1.124216	0.095287	H	2.988333	-1.172829	0.103429
H	2.985476	1.218378	-0.017236	H	2.988342	1.172811	0.10344
H	2.074651	1.159298	-1.520637	H	2.133537	1.202233	-1.433335
H	-1.968701	-2.260775	0.163574	H	-1.654937	-1.711308	0.93963
H	-2.205462	2.004017	-0.507062	H	-2.218658	-2.002384	-0.685553
H	-1.643534	1.469367	1.065365	H	-2.218658	2.00238	-0.685565
H	-3.248335	-0.107939	-0.962671	H	-1.654937	1.711313	0.93962
H	-3.389528	-0.141246	0.782137	H	-3.638055	0	0.281804

Atom	X	Y	Z	Atom	X	Y	Z
vdW1 sites 1-2 JP-10/AIO				vdW1 site 3 JP-10/AIO			
C	-1.845897	-0.620373	0.222476	C	1.094905	0.865603	-0.785911
C	-1.155568	0.139051	-0.966474	C	1.094954	0.86567	0.785849
C	-0.657847	-1.261778	0.958818	C	1.418394	-0.598591	-1.129651
C	0.336887	-0.164876	-0.752322	C	1.418461	-0.598445	1.129697
C	0.441198	-0.195486	0.785574	C	0.697759	-1.35731	0.000094
C	-0.102931	-2.400434	0.081327	C	2.897022	-0.854888	-0.779781
C	0.591991	-1.644321	-1.091889	C	2.897088	-0.854783	0.779727
C	-2.621317	0.455373	1.005694	C	-0.307657	1.352815	-1.193689
C	-1.568272	1.614827	-0.811679	C	-0.30763	1.352927	1.193644
C	-2.883426	1.55969	-0.025263	C	-0.772774	2.194939	-0.000063
H	-2.539274	-1.390332	-0.139299	H	1.86182	1.541789	-1.188571
H	-1.490872	-0.242427	-1.939263	H	1.861837	1.541958	1.188402
H	-0.879792	-1.556137	1.990638	H	1.145022	-0.881994	-2.153021
H	0.997202	0.529158	-1.287133	H	1.145236	-0.881835	2.153111
H	0.208346	0.756472	1.274112	H	-0.388584	-1.236181	0.00013
H	1.411559	-0.558918	1.145346	H	0.94209	-2.428048	0.000166
H	-0.897247	-3.073353	-0.257415	H	3.558086	-0.09098	-1.203832
H	0.621199	-3.001337	0.640958	H	3.22442	-1.824595	-1.171292
H	1.666924	-1.847015	-1.108146	H	3.224488	-1.824443	1.171351
H	0.183701	-1.911525	-2.071848	H	3.558166	-0.090816	1.203637
H	-2.002528	0.850581	1.820965	H	-0.987552	0.501466	-1.293879
H	-3.535386	0.057114	1.457996	H	-0.291579	1.904081	-2.141517
H	-1.660507	2.121025	-1.778144	H	-0.291498	1.904308	2.141399
H	-0.813483	2.160882	-0.231675	H	-0.987503	0.501595	1.29398
H	-3.700804	1.258237	-0.691517	H	-0.271678	3.172442	-0.000097
H	-3.159462	2.518372	0.426088	H	-1.854736	2.369116	-0.00003
Al	3.328476	1.550786	0.265866	Al	-4.219396	-0.900399	-0.000009
O	3.638917	-0.215132	0.106815	O	-2.672378	-0.835037	0.000085

Atom	X	Y	Z	Atom	X	Y	Z
vdW1 site 4 JP-10/AIO				vdW1 sites 5-6 JP-10/AIO			
C	0.665171	0.357543	0.784778	C	0.374399	0.225682	0.784799
C	0.665205	0.357554	-0.784777	C	0.374378	0.22567	-0.784776
C	0.912678	-1.121426	1.130932	C	1.763555	-0.336618	1.131767
C	0.912668	-1.121412	-1.130933	C	1.763558	-0.336612	-1.131748
C	1.857914	-1.565132	-0.00001	C	2.636416	0.235031	0.000013
C	-0.365245	-1.908466	0.778975	C	1.76887	-1.836983	0.779783
C	-0.365315	-1.908384	-0.778949	C	1.768903	-1.836966	-0.779809
C	1.777072	1.338172	1.199812	C	0.114403	1.685441	1.198245
C	1.777167	1.338165	-1.199739	C	0.114387	1.68541	-1.198241
C	1.911507	2.284429	0.000037	C	-0.631229	2.284209	0.000004
H	-0.307568	0.691771	1.158514	H	-0.430733	-0.409704	1.166424
H	-0.307488	0.691877	-1.158554	H	-0.430734	-0.40974	-1.166379
H	1.273122	-1.285785	2.15384	H	2.093661	-0.117393	2.154157
H	1.273076	-1.285804	-2.153848	H	2.093646	-0.117339	-2.154134
H	2.822474	-1.047768	-0.000016	H	2.696645	1.327245	0.000002
H	2.043222	-2.646375	-0.000018	H	3.655761	-0.170354	0.000015
H	-1.259169	-1.424885	1.179056	H	0.901744	-2.354158	1.20369
H	-0.3114	-2.928887	1.177378	H	2.667964	-2.325892	1.171656
H	-0.311632	-2.928762	-1.177467	H	2.66805	-2.325818	-1.171635
H	-1.259203	-1.42461	-1.178874	H	0.901837	-2.354197	-1.203768
H	2.723101	0.802899	1.35425	H	1.064672	2.214131	1.354065
H	1.542938	1.857442	2.135851	H	-0.452031	1.750104	2.133644
H	1.543087	1.85743	-2.135794	H	-0.452064	1.750079	-2.133623
H	2.72321	0.802897	-1.354106	H	1.064656	2.214088	-1.354078
H	1.078668	2.998295	0	H	-1.65978	1.912552	-0.000001
H	2.844591	2.859499	0.000071	H	-0.644884	3.380763	-0.000023
Al	-4.166579	0.716618	0.000167	Al	-4.12735	-1.111835	0.000055
O	-2.554806	0.59856	-0.000402	O	-2.796088	-0.184513	-0.00012

Atom	X	Y	Z	Atom	X	Y	Z
TS1 JP-10/AIO				TS2 JP-10/AIO			
C	1.116564	-0.655207	0.663072	Al	4.359131	-0.373861	0.151823
C	1.802351	0.729226	0.378115	C	-0.548599	-0.404625	-0.785763
C	-0.259943	-0.506549	-0.014586	C	-2.005954	-0.145166	-0.243774
C	0.720156	1.495932	-0.401738	C	0.24915	0.717371	-0.11765
C	0.06467	0.377051	-1.23166	C	-1.826592	1.093828	0.653966
C	-1.085295	0.469326	0.826796	C	-0.425805	0.85305	1.252053
C	-0.413142	1.843793	0.584734	C	-0.104063	2.053387	-0.779919
C	2.047301	-1.715498	0.043943	C	-1.554762	2.31116	-0.254639
C	3.090234	0.399492	-0.398814	C	-0.191037	-1.836072	-0.348234
C	3.42312	-1.039077	0.014456	C	-2.412091	-1.444405	0.476954
H	1.005074	-0.838427	1.73951	C	-1.547769	-2.529467	-0.177181
H	2.055022	1.251551	1.309739	H	-0.500966	-0.320255	-1.87866
H	-0.754045	-1.46255	-0.223745	H	-2.707421	0.063726	-1.06194
H	1.099307	2.356105	-0.964233	H	1.392976	0.487391	-0.084981
H	0.741049	-0.093553	-1.950479	H	-2.642549	1.244229	1.370641
H	-0.838832	0.706018	-1.754623	H	-0.353345	-0.04366	1.872937
H	-1.206764	0.18254	1.876206	H	-0.052647	1.708771	1.825371
H	-2.156302	0.543751	0.375681	H	-0.048411	1.997422	-1.871404
H	-1.123485	2.545609	0.136274	H	0.580359	2.842184	-0.451711
H	-0.034412	2.294727	1.507817	H	-1.601872	3.241279	0.321697
H	1.727484	-1.946646	-0.979579	H	-2.289207	2.387657	-1.063189
H	2.035656	-2.654143	0.607232	H	0.346214	-1.811443	0.606663
H	3.894173	1.110474	-0.182791	H	0.466141	-2.329638	-1.07088
H	2.902877	0.440044	-1.478769	H	-3.48696	-1.639164	0.399101
H	3.860329	-1.044114	1.020287	H	-2.171833	-1.374885	1.54499
H	4.132985	-1.530992	-0.658618	H	-1.95988	-2.787048	-1.16069
Al	-4.100233	-1.089066	-0.030696	H	-1.493293	-3.451866	0.410987
O	-3.384149	0.488316	-0.345846	O	2.757389	0.078891	0.032811

Atom	X	Y	Z	Atom	X	Y	Z
TS3 JP-10/AIO				TS4 JP-10/AIO			
C	1.049354	0.881022	-0.785793	C	0.155667	0.3486	0.505311
C	1.049191	0.880943	0.785963	C	0.853518	0.378237	-0.891863
C	1.181733	-0.611337	-1.135446	C	0.764756	-0.876448	1.193412
C	1.181587	-0.611449	1.135446	C	1.804295	-0.830742	-0.82097
C	0.409667	-1.289585	-0.000086	C	2.212993	-0.832689	0.663428
C	2.619517	-1.053605	-0.78053	C	0.22272	-2.135075	0.48736
C	2.619473	-1.05352	0.780627	C	0.947268	-2.109532	-0.892939
C	-0.273364	1.552272	-1.198781	C	0.397304	1.721078	1.143645
C	-0.273623	1.552117	1.198756	C	1.509325	1.768156	-0.983183
C	-0.635485	2.43752	0.000006	C	0.657211	2.642763	-0.054213
H	1.899487	1.448272	-1.186898	H	-0.97904	0.206681	0.369911
H	1.899214	1.448198	1.187295	H	0.123228	0.256281	-1.701825
H	0.871641	-0.865458	-2.154516	H	0.644528	-0.882989	2.282302
H	0.871414	-0.865735	2.15445	H	2.623218	-0.798137	-1.548967
H	-0.750295	-1.067259	-0.000128	H	2.767446	0.058809	0.972009
H	0.468856	-2.38491	-0.000149	H	2.793657	-1.719728	0.943942
H	3.36656	-0.375137	-1.205997	H	-0.865033	-2.092346	0.394745
H	2.823256	-2.055487	-1.172413	H	0.482922	-3.037276	1.051776
H	2.823464	-2.055287	1.172671	H	1.583646	-2.99221	-1.020101
H	3.366319	-0.374793	1.206025	H	0.248535	-2.083338	-1.735341
H	-1.047711	0.791467	-1.332078	H	1.286007	1.685953	1.789457
H	-0.177111	2.107535	-2.138111	H	-0.446707	2.038104	1.764581
H	-0.177571	2.107256	2.13818	H	1.55156	2.139276	-2.012765
H	-1.047992	0.791291	1.331785	H	2.540071	1.726268	-0.608853
H	-0.015482	3.342995	0.000132	H	-0.294981	2.880901	-0.542901
H	-1.684557	2.75434	-0.000091	H	1.140844	3.586861	0.21901
Al	-3.82982	-0.95691	0.000036	Al	-4.063433	-0.134438	-0.253408
O	-2.158767	-1.051718	-0.000199	O	-2.440701	0.041061	0.072175

Atom	X	Y	Z	Atom	X	Y	Z
TS5 JP-10/AIO				TS6 JP-10/AIO			
C	0.020121	0.050079	-0.349404	Al	5.233121	-0.000056	-0.236816
C	1.340017	0.872062	-0.588349	C	-0.904529	0.78603	-0.620168
C	0.50375	-1.149724	0.483128	C	-0.904495	-0.78603	-0.620033
C	2.403076	0.032033	0.140718	C	-2.108321	1.128406	0.279118
C	1.611775	-0.515369	1.341925	C	-2.108135	-1.128326	0.279502
C	1.325824	-2.06745	-0.441635	C	-2.083838	0.000218	1.324306
C	2.636201	-1.254735	-0.673887	C	-3.39188	0.779333	-0.498987
C	-0.927217	1.018915	0.362575	C	-3.391819	-0.77976	-0.498609
C	1.071672	2.270156	0.001992	C	0.473292	1.21582	-0.068559
C	-0.457408	2.417176	-0.029266	C	0.47347	-1.215654	-0.068697
H	-0.431221	-0.274711	-1.294879	C	1.055739	0.000082	0.652848
H	1.571388	0.955695	-1.65749	H	-1.058132	1.19858	-1.625128
H	-0.292114	-1.66834	1.031526	H	-1.058302	-1.198748	-1.624893
H	3.318878	0.585523	0.376283	H	-2.089052	2.152894	0.667544
H	1.252078	0.259308	2.025864	H	-2.088637	-2.152678	0.668273
H	2.175899	-1.255509	1.920506	H	-1.197566	0.0004	1.96182
H	0.792889	-2.289723	-1.371566	H	-2.974603	0.000245	1.964035
H	1.537519	-3.021861	0.051266	H	-3.385766	1.203874	-1.508078
H	3.506946	-1.799027	-0.293883	H	-4.274245	1.173206	0.016606
H	2.820444	-1.039474	-1.731179	H	-4.274072	-1.173437	0.017329
H	-0.946449	0.87409	1.449022	H	-3.385839	-1.204805	-1.507488
H	-2.027036	0.855289	-0.005625	H	0.401857	2.099578	0.575449
H	1.588158	3.058554	-0.555025	H	1.132124	1.477666	-0.904439
H	1.427016	2.317903	1.038364	H	1.132238	-1.477162	-0.904735
H	-0.791287	2.640835	-1.048698	H	0.402355	-2.099573	0.575125
H	-0.837812	3.20276	0.630031	H	2.213322	0.00013	0.545813
Al	-3.526499	-1.257558	0.137845	H	0.871088	0.000024	1.731274
O	-3.24846	0.363509	-0.480411	O	3.618218	-0.000023	0.183222

Atom	X	Y	Z	Atom	X	Y	Z
vdW2 JP-10/R1				vdW2 JP-10/R2			
C	1.63335	-0.51238	0.808329	Al	4.51426	0.017514	0.151504
C	1.862562	0.875495	0.108984	C	-0.765515	-0.382176	-0.960334
C	0.132283	-0.795691	0.519682	C	-1.997021	-0.457327	0.04067
C	0.481968	1.20241	-0.49301	C	-0.132211	0.911417	-0.498812
C	-0.030362	-0.193318	-0.891683	C	-1.823516	0.806745	0.910961
C	-0.637124	0.203396	1.338856	C	-0.281742	0.910097	1.016267
C	-0.474411	1.550599	0.668824	C	-0.925196	2.122866	-0.943274
C	2.633737	-1.483462	0.152321	C	-2.146213	2.046433	0.045553
C	2.994568	0.640793	-0.908536	C	0.025654	-1.684586	-0.734965
C	3.756118	-0.571905	-0.359314	C	-1.840484	-1.80197	0.773014
H	1.81814	-0.457129	1.887961	C	-1.015603	-2.667495	-0.186336
H	2.164553	1.643809	0.832121	H	-1.100482	-0.311698	-2.001755
H	-0.156394	-1.843527	0.651866	H	-2.949547	-0.431001	-0.503528
H	0.508821	1.952717	-1.290318	H	-2.373238	0.768289	1.858431
H	0.583784	-0.68679	-1.649704	H	0.193528	0.065584	1.517824
H	-1.071172	-0.186587	-1.226731	H	0.054431	1.839641	1.48598
H	-0.816588	0.081283	2.404653	H	-1.223759	2.065169	-1.993417
H	-2.665978	-0.126502	0.538375	H	-0.363069	3.050633	-0.798927
H	-1.432064	1.928718	0.283161	H	-2.201516	2.947873	0.664223
H	-0.069012	2.32003	1.337799	H	-3.101353	1.943999	-0.47896
H	2.163178	-2.002129	-0.691572	H	0.822374	-1.525147	-0.001692
H	2.981397	-2.250161	0.852086	H	0.504181	-2.030238	-1.656688
H	3.624802	1.526949	-1.035111	H	-2.809624	-2.241565	1.03076
H	2.574628	0.398878	-1.892552	H	-1.288075	-1.660176	1.70973
H	4.391779	-0.261909	0.478938	H	-1.653954	-3.028678	-1.001914
H	4.399594	-1.053192	-1.103238	H	-0.568712	-3.541937	0.297648
Al	-5.044944	-0.439893	-0.448413	O	2.8453	0.302666	0.16759
O	-3.441417	-0.095185	-0.026884	H	2.022119	0.616211	-0.214443

Atom	X	Y	Z	Atom	X	Y	Z
vdW2 JP-10/R3				vdW2 JP-10/R4			
Al	4.095524	-0.69772	-0.000129	C	0.430832	0.376646	0.635545
C	-1.088607	0.887382	0.786423	C	0.786479	0.379587	-0.852382
C	-1.087972	0.886736	-0.787095	C	1.030918	-0.872995	1.223273
C	-1.379	-0.584568	1.138781	C	1.657814	-0.888466	-0.964546
C	-1.377783	-0.585652	-1.138361	C	2.35191	-0.928228	0.411189
C	-0.699266	-1.310212	0.000885	C	0.285709	-2.09836	0.644126
C	-2.861715	-0.871703	0.780555	C	0.71297	-2.103384	-0.85505
C	-2.860897	-0.872419	-0.781416	C	0.580955	1.763759	1.207038
C	0.305547	1.395537	1.195541	C	1.45139	1.754653	-1.048029
C	0.306204	1.395255	-1.195751	C	0.712478	2.65329	-0.043653
C	0.768171	2.235265	-0.000031	H	-1.633192	0.132118	0.231936
H	-1.867297	1.545808	1.191469	H	-0.0972	0.307527	-1.502862
H	-1.86677	1.544285	-1.193337	H	1.129034	-0.872016	2.313182
H	-1.097301	-0.872298	2.155848	H	2.315742	-0.907387	-1.839944
H	-1.094942	-0.874355	-2.154832	H	3.012134	-0.076078	0.601445
H	-0.514711	-2.384328	0.001415	H	2.913338	-1.854801	0.580693
H	-3.529249	-0.115547	1.206827	H	-0.79604	-2.016299	0.769966
H	-3.171417	-1.84535	1.172437	H	0.614111	-3.010637	1.153174
H	-3.170353	-1.846368	-1.172744	H	1.242461	-3.027258	-1.10989
H	-3.527907	-0.116581	-1.209065	H	-0.143269	-2.014138	-1.530201
H	0.984735	0.545272	1.321992	H	1.497296	1.814299	1.817067
H	0.286597	1.947269	2.140998	H	-0.247031	2.056055	1.864232
H	0.287188	1.947224	-2.141062	H	1.380745	2.110769	-2.080704
H	0.985684	0.545213	-1.322272	H	2.51522	1.700133	-0.786139
H	0.255492	3.205005	-0.000355	H	-0.285066	2.889969	-0.430898
H	1.846117	2.429943	0.000291	H	1.227481	3.598333	0.154087
O	2.5291	-1.342602	0.000644	Al	-4.199599	-0.066018	-0.095101
H	1.57142	-1.297743	0.001731	O	-2.507463	-0.023921	-0.139237

Atom	X	Y	Z	Atom	X	Y	Z
vdW2 JP-10/R5				vdW2 JP-10/R6			
Al	-4.290743	-1.127192	-0.247615	Al	-4.292772	-1.099693	-0.000807
C	0.270918	-0.031515	0.617712	C	0.397964	0.082639	0.786753
C	0.601366	0.346557	-0.868319	C	0.396683	0.080381	-0.785972
C	1.63325	-0.513924	1.177344	C	1.877341	-0.164207	1.129895
C	2.083795	-0.047785	-0.989595	C	1.875496	-0.167448	-1.130826
C	2.627245	0.355712	0.393559	C	2.59365	0.593325	-0.002137
C	1.907787	-1.903365	0.575169	C	2.214909	-1.625428	0.780591
C	2.189179	-1.584323	-0.924588	C	2.213631	-1.627662	-0.777889
C	-0.283501	1.222935	1.213093	C	-0.143666	1.45926	1.232616
C	0.348189	1.865342	-1.007505	C	-0.145662	1.455722	-1.234909
C	-0.538079	2.282102	0.184549	C	-0.727353	2.074559	-0.00156
H	-0.452621	-0.859384	0.674577	H	-0.242706	-0.713057	1.180435
H	-0.026535	-0.212149	-1.57203	H	-0.244608	-0.71646	-1.176319
H	1.702099	-0.47122	2.269488	H	2.145919	0.123632	2.152527
H	2.585746	0.397193	-1.856026	H	2.142402	0.117459	-2.154716
H	2.534836	1.423371	0.614731	H	2.396382	1.670702	-0.003517
H	3.669562	0.052976	0.545816	H	3.678528	0.437421	-0.002801
H	1.063239	-2.586025	0.714076	H	1.487169	-2.322999	1.207143
H	2.781716	-2.361704	1.049936	H	3.200119	-1.89846	1.173063
H	3.191057	-1.915956	-1.216206	H	3.198194	-1.901824	-1.171197
H	1.475511	-2.065552	-1.60109	H	1.485192	-2.326451	-1.201246
H	-0.494285	1.340434	2.272854	H	0.674319	2.086163	1.626705
H	-2.340756	0.309184	0.671533	H	-0.871891	1.369643	2.048088
H	1.30062	2.404305	-0.967878	H	-0.875183	1.363794	-2.04897
H	-1.596105	2.296382	-0.118857	H	0.671696	2.081475	-1.632113
H	-0.30956	3.290211	0.549702	H	-1.21408	3.047061	-0.00256
O	-3.02891	-0.055467	0.116179	O	-2.852151	-0.210196	0.004287
H	-0.114484	2.104754	-1.969581	H	-2.32617	0.592633	0.002295

Atom	X	Y	Z	Atom	X	Y	Z
vdW1 Site 1 JP-10/BO				vdW1 Site 2 JP-10/BO			
C	-1.286342	-0.786229	-0.500869	C	-0.088229	-0.301962	-0.772602
C	-1.286011	0.785302	-0.502464	C	-1.537642	-0.633887	-0.264029
C	0.148561	-1.131535	-0.06581	C	0.229213	1.034954	-0.079758
C	0.149023	1.130911	-0.068073	C	-1.862899	0.559166	0.651504
C	0.468168	0.000617	0.92678	C	-0.48917	0.870544	1.271403
C	1.098476	-0.781059	-1.227126	C	-0.63346	2.127191	-0.740032
C	1.098865	0.777729	-1.228635	C	-2.073633	1.798961	-0.239057
C	-2.40296	-1.198466	0.476515	C	0.784279	-1.497705	-0.347518
C	-2.402473	1.199985	0.47406	C	-1.428503	-2.004235	0.430589
C	-3.358119	0.000968	0.489536	C	-0.205062	-2.661997	-0.219328
H	-1.498827	-1.190246	-1.499225	H	-0.059714	-0.190731	-1.864328
H	-1.498315	1.187373	-1.501643	H	-2.2538	-0.694355	-1.093826
H	0.263197	-2.153772	0.312784	H	1.298561	1.260411	-0.035613
H	0.264065	2.153855	0.308485	H	-2.68191	0.368736	1.354639
H	-0.168294	0.001641	1.816957	H	-0.087696	0.062241	1.889512
H	1.517319	0.000729	1.238689	H	-0.490971	1.792087	1.865269
H	0.756809	-1.208964	-2.175669	H	-0.549549	2.108336	-1.83161
H	2.104136	-1.163338	-1.02867	H	-0.319238	3.12161	-0.40535
H	2.104705	1.1599	-1.030842	H	-2.484583	2.628792	0.345929
H	0.757475	1.203941	-2.178032	H	-2.773151	1.597961	-1.057153
H	-1.988366	-1.350936	1.480711	H	1.253237	-1.295036	0.622632
H	-2.886069	-2.135383	0.179918	H	1.594264	-1.687357	-1.059009
H	-2.885201	2.136491	0.175553	H	-2.345631	-2.593702	0.32729
H	-1.987816	1.354335	1.477941	H	-1.248385	-1.870349	1.50446
H	-3.966171	0.000156	-0.42348	H	-0.471591	-3.03429	-1.216281
H	-4.042879	0.00198	1.344385	H	0.189167	-3.506935	0.355611
B	5.330651	0.001592	0.823605	B	4.975952	0.313481	0.215318
O	4.142231	0.000618	0.592579	O	3.797735	0.577375	0.134276

Atom	X	Y	Z	Atom	X	Y	Z
vdW1 Site 3 JP-10/BO				vdW1 Site 4 JP-10/BO			
C	0.637902	0.879564	-0.785759	C	0.379974	0.333007	0.785312
C	0.637879	0.879491	0.785824	C	0.379837	0.333122	-0.785227
C	1.139565	-0.533352	-1.131277	C	0.331391	-1.165736	1.131349
C	1.139535	-0.533457	1.13124	C	0.331193	-1.16558	-1.131472
C	0.524033	-1.37646	-0.000063	C	1.171149	-1.784644	-0.000182
C	2.637861	-0.607415	-0.779689	C	-1.074783	-1.689172	0.779331
C	2.637834	-0.607533	0.779686	C	-1.074915	-1.689074	-0.779284
C	-0.811963	1.194611	-1.198703	C	1.663274	1.076766	1.199455
C	-0.812002	1.194486	1.198747	C	1.663058	1.076937	-1.199488
C	-1.392189	1.954425	0.000052	C	1.981561	1.977751	0.000021
H	1.315887	1.643402	-1.188582	H	-0.501502	0.853022	1.178088
H	1.315853	1.64329	1.188739	H	-0.501717	0.853179	-1.177772
H	0.903344	-0.849141	-2.153881	H	0.652307	-1.396038	2.153884
H	0.903274	-0.849327	2.15381	H	0.651931	-1.395722	-2.154099
H	-0.56872	-1.389443	-0.000073	H	2.21806	-1.46682	-0.000252
H	0.888036	-2.410971	-0.000101	H	1.141007	-2.880617	-0.000252
H	3.198463	0.231959	-1.204142	H	-1.861519	-1.052786	1.19445
H	3.081582	-1.528928	-1.171678	H	-1.219019	-2.701138	1.173573
H	3.081484	-1.529141	1.171537	H	-1.219204	-2.700995	-1.173623
H	3.198484	0.231732	1.204288	H	-1.861729	-1.052647	-1.194191
H	-1.375131	0.265998	-1.342899	H	2.483241	0.363983	1.35301
H	-0.858888	1.759385	-2.136038	H	1.535833	1.629902	2.136026
H	-0.858971	1.759157	2.136141	H	1.535454	1.630212	-2.135954
H	-1.375164	0.265849	1.34282	H	2.482999	0.364178	-1.353294
H	-1.02755	2.989375	0.00011	H	1.308788	2.844185	0.000143
H	-2.486873	1.984457	0.000034	H	3.009896	2.355101	-0.000045
B	-4.336747	-1.726171	-0.00014	B	-4.04504	1.927611	-0.000238
O	-3.210262	-1.281621	0.000034	O	-3.017507	1.286835	0.000325

Atom	X	Y	Z	Atom	X	Y	Z
vdW1 Site 5 JP-10/BO				vdW1 Site 6 JP-10/BO			
C	0.162527	0.205488	0.426204	C	0.637852	0.879442	-0.78586
C	-0.368143	-0.523045	-0.860937	C	0.637917	0.87957	0.785708
C	-1.13012	0.68876	1.106199	C	1.139585	-0.533504	-1.13123
C	-1.894106	-0.359941	-0.748451	C	1.139677	-0.533324	1.131267
C	-2.11461	-0.445938	0.772322	C	0.524162	-1.376503	0.000113
C	-1.708318	1.841577	0.263033	C	2.637908	-0.60743	-0.779722
C	-2.235827	1.118831	-1.014159	C	2.63797	-0.607316	0.779648
C	0.974317	-0.851769	1.196573	C	-0.812056	1.194328	-1.198756
C	0.162958	-1.965522	-0.768713	C	-0.811956	1.194523	1.198678
C	1.407845	-1.852431	0.119306	C	-1.392267	1.954273	-0.000074
H	0.815736	1.046829	0.169896	H	1.315775	1.643256	-1.188833
H	0.008773	-0.04685	-1.775208	H	1.315882	1.643444	1.188495
H	-1.010077	0.928408	2.168908	H	0.90332	-0.849413	-2.153785
H	-2.46356	-1.067913	-1.361481	H	0.90349	-0.849062	2.153892
H	-1.838356	-1.411742	1.205264	H	-0.568595	-1.389536	0.000163
H	-3.145644	-0.21559	1.065486	H	0.888195	-2.411005	0.000181
H	-0.950372	2.599159	0.039176	H	3.198459	0.231897	-1.204337
H	-2.524614	2.34076	0.796245	H	3.081648	-1.52899	-1.171585
H	-3.317676	1.252281	-1.121702	H	3.081734	-1.528824	1.171607
H	-1.767558	1.485479	-1.933409	H	3.198565	0.232066	1.204094
H	0.340824	-1.353571	1.939326	H	-1.375171	0.265653	-1.342777
H	1.81882	-0.40456	1.729633	H	-0.859089	1.758955	-2.136174
H	0.370123	-2.392356	-1.755838	H	-0.858909	1.759304	2.136007
H	-0.58025	-2.612251	-0.285461	H	-1.375067	0.265878	1.342897
H	2.237088	-1.424372	-0.454464	H	-1.027715	2.989254	-0.000177
H	1.73815	-2.814426	0.526364	H	-2.486951	1.984195	-0.000031
B	4.557266	1.646835	-0.392524	B	-4.336727	-1.72652	-0.000581
O	3.492891	1.09006	-0.242297	O	-3.210586	-1.281103	0.00058

Atom	X	Y	Z	Atom	X	Y	Z
TS1 JP-10/BO				TS2 JP-10/BO			
C	1.014145	-0.652867	0.684473	C	0.272786	0.43704	-0.773867
C	1.412093	0.825558	0.331264	C	1.657749	-0.134243	-0.264942
C	-0.397908	-0.788092	0.069935	C	-0.693408	-0.527298	-0.104895
C	0.177615	1.347016	-0.42613	C	1.2437	-1.321391	0.629803
C	-0.285182	0.092351	-1.187829	C	-0.06892	-0.804004	1.260335
C	-1.32501	0.059418	0.9287	C	-0.662033	-1.890188	-0.785316
C	-0.967	1.516019	0.595009	C	0.709879	-2.45188	-0.276863
C	2.099818	-1.541239	0.046702	C	0.231941	1.90266	-0.303205
C	2.709671	0.717782	-0.490835	C	2.342391	1.042589	0.454247
C	3.321461	-0.620345	-0.058791	C	1.708923	2.292448	-0.167823
H	0.986729	-0.818203	1.76875	H	0.190162	0.385513	-1.866026
H	1.59341	1.419609	1.235961	H	2.276986	-0.475944	-1.103781
H	-0.724379	-1.823657	-0.075957	H	-1.953494	-0.0197	-0.031817
H	0.367808	2.238616	-1.033146	H	2.023053	-1.640091	1.33136
H	0.443807	-0.276043	-1.914298	H	0.056591	0.082014	1.887152
H	-1.242477	0.232569	-1.702623	H	-0.600989	-1.573018	1.830007
H	-1.404032	-0.214336	1.984575	H	-0.714841	-1.810656	-1.874767
H	-2.517852	-0.158877	0.496746	H	-1.493793	-2.520139	-0.452655
H	-1.818766	2.041493	0.143712	H	0.563981	-3.372628	0.296965
H	-0.663231	2.088068	1.477839	H	1.398352	-2.677988	-1.096942
H	1.789051	-1.860625	-0.955434	H	-0.261933	1.977905	0.672902
H	2.286088	-2.446937	0.632428	H	-0.324796	2.540656	-0.996547
H	3.373575	1.572145	-0.325028	H	3.431321	1.008911	0.347088
H	2.479133	0.690212	-1.562858	H	2.121365	1.010836	1.528122
H	3.790896	-0.512868	0.926467	H	2.137468	2.470948	-1.161349
H	4.084101	-0.991898	-0.750866	H	1.8629	3.19803	0.427544
B	-3.871099	-0.402171	-0.015786	B	-3.248166	0.498339	0.093944
O	-5.003323	-0.612752	-0.402791	O	-4.366196	0.956156	0.223522

Atom	X	Y	Z	Atom	X	Y	Z
TS3 JP-10/BO				TS4 JP-10/BO			
C	0.607771	0.923543	-0.785755	C	-0.213747	0.326327	0.446942
C	0.607835	0.923685	0.785556	C	0.580804	0.435358	-0.878368
C	0.960913	-0.531952	-1.139281	C	0.388763	-0.863395	1.18003
C	0.960789	-0.531802	1.139312	C	1.615488	-0.696317	-0.7262
C	0.327335	-1.322277	0.000038	C	1.876298	-0.689633	0.792031
C	2.451824	-0.753161	-0.781217	C	0.041769	-2.157509	0.415164
C	2.45174	-0.753098	0.781417	C	0.875465	-2.037511	-0.896373
C	-0.793095	1.408137	-1.201704	C	-0.231158	1.702107	1.100175
C	-0.792854	1.408697	1.201659	C	1.110893	1.880914	-0.888424
C	-1.283753	2.22551	-0.000164	C	0.081733	2.660094	-0.058036
H	1.368206	1.605911	-1.185579	H	-1.443723	0.078661	0.157731
H	1.368468	1.605956	1.185159	H	-0.058388	0.268589	-1.757413
H	0.694378	-0.832984	-2.157382	H	0.16448	-0.894361	2.251059
H	0.694161	-0.832682	2.157432	H	2.494635	-0.58278	-1.369499
H	-1.033643	-1.319837	-0.000488	H	2.321424	0.237993	1.164174
H	0.502984	-2.403813	0.000131	H	2.493891	-1.532413	1.123634
H	3.084718	0.031883	-1.207289	H	-1.031683	-2.259664	0.231199
H	2.805394	-1.711781	-1.173338	H	0.352543	-3.02936	0.999574
H	2.805291	-1.711671	1.17367	H	1.588585	-2.863416	-0.983993
H	3.084573	0.032002	1.207475	H	0.251941	-2.047171	-1.795831
H	-1.461472	0.555638	-1.368372	H	0.556355	1.754419	1.86466
H	-0.76841	1.980828	-2.134342	H	-1.181778	1.914116	1.603746
H	-0.767684	1.982027	2.133898	H	1.231577	2.268912	-1.904728
H	-1.461329	0.556454	1.369348	H	2.092244	1.9255	-0.400604
H	-0.801824	3.210716	-0.000412	H	-0.823645	2.82898	-0.653066
H	-2.366632	2.385119	-0.000092	H	0.44466	3.636396	0.277851
B	-2.4122	-1.581556	-0.000581	O	-3.997019	-0.515425	-0.371026
O	-3.584652	-1.90121	0.00049	B	-2.846961	-0.188723	-0.152387

Atom	X	Y	Z	Atom	X	Y	Z
TS5 JP-10/BO				TS6 JP-10/BO			
C	-0.152024	-0.259404	-0.170492	O	4.426367	-1.442731	0.000026
C	0.812778	0.85797	-0.716938	C	-0.127232	-0.092518	-0.786394
C	0.771813	-1.135205	0.692661	C	-0.127238	-0.092561	0.786382
C	2.165082	0.465655	-0.095756	C	-1.619648	0.053471	-1.131741
C	1.739701	-0.090964	1.275111	C	-1.619654	0.053449	1.131734
C	1.702745	-1.91494	-0.255038	C	-2.119705	0.968621	0.000005
C	2.663101	-0.812678	-0.796707	C	-2.322109	-1.271409	-0.779523
C	-1.23555	0.499338	0.583969	C	-2.32216	-1.2714	0.779494
C	0.227604	2.197526	-0.225448	C	0.767042	1.087868	-1.214427
C	-1.262852	1.911628	0.025405	C	0.767054	1.087789	1.214479
H	-0.599986	-0.843706	-0.986697	C	1.628388	1.368854	0.00003
H	0.8627	0.847086	-1.81272	H	0.278234	-1.029132	-1.188688
H	0.238709	-1.762772	1.415296	H	0.278203	-1.029204	1.18863
H	2.895027	1.282631	-0.08107	H	-1.804179	0.400179	-2.154554
H	1.255548	0.646406	1.923056	H	-1.804175	0.400144	2.154554
H	2.571818	-0.543889	1.825561	H	-1.663917	1.963818	0.000015
H	1.144948	-2.421675	-1.048866	H	-3.209013	1.087544	0.000006
H	2.256088	-2.682014	0.296202	H	-1.800546	-2.134681	-1.204705
H	3.70039	-1.024896	-0.518109	H	-3.34413	-1.280895	-1.172019
H	2.630303	-0.71854	-1.886752	H	-3.344215	-1.280803	1.171914
H	-1.190312	0.42443	1.674835	H	-1.800692	-2.134704	1.204731
H	-2.364228	-0.073817	0.30207	H	0.158079	1.974289	-1.442602
H	0.386736	3.006316	-0.945966	H	1.351638	0.864823	-2.113895
H	0.7092	2.498045	0.712201	H	1.351648	0.864692	2.113936
H	-1.804703	1.919939	-0.929448	H	0.158095	1.9742	1.442706
H	-1.744205	2.63561	0.689125	H	2.236527	2.277895	0.000061
O	-4.680504	-1.251177	-0.275972	B	3.522055	-0.631545	-0.000096
B	-3.619678	-0.698657	-0.06431	H	2.508793	0.428426	-0.000059

Atom	X	Y	Z	Atom	X	Y	Z
vdW2 HBO/R1				vdW2 HBO/R2			
C	1.06015	-0.422629	0.874749	O	5.123371	0.217198	0.069428
C	1.683835	0.746792	0.030983	C	-0.064226	-0.294278	-0.661145
C	-0.447076	-0.34187	0.505197	C	-1.607255	-0.560083	-0.393209
C	0.47096	1.331998	-0.719007	C	0.120752	1.001773	0.098204
C	-0.375063	0.072691	-0.979292	C	-2.01886	0.628464	0.502696
C	-0.961317	0.928626	1.122785	C	-0.736988	0.852064	1.345055
C	-0.411005	2.076819	0.307074	C	-0.504482	2.174161	-0.632254
C	1.794445	-1.701016	0.426944	C	-2.030907	1.910148	-0.360746
C	2.758687	0.087681	-0.853518	C	0.662111	-1.543373	-0.127899
C	3.142105	-1.191146	-0.098638	C	-1.672044	-1.950518	0.263717
H	1.203123	-0.265511	1.950526	C	-0.392275	-2.654465	-0.201505
H	2.14507	1.50528	0.676069	H	0.137807	-0.164145	-1.730847
H	-1.008942	-1.251622	0.74221	H	-2.176664	-0.558352	-1.331137
H	0.736193	1.925971	-1.600145	H	-2.945215	0.458197	1.063345
H	0.117556	-0.665117	-1.618125	H	-0.473669	0.00559	1.983041
H	-1.357337	0.302588	-1.405502	H	-0.783447	1.760263	1.954103
H	-1.238685	1.012076	2.170177	H	-0.258675	2.183856	-1.69766
H	-3.460249	0.091031	0.410367	H	-0.19172	3.131172	-0.203107
H	-1.20955	2.639341	-0.199864	H	-2.478231	2.744478	0.189121
H	0.156621	2.801451	0.904573	H	-2.602531	1.777103	-1.284574
H	1.242945	-2.194333	-0.382556	H	0.968324	-1.390562	0.913524
H	1.891883	-2.425714	1.24156	H	1.565789	-1.768771	-0.702901
H	3.607766	0.754251	-1.035732	H	-2.585908	-2.488655	-0.008163
H	2.336615	-0.173242	-1.83184	H	-1.665447	-1.854239	1.356303
H	3.797298	-0.941438	0.744653	H	-0.508084	-2.986775	-1.2402
H	3.668159	-1.921403	-0.722332	H	-0.137093	-3.532153	0.401065
O	-5.36655	-1.047284	-0.458145	B	3.957036	0.541682	0.122606
B	-4.398078	-0.468602	-0.016509	H	2.827653	0.853644	0.172148

Atom	X	Y	Z	Atom	X	Y	Z
vdW2 HBO/R3				vdW2 HBO/R4			
O	4.86964	-1.191161	0.000139	C	0.055228	0.229493	0.623954
C	-0.916675	0.832268	0.786703	C	0.392086	0.438239	-0.851985
C	-0.916611	0.83217	-0.786787	C	1.159863	-0.613511	1.202806
C	-1.132834	-0.653066	1.137569	C	1.756555	-0.273995	-0.966436
C	-1.132695	-0.653216	-1.137485	C	2.368497	-0.027724	0.426916
C	-0.410766	-1.33718	0.000132	C	1.073264	-2.026124	0.579827
C	-2.59959	-1.013041	0.780758	C	1.48999	-1.791639	-0.904436
C	-2.59949	-1.013165	-0.780807	C	-0.458308	1.51323	1.224355
C	0.450905	1.407005	1.19697	C	0.349647	1.969673	-1.00975
C	0.450982	1.406901	-1.197024	C	-0.726992	2.405464	-0.003088
C	0.879488	2.262628	-0.00005	H	-2.359343	-0.675068	0.235686
H	-1.726187	1.451752	1.192834	H	-0.342831	-0.017667	-1.534108
H	-1.726112	1.451575	-1.193061	H	1.230797	-0.601632	2.294703
H	-0.838361	-0.924515	2.155738	H	2.359935	0.041573	-1.824303
H	-0.838096	-0.924792	-2.155583	H	2.5543	1.027321	0.651442
H	-0.146682	-2.393335	0.00022	H	3.294455	-0.591683	0.591728
H	-3.304847	-0.291973	1.207396	H	0.070275	-2.450357	0.677825
H	-2.859906	-2.00122	1.172397	H	1.76995	-2.704924	1.082837
H	-2.859732	-2.001413	-1.172321	H	2.398757	-2.351273	-1.148827
H	-3.304709	-0.292181	-1.207651	H	0.716051	-2.098886	-1.614862
H	1.165834	0.586874	1.336487	H	0.318075	1.962923	1.864127
H	0.402615	1.963669	2.138547	H	-1.340777	1.375557	1.861634
H	0.402733	1.963488	-2.138649	H	0.13442	2.282177	-2.036644
H	1.165933	0.586773	-1.336439	H	1.317503	2.401432	-0.727178
H	0.324739	3.208829	-0.000109	H	-1.720778	2.187241	-0.411151
H	1.947456	2.504643	-0.000027	H	-0.694247	3.474361	0.228918
B	3.661678	-1.282694	-0.00009	O	-4.634075	-1.193439	-0.260676
H	2.493526	-1.373227	-0.000319	B	-3.478583	-0.930444	-0.007882

Atom	X	Y	Z	Atom	X	Y	Z
vdW2 HBO/R5				vdW2 HBO/R6			
O	-5.066482	-1.266714	-0.438997	O	3.113165	1.684621	-0.057578
C	-0.034586	-0.172982	0.443366	C	0.065817	0.388285	0.594482
C	0.509464	0.483381	-0.875785	C	-0.062709	-0.295893	-0.816015
C	1.244805	-0.717143	1.124697	C	-1.384372	0.384472	1.109777
C	2.017515	0.184796	-0.801045	C	-1.570006	-0.588815	-0.921993
C	2.291679	0.326607	0.707343	C	-1.922005	-0.937643	0.535148
C	1.708459	-1.948575	0.325934	C	-2.186724	1.418037	0.298252
C	2.225711	-1.328174	-1.007438	C	-2.311302	0.748678	-1.103608
C	-0.740083	0.938098	1.15163	C	1.047508	-0.471802	1.420263
C	0.158132	1.986007	-0.793714	C	0.832324	-1.555289	-0.784347
C	-0.971499	2.10785	0.247828	C	1.683813	-1.401938	0.436901
H	-0.718435	-1.01278	0.233852	H	0.453939	1.408295	0.509897
H	0.059486	0.032983	-1.769112	H	0.260856	0.377793	-1.61905
H	1.131223	-0.890707	2.199964	H	-1.464272	0.510115	2.195273
H	2.621625	0.81316	-1.464983	H	-1.819224	-1.343749	-1.676288
H	2.087644	1.324569	1.106742	H	-1.402322	-1.824194	0.913634
H	3.312916	0.03832	0.981279	H	-2.998368	-1.069053	0.694926
H	0.898477	-2.669341	0.173873	H	-1.680481	2.387816	0.262962
H	2.513533	-2.468514	0.855524	H	-3.173399	1.57874	0.745387
H	3.286041	-1.554008	-1.160518	H	-3.360503	0.575163	-1.364915
H	1.683695	-1.695621	-1.884826	H	-1.870699	1.352566	-1.903462
H	-1.177651	0.83472	2.140656	H	0.504657	-1.038368	2.196117
H	-3.150043	-0.200397	0.492309	H	1.780423	0.148164	1.949135
H	1.031857	2.552422	-0.454529	H	1.416517	-1.672533	-1.706469
H	-1.952938	2.035556	-0.251179	H	0.209439	-2.463398	-0.713237
H	-0.966122	3.0691	0.773844	H	2.447486	-2.124095	0.716566
B	-4.092356	-0.72466	0.034675	B	3.387029	0.741116	-0.769686
H	-0.125254	2.388358	-1.771188	H	3.701412	-0.114369	-1.50458

Atom	X	Y	Z	Atom	X	Y	Z
vdW1 JP-10/BO ₂				vdW2 JP-10/BO ₂			
C	-1.733966	-0.657576	-0.622443	C	0.16166	0.488401	-0.225288
C	-1.572927	0.888352	-0.38956	C	1.61713	0.09062	-0.665799
C	-0.356978	-1.214031	-0.220451	C	-0.287904	-0.727438	0.605263
C	-0.121189	1.013045	0.10502	C	1.805067	-1.299511	-0.033957
C	0.049713	-0.275864	0.929334	C	1.024377	-1.159991	1.283854
C	0.662361	-0.80827	-1.301609	C	-0.527164	-1.904632	-0.360868
C	0.807975	0.730204	-1.092168	C	0.916766	-2.298162	-0.800377
C	-2.915717	-1.088308	0.266403	C	0.305033	1.81454	0.543347
C	-2.665862	1.270216	0.625946	C	2.529535	1.206896	-0.124616
C	-3.740746	0.191289	0.447992	C	1.604452	2.423289	0.002806
H	-1.955502	-0.886144	-1.672926	H	-0.491735	0.637905	-1.093349
H	-1.717476	1.453584	-1.319335	H	1.704589	0.036342	-1.758443
H	-0.359232	-2.285425	0.008786	H	-1.118391	-0.526642	1.29461
H	0.090196	1.954859	0.624349	H	2.852316	-1.609528	0.055029
H	-0.608634	-0.332159	1.801124	H	1.434645	-0.410192	1.966064
H	1.080443	-0.4452	1.257632	H	0.92807	-2.108407	1.824637
H	0.318897	-1.068645	-2.308095	H	-1.158864	-1.6201	-1.209037
H	1.61446	-1.320514	-1.13157	H	-1.023697	-2.734528	0.152676
H	1.841191	1.006651	-0.85549	H	1.148209	-3.326944	-0.5052
H	0.516654	1.307739	-1.975694	H	1.063894	-2.226617	-1.882719
H	-2.548847	-1.432592	1.241258	H	0.407146	1.621636	1.618858
H	-3.484595	-1.913231	-0.174819	H	-0.568769	2.458919	0.406117
H	-3.039899	2.286842	0.466268	H	3.393284	1.383558	-0.773895
H	-2.266129	1.228213	1.646627	H	2.91791	0.932764	0.864127
H	-4.319547	0.391585	-0.461991	H	1.424185	2.857821	-0.987865
H	-4.445422	0.13849	1.284627	H	2.012192	3.212981	0.642482
O	3.763701	-1.111134	0.865873	O	-3.517514	-0.662742	0.521782
B	4.21371	-0.058002	0.447736	B	-3.30461	0.494362	-0.113511
O	4.703664	1.100087	-0.0109	O	-3.144441	1.555885	-0.695874

Atom	X	Y	Z	Atom	X	Y	Z
vdW3 JP-10/BO ₂				vdW4 JP-10/BO ₂			
C	-1.848	-0.062721	-0.280286	C	0.15811	0.268219	0.783547
C	-0.950366	-0.22457	0.999284	C	0.165566	0.382358	-0.785028
C	-1.119511	1.031777	-1.079208	C	1.571567	-0.250323	1.101434
C	0.176726	0.795086	0.761763	C	1.581782	-0.089987	-1.156651
C	0.356206	0.722168	-0.767665	C	2.41678	0.444834	0.019701
C	-1.306264	2.371276	-0.342078	C	1.65339	-1.7195	0.645209
C	-0.409167	2.210726	0.9226	C	1.655182	-1.609471	-0.910213
C	-1.890031	-1.456714	-0.933685	C	-0.180507	1.679169	1.300142
C	-0.523211	-1.704702	1.022775	C	-0.161088	1.855534	-1.09302
C	-1.614743	-2.425451	0.222509	C	-0.934201	2.339986	0.139337
H	-2.865102	0.258149	-0.021267	H	-0.590145	-0.448811	1.151319
H	-1.505228	0.018856	1.914346	H	-0.58526	-0.265417	-1.255247
H	-1.389488	1.061417	-2.140692	H	1.87911	-0.084191	2.139839
H	1.065389	0.617618	1.378821	H	1.901164	0.218486	-2.158299
H	0.676365	-0.257269	-1.135205	H	2.425625	1.535854	0.097041
H	1.034818	1.490442	-1.158953	H	3.453483	0.089661	0.000418
H	-2.356818	2.55661	-0.096523	H	0.816974	-2.313907	1.026711
H	-0.962861	3.205303	-0.963089	H	2.576765	-2.183949	1.006883
H	0.389595	2.959844	0.934849	H	2.57572	-2.025727	-1.332605
H	-0.969154	2.313094	1.857577	H	0.814828	-2.138035	-1.371825
H	-1.09728	-1.547386	-1.686561	H	0.743523	2.233067	1.507398
H	-2.841563	-1.644706	-1.441659	H	-0.75556	1.649868	2.231423
H	-0.413402	-2.084165	2.043971	H	-0.724208	1.963283	-2.025526
H	0.445349	-1.833515	0.525064	H	0.765522	2.43249	-1.202677
H	-2.516435	-2.534639	0.837519	H	-1.963399	1.966205	0.099447
H	-1.316364	-3.424513	-0.111398	H	-0.978196	3.431094	0.220026
O	3.156471	-1.643754	-0.445984	O	-3.608864	-0.278832	-0.369134
B	3.285811	-0.455079	-0.195834	B	-2.87082	-1.190403	-0.029947
O	3.46394	0.84113	0.081774	O	-2.086302	-2.210278	0.337718

Atom	X	Y	Z	Atom	X	Y	Z
vdW5 JP-10/BO ₂				vdW6 JP-10/BO ₂			
C	0.403328	0.446756	0.709745	C	-0.977908	-0.877496	-0.785649
C	0.521435	0.320123	-0.851471	C	-0.977702	-0.87734	0.785796
C	0.628772	-1.000127	1.193848	C	-1.606552	0.483743	-1.131251
C	0.775776	-1.187054	-1.050657	C	-1.606257	0.483964	1.131272
C	1.634975	-1.555126	0.17028	C	-1.071808	1.38053	-0.000147
C	-0.626421	-1.815944	0.829046	C	-3.105186	0.418825	-0.779469
C	-0.534373	-1.931596	-0.724021	C	-3.104983	0.418927	0.779897
C	1.465413	1.479047	1.139874	C	0.494623	-1.056724	-1.199686
C	1.678953	1.253968	-1.267317	C	0.49493	-1.056482	1.19949
C	2.493992	1.557888	0.000803	C	1.14034	-1.761253	-0.000111
H	-0.590268	0.78773	1.035101	H	-1.581585	-1.700803	-1.189035
H	-0.40059	0.609864	-1.368139	H	-1.581271	-1.700569	1.189506
H	0.914753	-1.071191	2.249182	H	-1.40071	0.819608	-2.153928
H	1.192741	-1.434454	-2.033104	H	-1.40018	0.820038	2.153832
H	2.61406	-1.074466	0.193819	H	0.01465	1.501226	-0.000314
H	1.777241	-2.637579	0.272452	H	-1.531306	2.375952	-0.000191
H	-1.545006	-1.329964	1.175753	H	-3.586269	-0.468416	-1.204047
H	-0.592346	-2.80425	1.299583	H	-3.631519	1.295575	-1.171439
H	-0.469013	-2.979685	-1.034255	H	-3.631241	1.295708	1.171895
H	-1.39195	-1.490182	-1.240336	H	-3.585915	-0.468278	1.204724
H	1.915997	1.224827	2.105971	H	0.961262	-0.075996	-1.346622
H	0.98355	2.456655	1.258657	H	0.594282	-1.614165	-2.137056
H	1.259603	2.18722	-1.660522	H	0.594819	-1.613738	2.136944
H	2.287329	0.816406	-2.066956	H	0.961606	-0.075725	1.346123
H	2.974819	2.540358	-0.047577	H	0.86373	-2.822782	0.000032
H	3.29245	0.825396	0.141918	H	2.235396	-1.711873	-0.000259
O	-3.063842	0.977132	1.230449	O	2.706157	1.68228	-0.00058
B	-3.080373	0.84876	-0.099884	B	3.6617	0.923826	-0.000087
O	-3.120234	0.738106	-1.315814	O	4.708689	0.090837	0.000506

Atom	X	Y	Z	Atom	X	Y	Z
TS1 JP-10/BO ₂				TS2 JP-10/BO ₂			
C	1.461748	-0.733085	0.563655	C	0.093937	0.463436	-0.416197
C	1.555716	0.832737	0.479819	C	1.637901	0.196117	-0.587296
C	0.098788	-1.036427	-0.092018	C	-0.34347	-0.772204	0.37499
C	0.228045	1.222832	-0.192899	C	1.846976	-1.148913	0.133745
C	0.008014	0.055638	-1.17138	C	0.848113	-1.044085	1.30439
C	-0.983926	-0.565673	0.886173	C	-0.333849	-1.999313	-0.543368
C	-0.906085	0.98041	0.824477	C	1.197012	-2.259471	-0.716601
C	2.691874	-1.265256	-0.196379	C	-0.018912	1.816779	0.30928
C	2.833431	1.126826	-0.327854	C	2.334867	1.413904	0.047065
C	3.705664	-0.117218	-0.121321	C	1.292152	2.534703	-0.033508
H	1.484092	-1.086159	1.602393	H	-0.42108	0.512641	-1.382413
H	1.634354	1.285308	1.476397	H	1.91195	0.116686	-1.646604
H	-0.016876	-2.072452	-0.42654	H	-1.328697	-0.641096	0.944487
H	0.224305	2.227651	-0.628425	H	2.888452	-1.347819	0.409848
H	0.77758	-0.025058	-1.943699	H	1.061077	-0.231058	2.002122
H	-0.971197	0.08674	-1.662039	H	0.744556	-1.978725	1.864942
H	-0.896129	-0.990443	1.891441	H	-0.845391	-1.804541	-1.490463
H	-1.981254	-0.952422	0.50525	H	-0.828408	-2.849203	-0.063256
H	-1.843886	1.425754	0.474011	H	1.467796	-3.248704	-0.334118
H	-0.688094	1.421461	1.802388	H	1.515624	-2.211219	-1.762296
H	2.433546	-1.462564	-1.243937	H	-0.089074	1.665696	1.393678
H	3.063523	-2.203324	0.227974	H	-0.909247	2.370339	-0.003625
H	3.317527	2.054874	-0.007511	H	3.274313	1.656983	-0.459686
H	2.593016	1.23759	-1.392298	H	2.576923	1.207752	1.096903
H	4.161169	-0.089399	0.875909	H	1.242573	2.922926	-1.057762
H	4.514842	-0.20632	-0.853454	H	1.509437	3.377218	0.630821
O	-3.405046	-1.363598	-0.178396	O	-2.849437	-0.34976	1.145073
B	-3.91876	-0.137198	-0.216502	B	-3.10113	0.267469	-0.00844
O	-4.391497	0.992354	-0.262727	O	-3.349753	0.842143	-1.061996

Atom	X	Y	Z	Atom	X	Y	Z
TS3 JP-10/BO ₂				TS4 JP-10/BO ₂			
C	1.473689	0.172466	-0.778193	C	-0.444979	0.324198	-0.691828
C	1.457155	0.171799	0.79412	C	-0.423126	0.276705	0.843049
C	0.473715	-0.937825	-1.14212	C	-0.807513	-1.062977	-1.174787
C	0.449386	-0.938525	1.135946	C	-0.888796	-1.169455	1.103095
C	-0.557811	-0.832391	-0.013905	C	-1.85288	-1.408409	-0.07393
C	1.110152	-2.297323	-0.777012	C	0.325257	-2.047677	-0.814709
C	1.093347	-2.297867	0.783749	C	0.282278	-2.105768	0.742359
C	1.076681	1.60135	-1.195021	C	-1.15478	1.589083	-1.14743
C	1.051985	1.60047	1.203803	C	-1.352682	1.438944	1.245858
C	1.469445	2.466121	0.008875	C	-1.170699	2.461615	0.115002
H	2.470235	-0.067359	-1.169414	H	0.824718	0.52662	-1.135105
H	2.44517	-0.068761	1.205979	H	0.57703	0.44793	1.264183
H	0.084412	-0.88238	-2.163557	H	-1.148107	-1.104823	-2.212929
H	0.038501	-0.883692	2.148941	H	-1.2994	-1.32494	2.105511
H	-1.097534	0.184839	-0.020238	H	-2.729179	-0.752984	-0.077701
H	-1.335245	-1.604329	-0.022433	H	-2.189747	-2.447031	-0.160914
H	2.118605	-2.387753	-1.192168	H	1.288063	-1.716321	-1.208457
H	0.51353	-3.123611	-1.176067	H	0.105127	-3.024928	-1.254782
H	0.48813	-3.124326	1.169276	H	0.079486	-3.123646	1.08929
H	2.092612	-2.38877	1.220449	H	1.218519	-1.776324	1.199953
H	-0.005082	1.666778	-1.35561	H	-2.176208	1.298894	-1.437058
H	1.563873	1.905712	-2.126946	H	-0.691871	2.054015	-2.022654
H	1.520056	1.904021	2.145738	H	-1.096634	1.834191	2.232388
H	-0.032795	1.66596	1.342189	H	-2.395012	1.099058	1.280766
H	2.555698	2.618377	0.020085	H	-0.205829	2.968082	0.22338
H	0.994522	3.452237	0.004353	H	-1.951887	3.226575	0.090591
O	-2.249682	1.193759	-0.026215	O	2.366794	0.724818	-1.26286
B	-3.313376	0.391132	-0.006537	B	2.706408	0.570636	-0.020667
O	-4.304602	-0.327792	0.011297	O	3.031508	0.423293	1.168709

Atom	X	Y	Z	Atom	X	Y	Z
TS5 JP-10/BO ₂				TS6 JP-10/BO ₂			
C	0.071036	-0.107928	0.655572	C	-0.6221	0.242391	1.145214
C	0.261834	0.019994	-0.896666	C	-1.25705	1.230288	0.103144
C	1.513979	0.022421	1.198059	C	-0.687303	-1.120015	0.416646
C	1.792314	0.100544	-1.04137	C	-1.758148	0.281997	-0.998177
C	2.197153	0.948066	0.175925	C	-0.609625	-0.735331	-1.073157
C	2.225348	-1.309672	0.892464	C	-2.149219	-1.594084	0.502559
C	2.378046	-1.274084	-0.658891	C	-2.898026	-0.576003	-0.41127
C	-0.884744	1.019391	1.052585	C	0.784274	0.777413	1.46071
C	-0.504735	1.295287	-1.321317	C	-0.122676	2.179396	-0.350183
C	-0.825955	2.085851	-0.039957	C	1.14675	1.711751	0.335072
H	-0.335412	-1.086188	0.939478	H	-1.210665	0.194428	2.068531
H	-0.129378	-0.856396	-1.425102	H	-2.082584	1.810211	0.532439
H	1.567087	0.32727	2.2491	H	0.052474	-1.845506	0.767664
H	2.12024	0.466932	-2.02035	H	-2.019477	0.794391	-1.930776
H	1.813721	1.969845	0.157613	H	0.344775	-0.31488	-1.392966
H	3.283362	0.989451	0.318598	H	-0.838284	-1.58361	-1.727985
H	1.653634	-2.173771	1.244574	H	-2.525305	-1.602268	1.530477
H	3.20367	-1.339798	1.383573	H	-2.241004	-2.612413	0.111697
H	3.430288	-1.341325	-0.953525	H	-3.445207	-1.086609	-1.209635
H	1.84535	-2.092073	-1.153734	H	-3.620937	0.035073	0.139524
H	-0.745007	1.390622	2.074571	H	1.521281	-0.015226	1.634808
H	-1.949186	0.614591	1.05655	H	0.763467	1.384754	2.379045
H	-1.439347	1.011728	-1.81748	H	-0.313603	3.210254	-0.019625
H	0.068411	1.888561	-2.042428	H	-0.023479	2.223581	-1.440695
H	-1.764468	2.642756	-0.118957	H	1.945434	2.439927	0.504286
H	-0.042865	2.814593	0.188559	H	1.8313	0.984422	-0.587957
O	-3.374455	0.075284	0.461825	O	2.848651	0.031577	-1.288445
B	-2.931365	-1.08289	-0.021543	B	2.90094	-0.895152	-0.369275
O	-2.534162	-2.151732	-0.470794	O	2.95083	-1.772526	0.501469

Atom	X	Y	Z	Atom	X	Y	Z
vdW2 BO ₂ /R1				vdW2 BO ₂ /R2			
C	-1.145326	-0.498976	-0.822161	C	0.065223	0.365085	-0.467204
C	-1.910508	0.708415	-0.172209	C	1.640829	0.569357	-0.542133
C	0.312293	-0.294249	-0.318987	C	0.021697	-0.955831	0.269699
C	-0.808716	1.443633	0.614952	C	2.198373	-0.665873	0.199181
C	0.072618	0.276784	1.094174	C	1.131769	-0.883022	1.303993
C	0.810904	0.930558	-1.03766	C	0.410667	-2.121412	-0.617461
C	0.128733	2.12542	-0.405965	C	1.968788	-1.913939	-0.683122
C	-1.848343	-1.77	-0.307723	C	-0.477271	1.613032	0.255581
C	-3.028493	0.076062	0.677497	C	1.902739	1.929127	0.129131
C	-3.266313	-1.295353	0.033339	C	0.580385	2.690098	-0.014491
H	-1.186787	-0.464961	-1.917362	H	-0.378273	0.281381	-1.465938
H	-2.347663	1.364228	-0.935655	H	1.982679	0.587437	-1.584285
H	0.934914	-1.191428	-0.400543	H	-1.878316	-1.120725	0.86894
H	-1.185965	2.115398	1.392873	H	3.231623	-0.545001	0.543495
H	-0.440962	-0.419185	1.761751	H	1.047619	-0.052722	2.007636
H	0.994247	0.609259	1.582448	H	1.277298	-1.81586	1.856936
H	1.12013	0.908097	-2.081592	H	-0.068066	-2.078157	-1.599034
H	2.666387	0.866524	-0.243965	H	0.163848	-3.083545	-0.158218
H	0.845959	2.784929	0.105531	H	2.491572	-2.783002	-0.271724
H	-0.407131	2.745804	-1.134512	H	2.324172	-1.764345	-1.707027
H	-1.35236	-2.141163	0.596925	H	-0.555024	1.428744	1.333838
H	-1.824641	-2.578269	-1.045094	H	-1.472768	1.886663	-0.10483
H	-3.925784	0.702188	0.707892	H	2.753885	2.447837	-0.323666
H	-2.690223	-0.055176	1.712581	H	2.136453	1.788506	1.191489
H	-3.848863	-1.176514	-0.888106	H	0.473639	3.06144	-1.040555
H	-3.809671	-1.990034	0.681948	H	0.500106	3.549174	0.658941
O	3.49541	0.65503	0.227456	O	-2.851599	-1.038372	0.927254
B	3.834296	-0.626647	0.179462	B	-3.369869	-0.240397	0.004668
O	4.177821	-1.800058	0.157047	O	-3.878438	0.495175	-0.830801

Atom	X	Y	Z	Atom	X	Y	Z
vdW2 BO ₂ /R3				vdW2 BO ₂ /R4			
C	-0.881412	0.968179	0.764356	C	0.497429	0.364124	0.675806
C	-0.896361	0.922574	-0.807796	C	0.463726	0.276913	-0.853881
C	-1.378623	-0.434644	1.163495	C	0.963232	-0.977249	1.179198
C	-1.399997	-0.501022	-1.115107	C	1.006145	-1.147444	-1.091224
C	-0.830794	-1.288451	0.043029	C	2.001088	-1.311445	0.073897
C	-2.890684	-0.517608	0.821181	C	-0.121955	-2.036009	0.875596
C	-2.905293	-0.563273	-0.740169	C	-0.105877	-2.1356	-0.680839
C	0.573829	1.281861	1.15609	C	1.076568	1.691355	1.104385
C	0.5513	1.212325	-1.244838	C	1.324443	1.478538	-1.28872
C	1.167502	1.982667	-0.071123	C	1.065846	2.522353	-0.191369
H	-1.554321	1.741944	1.153641	H	-1.384343	0.638854	1.160588
H	-1.577253	1.672583	-1.228412	H	-0.542131	0.381243	-1.287327
H	-1.132528	-0.73177	2.186977	H	1.330383	-0.981686	2.209871
H	-1.172822	-0.857705	-2.123825	H	1.404814	-1.311955	-2.097553
H	1.256786	-1.634737	-0.037477	H	2.842538	-0.612269	0.044206
H	-0.843801	-2.379492	0.074897	H	2.392969	-2.331209	0.164186
H	-3.436281	0.33925	1.229193	H	-1.098758	-1.75822	1.279716
H	-3.333587	-1.42433	1.244112	H	0.156261	-2.990406	1.334099
H	-3.355263	-1.493033	-1.101054	H	0.143871	-3.15125	-1.003456
H	-3.459089	0.268454	-1.187277	H	-1.068208	-1.875865	-1.132033
H	1.115938	0.348997	1.354467	H	2.108165	1.536443	1.458533
H	0.637563	1.880118	2.070486	H	0.533385	2.1632	1.932326
H	0.596381	1.756955	-2.193232	H	1.067155	1.831576	-2.291924
H	1.087736	0.268545	-1.399336	H	2.384993	1.199269	-1.29467
H	0.832793	3.026549	-0.098272	H	0.075246	2.968844	-0.334616
H	2.261023	1.977146	-0.079142	H	1.798527	3.33469	-0.184171
O	2.169193	-1.963546	-0.115308	O	-2.359706	0.754129	1.168158
B	3.131357	-1.061962	0.022654	B	-2.923656	0.396657	0.022903
O	4.051199	-0.264618	0.141092	O	-3.459101	0.073651	-1.029332

Atom	X	Y	Z	Atom	X	Y	Z
vdW2 BO ₂ /R5				vdW2 BO ₂ /R6			
C	0.232005	0.155898	0.78197	C	-0.720762	0.305292	1.143938
C	0.202568	-0.254542	-0.733478	C	-1.463548	1.138442	0.036263
C	1.750149	0.322439	1.073321	C	-0.573614	-1.086552	0.4893
C	1.698054	-0.303682	-1.096	C	-1.77114	0.077428	-1.03408
C	2.274444	0.857216	-0.268737	C	-0.480936	-0.756511	-1.011676
C	2.369102	-1.08688	1.104465	C	-1.954413	-1.76346	0.544475
C	2.324952	-1.521811	-0.391131	C	-2.797547	-0.917374	-0.456967
C	-0.538874	1.436646	0.859617	C	0.601998	1.039164	1.436649
C	-0.604844	0.837576	-1.477996	C	-0.469398	2.225049	-0.440966
C	-0.839172	2.006011	-0.493418	C	0.822746	1.959497	0.273584
H	-0.181415	-0.615794	1.447974	H	-1.316676	0.223728	2.06019
H	-0.265108	-1.23365	-0.883806	H	-2.384805	1.59775	0.413078
H	1.960842	0.928707	1.960608	H	0.241552	-1.689119	0.902631
H	1.883768	-0.271486	-2.174903	H	-2.058876	0.504165	-2.001374
H	1.876965	1.839051	-0.541918	H	0.407959	-0.188832	-1.295989
H	3.368972	0.901391	-0.303676	H	-0.533609	-1.6511	-1.642239
H	1.815275	-1.764008	1.762361	H	-2.371867	-1.769434	1.556298
H	3.39912	-1.042386	1.473128	H	-1.881144	-2.804645	0.213929
H	3.332333	-1.712353	-0.77507	H	-3.216973	-1.543895	-1.250482
H	1.735612	-2.429816	-0.551926	H	-3.633053	-0.39904	0.025061
H	-0.545075	2.046932	1.762337	H	1.429366	0.343775	1.628503
H	-2.30947	0.510945	1.238023	H	0.504391	1.640313	2.355908
H	-1.558864	0.420108	-1.811805	H	-0.838547	3.230815	-0.188167
H	-0.075149	1.170319	-2.37664	H	-0.35494	2.217422	-1.533775
H	-1.855205	2.415788	-0.563377	H	1.630908	2.691556	0.269907
H	-0.168247	2.85227	-0.705922	H	2.313547	0.880688	-0.790405
O	-3.086456	-0.080058	1.231324	O	3.028747	0.270043	-1.041284
B	-3.115787	-0.911733	0.199414	B	3.083416	-0.820381	-0.286511
O	-3.16926	-1.688765	-0.744341	O	3.156925	-1.833555	0.394579

Normal modes	R1		R2	
	Frequencies(cm^{-1})	IR Inten	Frequencies(cm^{-1})	IR Inten
v1	150.80	0.0565	135.47	0.0973
v2	178.27	0.1355	178.27	0.0472
v3	276.22	3.2021	263.61	0.2159
v4	305.30	3.5611	316.98	0.4626
v5	329.67	0.0812	330.64	0.0729
v6	385.28	3.6049	402.51	0.0998
v7	468.04	17.5334	494.82	0.6943
v8	496.17	2.2611	522.67	0.6841
v9	550.62	0.174	554.93	0.553
v10	575.95	5.5816	662.09	1.3754
v11	668.40	0.8415	732.11	0.1221
v12	758.68	0.6212	763.99	0.3684
v13	780.21	0.5466	802.62	0.6862
v14	814.91	1.5443	838.60	0.6325
v15	880.23	0.2929	855.72	5.2264
v16	884.44	1.6787	878.64	0.491
v17	914.54	0.1984	899.11	0.0932
v18	924.55	0.6254	913.86	0.3485
v19	930.29	1.8682	934.44	0.0652
v20	941.29	1.2883	939.16	2.055
v21	956.05	0.3219	956.91	1.9992
v22	960.59	0.1298	976.43	1.666
v23	984.53	2.9519	995.74	0.7941
v24	1007.97	0.7206	1022.11	0.8302
v25	1022.76	1.445	1026.22	2.4999
v26	1037.13	3.1683	1063.26	0.2115
v27	1057.54	0.121	1071.96	0.0572
v28	1064.38	0.1548	1079.74	0.2131
v29	1075.16	0.1396	1107.09	0.2356
v30	1095.46	0.7303	1127.42	0.2747
v31	1141.55	0.592	1158.68	1.0416
v32	1163.39	0.3808	1181.18	0.396
v33	1170.34	0.6483	1212.36	0.2153
v34	1202.49	1.5431	1214.67	0.5124
v35	1215.52	0.2356	1225.81	4.9354
v36	1230.44	0.3789	1236.31	1.7613
v37	1255.23	1.6136	1251.59	3.2631

v38	1271.95	1.1613	1275.49	0.718
v39	1286.16	1.7483	1282.90	1.1925
v40	1292.83	1.9139	1302.39	2.6855
v41	1306.80	0.6116	1317.08	1.2727
v42	1318.04	0.5003	1321.47	2.0023
v43	1331.49	1.3477	1327.16	1.8236
v44	1341.74	1.6207	1333.56	2.3021
v45	1353.46	2.4893	1348.27	1.207
v46	1357.65	1.1672	1362.89	0.3059
v47	1362.39	0.7739	1376.43	0.5065
v48	1376.53	1.8215	1390.23	0.9305
v49	1385.20	0.4517	1521.19	2.1516
v50	1511.62	4.9085	1523.26	0.3473
v51	1525.26	3.0828	1528.21	3.9478
v52	1527.82	3.857	1532.92	11.1111
v53	1537.29	7.5991	1545.21	13.0778
v54	1553.92	13.0791	1556.85	8.698
v55	3034.07	39.922	3075.11	21.2737
v56	3074.04	23.7347	3075.39	33.6201
v57	3075.12	34.0002	3078.72	4.8542
v58	3075.90	21.3529	3082.96	28.5711
v59	3076.77	1.0908	3085.10	17.5351
v60	3089.05	11.0864	3094.57	31.8993
v61	3094.07	52.4341	3097.32	52.7881
v62	3096.64	17.4993	3101.15	24.5497
v63	3118.32	52.9796	3111.94	35.3399
v64	3125.42	17.7962	3131.21	27.5236
v65	3130.04	31.4355	3137.53	4.3181
v66	3135.61	29.4332	3138.78	29.9643
v67	3144.49	58.0494	3148.65	44.6576
v68	3159.25	27.6229	3158.39	49.6916
v69	3230.98	22.287	3170.19	26.1427

Normal modes	R3		R4	
	Frequencies(cm ⁻¹)	IR Inten	Frequencies(cm ⁻¹)	IR Inten
v1	104.16	0.0054	116.76	0.118
v2	185.23	0.1348	163.75	0.1894
v3	242.11	0.0313	236.22	0.2715
v4	316.87	0.078	298.48	0.4033
v5	318.54	0.7193	315.66	0.1367
v6	357.53	5.1519	389.96	0.0329
v7	448.13	5.6907	485.76	0.6848
v8	531.13	0.7104	540.63	0.2203
v9	545.67	1.1932	557.48	0.8622
v10	667.53	0.3373	627.20	3.2183
v11	721.19	17.1714	730.84	0.1909
v12	748.05	1.2071	752.93	0.3897
v13	784.07	1.1605	812.34	1.5299
v14	809.50	0.9972	838.90	1.329
v15	847.58	1.9684	865.35	0.4765
v16	876.58	0.9678	895.37	1.9823
v17	887.72	1.0122	902.41	0.509
v18	906.08	0.7601	915.23	0.764
v19	932.43	0.0221	919.73	0.5235
v20	944.46	2.5387	934.21	0.3669
v21	946.02	0.2079	946.63	1.4536
v22	975.61	0.6065	981.35	0.232
v23	976.18	1.8518	982.70	4.5103
v24	1018.18	2.246	1020.37	1.6645
v25	1023.41	1.485	1034.85	1.3566
v26	1038.80	0.0837	1059.75	0.2177
v27	1064.70	0.0626	1068.51	0.1557
v28	1071.56	0.0748	1077.45	0.054
v29	1074.56	0.4156	1114.04	2.0984
v30	1096.18	1.2723	1141.99	0.6795
v31	1172.68	0.5595	1147.14	0.077
v32	1182.00	1.5394	1169.76	0.1267
v33	1208.44	1.5999	1176.75	0.628
v34	1214.91	0.4279	1208.19	1.6476
v35	1223.76	0.5893	1230.04	1.535
v36	1225.05	1.104	1243.23	1.9789
v37	1249.99	0.9515	1250.17	0.797
v38	1263.31	0.7418	1267.13	0.2072

v39	1284.20	2.4545	1276.32	1.1544
v40	1285.33	0.0332	1289.14	1.0156
v41	1309.40	0.0009	1321.32	0.2401
v42	1319.45	0.0107	1323.00	0.2904
v43	1323.88	0.2876	1330.06	1.8542
v44	1344.33	2.2807	1333.94	4.3596
v45	1346.61	0.1505	1355.97	2.0529
v46	1362.80	0.8032	1357.53	0.2455
v47	1363.35	0.4823	1368.98	0.5108
v48	1380.09	3.6908	1385.34	0.7641
v49	1381.68	0.5039	1508.81	4.882
v50	1519.61	4.8805	1521.84	0.8681
v51	1522.90	1.0547	1524.58	1.8937
v52	1525.93	8.2565	1531.77	10.3184
v53	1541.13	2.9249	1541.39	12.7643
v54	1544.65	8.6682	1554.17	3.6726
v55	3071.89	33.7046	3022.95	27.8484
v56	3073.20	15.9668	3040.00	22.3692
v57	3073.57	0.2394	3074.05	12.9793
v58	3073.72	29.398	3080.31	40.2035
v59	3078.72	32.361	3081.79	21.9296
v60	3086.95	13.7399	3081.97	21.5085
v61	3089.82	76.3336	3092.26	55.7636
v62	3128.11	25.7678	3100.07	34.0208
v63	3130.08	27.7661	3118.08	50.8464
v64	3132.46	0.7636	3130.69	29.5244
v65	3132.82	38.8501	3134.21	32.1031
v66	3134.74	27.0655	3135.49	8.0411
v67	3144.21	44.897	3144.10	9.9717
v68	3149.73	57.6503	3148.39	51.6051
v69	3214.44	21.4684	3156.58	42.9328

Normal modes	R5		R6	
	Frequencies(cm ⁻¹)	IR Inten	Frequencies(cm ⁻¹)	IR Inten
v1	119.67	0.0683	96.11	0.6883
v2	137.09	0.2673	116.86	0.0028
v3	255.60	0.3586	252.25	0.0102
v4	296.94	0.6589	278.61	0.9791
v5	317.78	0.4154	325.99	0.0043
v6	400.86	0.4797	394.14	25.9986
v7	416.92	22.4569	402.77	2.3727
v8	500.82	0.597	499.95	0.238
v9	535.19	0.2082	531.09	0.0243
v10	622.92	0.7574	690.87	1.0594
v11	747.00	0.2122	703.96	0.5126
v12	764.39	1.9491	746.09	0.3311
v13	774.02	1.0861	785.70	0.0258
v14	813.54	0.674	810.63	0.8901
v15	846.25	0.5372	841.15	1.0587
v16	865.37	0.5833	861.12	0.9222
v17	888.39	1.7869	914.88	1.7527
v18	918.60	0.6405	920.74	0.3797
v19	935.38	0.2748	933.15	1.2003
v20	952.31	0.1458	952.28	1.303
v21	955.23	1.5834	953.68	0.138
v22	977.79	2.7445	973.02	1.4825
v23	986.25	0.4756	987.74	0.4554
v24	1006.20	1.9206	990.58	2.1979
v25	1028.10	1.5785	1040.77	2.2594
v26	1046.51	0.1983	1052.08	0.0364
v27	1064.92	0.1531	1067.31	0.6004
v28	1072.04	0.0441	1074.32	0.2662
v29	1085.22	0.3259	1086.33	0.0803
v30	1097.94	1.0807	1098.08	0.0279
v31	1139.79	0.0094	1150.21	0.7594
v32	1154.09	0.3539	1163.97	0
v33	1177.00	1.0117	1164.17	1.2014
v34	1205.45	0.4123	1203.35	0.7623
v35	1226.58	3.9673	1220.26	0.0001
v36	1235.12	0.5261	1231.93	2.394
v37	1251.63	0.6497	1255.07	2.0392
v38	1263.89	0.1499	1267.83	0.0303

v39	1291.28	1.5752	1288.24	0.8217
v40	1297.64	0.3781	1297.61	0.3828
v41	1308.16	0.4089	1311.85	0.1835
v42	1316.66	0.5451	1322.68	0.0186
v43	1331.37	0.0591	1326.88	0.2238
v44	1332.77	1.933	1334.64	0.2796
v45	1337.56	1.7659	1335.25	5.7763
v46	1346.72	5.3194	1365.77	0.3518
v47	1364.62	0.9899	1368.84	4.6962
v48	1377.67	1.9113	1378.67	0.4934
v49	1387.79	0.7712	1391.91	0.6535
v50	1511.01	2.9537	1510.27	6.8327
v51	1525.03	2.4332	1512.70	1.9299
v52	1526.88	5.0538	1525.31	1.5708
v53	1542.70	14.9919	1535.43	16.2584
v54	1554.72	4.037	1555.06	4.6516
v55	3004.31	39.6552	3000.43	30.893
v56	3014.09	29.3286	3001.66	22.8575
v57	3079.07	21.9037	3078.22	12.7894
v58	3083.14	13.082	3079.60	7.5315
v59	3086.14	37.6354	3082.85	19.3657
v60	3088.00	14.8897	3084.31	18.1288
v61	3088.98	58.1459	3088.78	53.0711
v62	3108.42	29.3292	3095.19	33.6013
v63	3113.96	65.594	3105.14	61.5819
v64	3123.04	17.8516	3112.49	77.948
v65	3128.97	1.0162	3118.55	2.9792
v66	3141.40	30.185	3129.12	0.0418
v67	3148.40	58.2285	3144.45	23.2414
v68	3152.21	26.7011	3148.97	61.8299
v69	3222.35	22.3624	3228.34	30.3967

JP-10 B3LYP/def2-TZVP				
Normal modes	Frequencies(cm^{-1})	IR Inten	Frequencies(cm^{-1})	IR Inten
v1	144.86	0.009		
v2	183.19	0.0031		
v3	278.68	0.0817		
v4	323.98	0.0513		
v5	331.23	0.0421		
v6	406.96	0.0462		
v7	505.76	0.2251		
v8	538.22	0.1734		
v9	562.37	0.5638		
v10	677.86	0.524		
v11	742.45	0.3066		
v12	759.89	0.3185		
v13	794.65	1.3279		
v14	835.78	0.5303		
v15	869.43	1.0147		
v16	870.56	0.0155		
v17	891.40	0.6079		
v18	899.24	0.0652		
v19	916.88	0.9298		
v20	924.82	0.077		
v21	927.57	1.1053		
v22	961.72	1.7838		
v23	965.13	0.0305		
v24	994.87	1.6714		
v25	1004.67	0.489		
v26	1047.38	0.2149		
v27	1055.60	0.6282		
v28	1057.47	0.0282		
v29	1058.01	0.0489		
v30	1080.23	0.5847		
v31	1140.77	0.1199		
v32	1157.37	0.0264		
v33	1173.26	1.0062		
v34	1193.87	0.2069		
v35	1207.72	0.0662		
v36	1214.09	1.3373		
v37	1232.45	1.2409		
v38	1254.23	0.0055		

v39	1264.61	0.7579
v40	1293.87	1.2094
v41	1303.64	0.0343
v42	1309.67	0.2175
v43	1316.68	0.412
v44	1321.65	0.0001
v45	1331.83	0.0798
v46	1334.48	1.6902
v47	1348.14	0.5566
v48	1353.50	0.9748
v49	1373.56	0.7613
v50	1377.82	0.4264
v51	1494.18	1.123
v52	1497.05	1.8945
v53	1499.72	1.9952
v54	1505.95	4.2672
v55	1516.87	10.7064
v56	1531.63	4.8919
v57	3018.20	20.496
v58	3024.48	29.4339
v59	3027.22	19.6381
v60	3033.56	1.1218
v61	3038.18	24.6142
v62	3046.39	55.0985
v63	3047.55	8.1301
v64	3049.67	72.3811
v65	3067.56	6.2772
v66	3070.81	44.6458
v67	3074.56	41.3424
v68	3077.32	97.7589
v69	3080.47	45.9135
v70	3083.92	10.4729
v71	3091.25	82.9497
v72	3092.16	50.3735

Normal modes	R1 B3LYP/def2-TZVP		R2 B3LYP/def2-TZVP	
	Frequencies(cm ⁻¹)	IR Inten	Frequencies(cm ⁻¹)	IR Inten
v1	154.52	0.0815	144.65	0.0886
v2	179.74	0.1742	181.25	0.0512
v3	269.30	7.1892	277.96	0.3358
v4	304.29	2.3774	321.93	0.3858
v5	328.29	0.0587	329.63	0.0731
v6	377.36	5.8178	404.89	0.0916
v7	444.94	14.5213	502.13	0.6129
v8	506.69	0.503	526.28	0.7013
v9	553.10	0.0862	559.77	0.5547
v10	573.17	3.5614	668.25	1.0893
v11	677.19	0.4164	716.25	0.1597
v12	747.23	0.6745	755.95	0.2605
v13	768.85	0.2578	773.22	0.646
v14	795.54	1.5931	830.80	0.453
v15	866.58	0.5031	837.16	3.4844
v16	869.54	0.2943	858.47	0.4177
v17	891.38	0.5595	875.94	0.2142
v18	904.31	1.3591	886.36	0.3154
v19	913.76	0.6825	913.01	1.7382
v20	916.62	0.5315	921.73	0.254
v21	934.59	0.1724	931.59	1.1531
v22	936.76	0.2314	950.69	1.4763
v23	960.23	2.2927	971.47	0.5595
v24	981.98	0.7657	995.61	0.8167
v25	998.40	1.0491	1007.00	1.632
v26	1011.99	1.1601	1042.38	0.5466
v27	1035.93	0.0162	1052.47	0.1851
v28	1045.81	0.87	1065.04	0.1349
v29	1053.22	0.014	1087.08	0.1698
v30	1074.12	0.716	1100.16	0.1386
v31	1122.61	0.4333	1143.07	1.0528
v32	1145.38	0.2268	1166.20	0.149
v33	1159.77	0.6362	1190.35	0.1553
v34	1188.11	0.597	1199.66	0.5433
v35	1193.46	0.3524	1212.04	4.2047
v36	1212.58	0.1555	1219.35	1.5739
v37	1234.56	1.1736	1236.52	1.5887
v38	1252.49	0.8133	1255.45	0.9149

v39	1272.05	0.4255	1264.39	0.6344
v40	1283.11	1.9975	1290.15	1.6759
v41	1300.32	0.1951	1303.74	0.7396
v42	1307.81	0.1164	1311.10	0.3102
v43	1319.44	0.5644	1315.93	0.8326
v44	1327.68	0.4021	1322.15	1.2636
v45	1337.67	1.5205	1336.45	0.4335
v46	1346.14	0.5283	1347.68	0.2288
v47	1347.44	0.6114	1364.89	0.4053
v48	1361.57	1.1002	1375.72	0.6912
v49	1372.57	0.3848	1492.06	1.5808
v50	1473.41	4.1523	1493.09	0.3995
v51	1494.66	2.2168	1497.95	2.5398
v52	1499.43	2.8636	1502.77	6.6318
v53	1508.59	4.6117	1514.00	8.3847
v54	1525.09	8.8149	1526.60	5.8937
v55	2967.58	46.9071	3019.50	25.6647
v56	3010.11	25.6347	3028.39	25.7544
v57	3019.34	21.4738	3036.56	16.9318
v58	3026.04	29.8635	3040.21	14.0374
v59	3029.27	22.6579	3042.05	14.3771
v60	3039.33	7.4462	3050.66	47.6343
v61	3054.03	42.901	3055.79	51.4164
v62	3055.90	18.2456	3058.66	24.7223
v63	3071.17	38.4271	3071.46	44.1276
v64	3076.30	43.1507	3074.56	32.5003
v65	3083.17	77.8015	3077.44	56.9166
v66	3084.22	93.2132	3078.55	9.3664
v67	3087.96	4.722	3087.58	51.0083
v68	3097.24	32.9053	3098.93	72.6197
v69	3196.12	21.3324	3109.20	32.3534

Normal modes	R3 B3LYP/def2-TZVP		R4 B3LYP/def2-TZVP	
	Frequencies(cm ⁻¹)	IR Inten	Frequencies(cm ⁻¹)	IR Inten
v1	111.86	0.0013	116.60	0.1225
v2	187.42	0.1451	161.82	0.1459
v3	261.45	0.0526	239.56	0.4748
v4	308.49	2.5297	291.98	0.3404
v5	321.25	0.0591	316.28	0.0869
v6	337.24	8.1255	390.16	0.0281
v7	429.89	4.7033	494.61	0.5806
v8	535.22	0.5368	542.14	0.1624
v9	548.59	0.9172	561.15	1.0262
v10	674.72	13.1661	628.85	3.203
v11	675.02	0.1795	723.59	0.1385
v12	739.90	1.2947	740.35	0.2311
v13	768.83	0.5191	795.26	2.1631
v14	794.66	0.812	831.53	0.7287
v15	836.73	1.476	849.30	0.1588
v16	855.58	0.3368	876.57	0.8024
v17	872.73	0.1344	882.40	0.6114
v18	878.33	1.0743	890.91	0.2136
v19	914.40	0.0633	896.22	0.7737
v20	919.24	1.9664	907.04	0.2267
v21	928.82	0.0444	917.41	0.915
v22	948.99	0.1656	957.27	0.018
v23	950.47	1.5318	964.24	2.8843
v24	991.11	1.5685	990.06	1.1328
v25	994.38	0.151	1019.21	0.2754
v26	998.52	0.991	1040.19	0.0326
v27	1041.85	0.154	1047.23	1.0466
v28	1052.21	0.1074	1062.80	0.2034
v29	1058.98	0.1418	1095.04	1.1335
v30	1078.17	0.6567	1124.00	0.3732
v31	1156.48	0.407	1133.89	0.2313
v32	1167.36	1.1113	1152.89	0.2065
v33	1191.32	0.2743	1166.31	0.6413
v34	1192.74	0.9488	1190.56	1.7135
v35	1208.06	0.3175	1208.27	1.4261
v36	1208.95	0.2456	1224.14	0.9616
v37	1239.71	1.0744	1234.37	0.3267

v38	1244.86	0.1264	1249.11	0.2375
v39	1263.13	1.5503	1252.67	0.6844
v40	1277.97	0.0017	1285.78	1.0408
v41	1299.40	0.0179	1305.34	0.4388
v42	1309.49	0.2732	1311.16	0.2227
v43	1316.00	0.0038	1315.06	0.4198
v44	1333.44	0.8227	1326.56	1.5901
v45	1333.73	0.0987	1339.45	0.3495
v46	1348.42	0.549	1342.06	1.0895
v47	1348.92	0.3872	1353.64	0.0348
v48	1369.20	1.9851	1366.69	0.2754
v49	1372.65	0.3784	1470.83	3.8874
v50	1489.88	3.4971	1492.19	1.2989
v51	1493.07	0.5015	1493.11	1.6532
v52	1493.30	5.8954	1502.73	3.198
v53	1508.94	2.6721	1509.56	9.2603
v54	1513.37	5.2584	1526.23	3.2276
v55	3015.69	19.1536	2953.46	34.79
v56	3020.86	30.4691	2983.86	26.3467
v57	3024.86	25.7237	3018.23	19.0731
v58	3033.21	7.9221	3025.50	11.6416
v59	3036.58	26.3054	3036.07	55.6529
v60	3045.15	22.3585	3038.69	26.2375
v61	3050.22	80.6865	3038.99	42.3396
v62	3069.62	0.05	3050.10	64.2788
v63	3071.10	39.3357	3073.37	2.7039
v64	3074.48	51.8496	3074.21	64.1029
v65	3082.09	58.3304	3083.28	23.1515
v66	3090.87	53.6016	3084.07	70.1505
v67	3094.27	73.0037	3088.13	45.8074
v68	3097.54	20.462	3093.95	20.2313
v69	3190.92	17.6983	3097.42	60.2549

Normal modes	R5 B3LYP/def2-TZVP		R6 B3LYP/def2-TZVP	
	Frequencies(cm ⁻¹)	IR Inten	Frequencies(cm ⁻¹)	IR Inten
v1	120.90	0.1143	83.3286	0.7531
v2	133.95	0.2081	127.021	0.0001
v3	267.23	0.6456	265.134	0.0173
v4	290.21	0.6426	278.9338	0.8025
v5	319.78	0.4363	329.4545	0.0017
v6	401.50	3.0735	393.905	26.4158
v7	418.33	18.4598	405.1738	0.3165
v8	507.86	0.6899	511.1193	0.1762
v9	538.59	0.1126	536.0017	0.0074
v10	629.92	0.6461	687.9005	0.6149
v11	740.16	0.0986	711.3315	0.3173
v12	755.04	1.5252	733.6506	0.269
v13	767.56	0.7481	772.9638	0.07
v14	799.35	0.7287	799.0063	0.9518
v15	836.68	0.3308	833.6046	0.7728
v16	850.60	0.4925	843.2213	0.3718
v17	873.21	0.8881	890.3232	0.5409
v18	889.38	0.6722	895.0157	0.8602
v19	909.53	0.3198	913.112	1.087
v20	925.48	0.1109	926.8657	1.072
v21	927.62	1.3552	937.1678	0.6358
v22	951.88	1.373	952.9848	0.6736
v23	963.46	0.1667	965.6014	0.0583
v24	980.57	1.6358	967.5085	1.422
v25	1004.68	0.8729	1016.724	1.7597
v26	1021.03	0.3603	1025.347	0.0102
v27	1051.39	0.3015	1048.893	0.5321
v28	1053.92	0.2798	1057.725	0.6523
v29	1066.83	0.3804	1064.171	0.5682
v30	1077.31	0.9804	1080.183	0.0102
v31	1124.62	0.0424	1134.295	0.48
v32	1145.43	0.2195	1147.262	0.7383
v33	1163.19	0.7098	1151.437	0.1079
v34	1187.08	0.2985	1180.725	0.5952
v35	1210.78	2.7293	1201.713	0.0212
v36	1220.17	0.3924	1217.232	1.1894
v37	1231.70	0.8385	1236.958	1.3549

v38	1247.32	0.0552	1252.339	0.0015
v39	1281.70	0.4092	1269.27	0.0068
v40	1287.27	1.3514	1294.831	0.9459
v41	1295.52	0.0518	1306.422	0.3764
v42	1301.97	0.4031	1308.093	0.1973
v43	1314.32	0.291	1311.509	0.2552
v44	1320.90	0.5354	1322.565	0.264
v45	1324.06	1.4645	1329.05	2.4189
v46	1335.12	2.6536	1348.758	0.0892
v47	1349.92	0.6291	1355.671	2.4239
v48	1364.35	0.9604	1366.202	0.0777
v49	1372.84	1.054	1379.298	0.9583
v50	1471.01	2.2939	1471.471	6.1364
v51	1496.30	1.0639	1473.821	2.0765
v52	1497.93	2.9445	1494.006	1.0736
v53	1510.55	11.4606	1509.049	8.826
v54	1524.97	3.0114	1529.677	4.1653
v55	2916.75	47.5025	2924.335	33.6158
v56	2951.25	36.524	2926.529	30.7142
v57	3027.39	26.0106	3003.138	35.8921
v58	3037.95	26.8405	3003.252	20.2755
v59	3043.45	24.5827	3037.463	19.2909
v60	3046.67	61.0348	3045.19	39.8441
v61	3047.88	31.953	3048.151	50.7679
v62	3049.81	32.8158	3048.603	20.2586
v63	3067.07	4.955	3064.499	52.0511
v64	3079.13	54.3734	3067.151	10.2821
v65	3081.46	63.1313	3077.834	83.6528
v66	3087.65	20.263	3084.06	2.7467
v67	3091.66	65.3797	3086.597	27.5414
v68	3092.51	39.0635	3091.189	86.8256
v69	3180.15	22.9516	3183.43	30.2786

Normal modes	vdW1 Site 1-2 JP-10/AlO		vdW1 Site 3 JP-10/AlO	
	Frequencies(cm ⁻¹)	IR Inten	Frequencies(cm ⁻¹)	IR Inten
v1	17.00	0.4753	22.26	40.7366
v2	35.15	1.1885	23.90	43.2182
v3	49.13	0.0313	64.50	21.057
v4	55.59	8.5907	76.93	17.9013
v5	87.80	11.4418	89.36	20.229
v6	134.82	0.1075	137.31	0.0738
v7	180.82	0.1409	187.66	0.5789
v8	264.48	0.1635	261.39	0.0542
v9	318.16	0.1256	318.91	0.069
v10	332.61	0.5765	337.33	0.8012
v11	403.97	0.3471	407.11	0.3409
v12	494.40	1.2699	506.61	2.5179
v13	535.14	0.687	532.81	0.1998
v14	556.78	0.1874	556.83	0.3803
v15	667.99	1.0001	670.24	1.8832
v16	739.50	189.6392	754.67	0.2978
v17	750.36	0.4272	767.97	0.4537
v18	767.11	1.3633	811.64	1.9791
v19	813.37	1.2643	844.24	1.4032
v20	846.27	1.0181	885.61	0.2994
v21	881.30	1.2427	886.59	3.4096
v22	882.73	3.5929	918.26	1.0571
v23	911.22	0.3099	922.32	0.2979
v24	917.71	0.5921	943.71	2.2284
v25	938.81	0.3408	944.17	0.6643
v26	941.44	1.8559	951.38	0.7174
v27	947.30	3.4493	984.48	1.0347
v28	982.98	4.0438	997.62	5.9699
v29	992.96	1.1196	1019.01	3.1737
v30	1020.81	2.166	1031.76	2.1451
v31	1029.20	2.1967	1068.78	1.5294
v32	1066.78	0.8177	1069.18	0.2915
v33	1069.90	0.5057	1074.08	0.3362
v34	1076.44	0.2632	1075.27	0.503
v35	1078.65	0.3722	1095.05	1.8937
v36	1096.24	0.4668	1163.26	0.0997
v37	1157.96	0.4134	1180.14	1.8224

v38	1164.44	1.4713	1181.75	2.1879
v39	1186.39	2.2199	1210.22	0.4979
v40	1216.15	0.281	1225.19	0.0252
v41	1219.50	2.4034	1226.55	1.7454
v42	1228.48	3.9328	1245.04	3.1783
v43	1243.29	1.8996	1270.61	0.358
v44	1268.65	0.222	1292.52	3.5423
v45	1284.31	1.4462	1297.17	0.5519
v46	1288.98	3.4556	1309.35	0.2272
v47	1307.00	0.066	1317.40	0.4321
v48	1321.88	0.2783	1325.13	1.8959
v49	1327.59	0.5068	1338.42	0.147
v50	1330.50	2.3581	1351.03	0.8046
v51	1340.76	4.2183	1360.10	18.9673
v52	1344.29	4.6308	1364.78	1.739
v53	1362.50	0.6689	1366.21	3.0975
v54	1364.98	2.0614	1390.27	15.9302
v55	1381.74	1.4265	1391.94	0.0243
v56	1386.63	0.5141	1520.36	3.1699
v57	1522.53	1.3694	1523.42	1.3134
v58	1525.60	1.285	1529.71	0.2951
v59	1527.57	2.7122	1536.86	18.1104
v60	1533.16	13.3134	1547.15	0.4491
v61	1547.12	16.0041	1576.79	34.3308
v62	1557.41	5.2029	3053.91	2.336
v63	3066.81	12.7887	3056.53	468.1902
v64	3070.91	20.8058	3064.41	1254.6599
v65	3073.99	12.2776	3069.02	22.5979
v66	3074.45	14.9103	3069.14	143.156
v67	3076.02	36.9065	3077.52	105.2997
v68	3083.44	15.6569	3078.68	1396.5983
v69	3087.14	130.3601	3079.65	85.9813
v70	3089.62	32.5941	3102.67	128.511
v71	3097.27	81.3895	3106.70	741.8283
v72	3116.84	29.8883	3117.71	0.5857
v73	3130.13	43.7406	3118.16	50.9124
v74	3134.06	29.6455	3138.34	82.4097
v75	3135.58	4.2558	3148.64	2513.5143
v76	3138.22	12.7946	3149.64	5.9911
v77	3145.96	53.4531	3163.34	52.8704

v78	3156.11	45.7328	4661.83	2192532.61
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Normal modes	vdW1 Site 4 JP-10/AIO		vdW1 Site 5-6 JP-10/AIO	
	Frequencies(cm ⁻¹)	IR Inten	Frequencies(cm ⁻¹)	IR Inten
v1	11.82	38.9297	13.05	25.6421
v2	20.20	27.8923	16.49	22.7448
v3	32.24	0.041	32.34	9.3207
v4	52.90	10.2654	46.63	11.857
v5	73.20	33.5366	68.05	6.2506
v6	130.81	0.0085	128.95	0.0589
v7	182.22	3.0835	187.74	14.9395
v8	261.41	0.0428	260.68	0.0245
v9	319.49	0.0316	318.52	0.0486
v10	331.98	33.427	331.21	12.709
v11	403.48	110.8308	402.78	2.5148
v12	491.99	46.0165	491.51	5.491
v13	534.03	0.2413	532.43	0.2685
v14	549.35	9303.529	550.50	346.0482
v15	555.16	526.3659	638.60	6249.947
v16	664.43	0.6812	667.04	1.2896
v17	750.26	0.2219	750.11	0.3906
v18	767.90	5.8968	767.86	1.5668
v19	812.32	0.0653	812.23	1.2026
v20	846.11	6.2705	844.69	0.877
v21	880.04	2.9536	881.33	3.0285
v22	881.38	0.6856	886.07	0.6862
v23	913.06	0.0055	915.13	0.1211
v24	923.50	0.5528	918.12	0.674
v25	939.24	0.1871	940.29	0.3208
v26	941.42	1.1771	941.84	1.3336
v27	953.82	1.9217	952.73	2.0928
v28	980.84	4.138	980.72	2.7818
v29	983.76	0.4794	984.10	0.5033
v30	1019.63	2.2591	1018.45	3.768
v31	1030.86	2.0966	1033.29	4.0835
v32	1066.86	0.2361	1063.61	0.047
v33	1068.73	2.2548	1073.19	2.1406
v34	1076.84	0.0542	1074.11	2.9419
v35	1086.14	0.1006	1079.26	0.1166
v36	1093.51	0.6018	1094.83	0.5983
v37	1147.93	0.1518	1149.57	0.0365
v38	1165.40	0.0213	1166.92	0.1203

v39	1191.20	27.0206	1183.86	5.4355
v40	1212.34	0.0018	1213.92	0.006
v41	1218.95	0.2744	1220.64	0.078
v42	1226.42	11.4189	1222.99	16.7433
v43	1242.53	8.0718	1244.95	4.1751
v44	1270.29	0.0004	1270.66	0.1602
v45	1287.03	0.4431	1282.61	2.1474
v46	1288.95	0.7887	1288.85	0.5635
v47	1300.35	0.479	1300.59	0.239
v48	1322.94	0.0307	1322.94	0.0271
v49	1328.06	3.0928	1325.88	0.2164
v50	1330.62	0.8392	1327.89	1.4072
v51	1338.17	2.6104	1338.38	1.7581
v52	1340.07	41.0957	1342.81	3.5069
v53	1359.76	0.3751	1361.71	10.8286
v54	1361.92	15.6515	1379.92	3.5039
v55	1394.97	3.2885	1386.85	17.5979
v56	1397.68	2.4414	1394.53	0.3925
v57	1516.74	0.0155	1516.80	48.4038
v58	1520.74	8.33	1522.56	1.9854
v59	1525.99	2.7749	1524.52	0.2317
v60	1529.52	10.3174	1528.25	18.0932
v61	1542.75	19.3734	1543.74	40.5805
v62	1553.73	45.4829	1555.35	13.3299
v63	3063.31	36.366	3058.13	34.325
v64	3063.37	30.0372	3058.38	56.1495
v65	3067.62	20.0712	3070.84	22.4837
v66	3069.95	48.7322	3077.74	68.6684
v67	3077.27	49.742	3079.80	53.9451
v68	3079.84	69.4691	3081.53	62.6216
v69	3097.51	103.6163	3102.49	83.2044
v70	3103.36	149.4729	3107.58	80.5284
v71	3111.86	1.4538	3110.68	6.5876
v72	3112.71	74.9856	3115.24	53.4766
v73	3127.68	6.0018	3121.68	2.3256
v74	3129.03	73.3502	3128.76	85.9346
v75	3136.03	121.7255	3133.07	53.095
v76	3143.02	104.1185	3142.69	124.8937
v77	3153.09	18.1559	3147.66	40.6011
v78	3166.08	104.5249	3153.78	186.3386

Normal modes	TS1 JP-10/AIO		TS2 JP-10/AIO	
	Frequencies(cm ⁻¹)	IR Inten	Frequencies(cm ⁻¹)	IR Inten
v1	-993.18	3271.0801	-868.58	19417.4124
v2	15.07	0.6036	31.73	0.2087
v3	37.91	1.3788	37.91	0.5568
v4	68.90	1.9381	133.74	0.041
v5	94.27	1.5553	177.30	0.5322
v6	141.69	1.8133	259.29	0.0381
v7	180.78	1.6986	312.03	18.2947
v8	260.90	7.1931	327.23	9.5249
v9	315.90	4.5934	401.99	9.111
v10	332.00	0.3452	454.51	360.8925
v11	389.81	6.4701	480.71	1157.0138
v12	495.85	0.5424	497.70	98.4125
v13	537.64	0.6849	537.57	1038.8907
v14	557.48	2.8863	548.80	68.351
v15	667.08	2.3878	568.20	19.153
v16	734.33	215.7418	668.08	11.068
v17	752.02	0.4921	748.01	12.8386
v18	768.47	4.2508	764.82	3.0538
v19	809.94	15.2431	817.49	18.4656
v20	842.54	48.3448	843.58	0.8002
v21	880.79	3.8704	875.91	8.954
v22	882.56	0.6114	879.48	0.8683
v23	912.87	3.1449	906.64	4.5759
v24	920.62	9.0941	914.69	25.4844
v25	934.72	5.702	937.09	9.5041
v26	941.74	0.9562	939.45	2.303
v27	951.71	2.1183	953.05	43.5399
v28	976.70	57.0062	977.54	2.5348
v29	986.48	9.5641	1002.14	6.134
v30	1018.09	5.002	1020.42	27.0318
v31	1034.54	1.8888	1027.08	6.9098
v32	1043.31	173.9589	1049.87	297.9475
v33	1067.46	9.9572	1063.05	13.122
v34	1069.52	3.8903	1072.76	2.8982
v35	1076.25	6.9806	1080.74	12.7665
v36	1095.15	335.7539	1091.84	54.0248

v37	1115.83	306.2841	1127.60	321.1419
v38	1159.23	54.201	1146.34	50.1873
v39	1167.65	3.5998	1168.83	1.2847
v40	1185.71	65.1352	1202.68	483.4916
v41	1213.93	18.7186	1213.82	0.3349
v42	1216.48	3.488	1217.38	1.1
v43	1236.12	51.9013	1233.93	37.4861
v44	1248.98	1.2905	1250.61	474.2419
v45	1267.63	350.9143	1265.50	255.1189
v46	1283.06	1.4906	1280.44	36.6831
v47	1290.68	47.9646	1288.33	684.0329
v48	1306.98	63.6984	1303.73	1305.6723
v49	1315.01	112.9603	1308.87	144.4434
v50	1322.52	0.5279	1320.04	1.4243
v51	1331.50	9.9816	1325.09	68.164
v52	1337.38	19.2741	1332.27	13.162
v53	1353.80	242.3153	1347.50	500.8126
v54	1361.44	12.7241	1360.21	181.3874
v55	1363.28	27.5868	1363.69	995.156
v56	1380.52	7.8964	1382.08	143.2575
v57	1387.71	36.7655	1390.27	1922.4873
v58	1405.49	88.9104	1522.28	11.3465
v59	1522.55	2.2965	1522.80	2.2441
v60	1527.27	4.6915	1527.11	11.0037
v61	1529.11	7.2459	1532.43	8.3384
v62	1539.75	7.4257	1546.16	54.4113
v63	1554.97	12.9158	1559.27	97.4121
v64	3071.97	11.5525	3072.42	7.1476
v65	3075.29	14.0227	3072.56	36.6055
v66	3076.26	27.7301	3074.06	20.0482
v67	3076.47	22.6662	3079.45	29.6881
v68	3086.36	10.6618	3085.48	13.9053
v69	3087.78	49.102	3088.45	27.1617
v70	3099.11	13.4361	3091.45	88.6767
v71	3107.87	43.1271	3094.45	9.3349
v72	3119.80	35.7314	3110.04	92.4328
v73	3125.77	8.2309	3127.94	38.4383
v74	3131.92	31.3563	3131.41	2.8344
v75	3136.69	28.2931	3136.60	27.8708
v76	3145.57	4.1161	3146.72	39.6767

v77	3146.67	70.8167	3152.27	65.8554
v78	3164.93	23.1997	3160.96	30.905

Normal modes	TS3		TS4	
	Frequencies(cm ⁻¹)	IR Inten	Frequencies(cm ⁻¹)	IR Inten
v1	-1325.81	28345.1992	-506.92	6870.1904
v2	58.12	0.4065	34.97	0.4676
v3	61.39	0.0571	38.78	0.3244
v4	142.33	0.035	127.23	0.1551
v5	177.69	1.3517	173.26	17.1732
v6	260.77	0.0079	258.67	3.0391
v7	314.03	0.035	313.37	1.6464
v8	319.86	79.8031	326.16	23.4841
v9	332.10	64.3034	401.84	0.4423
v10	371.01	210.3668	488.58	141.9445
v11	390.28	1.2096	525.22	8.6434
v12	464.01	365.815	552.02	28.4791
v13	535.35	0.9729	611.22	2719.5648
v14	552.10	39.291	686.53	705.7731
v15	619.19	30.318	743.56	213.5919
v16	671.96	0.0436	765.90	116.3752
v17	745.33	0.267	804.92	89.2432
v18	778.26	19.2688	834.89	146.2567
v19	810.55	2.8624	861.42	116.6038
v20	841.49	1.9319	875.21	136.7934
v21	882.58	0.0161	904.45	145.5968
v22	883.44	0.9171	917.89	8.2154
v23	908.65	6.8158	923.76	194.2148
v24	927.29	137.7507	937.05	155.6536
v25	930.50	0.1477	941.93	97.292
v26	943.54	17.9595	952.86	370.8626
v27	945.96	0.0018	977.12	78.0726
v28	966.58	18.4975	981.78	9.2994
v29	978.52	0.1233	1016.95	268.8318
v30	1019.48	1.8017	1031.01	143.5648
v31	1029.38	1.6633	1056.85	77.6382
v32	1059.41	46.0838	1067.63	25.842
v33	1061.90	0.1181	1074.80	6.3745
v34	1071.01	48.6169	1092.43	44.6204
v35	1076.45	0.0508	1133.45	186.6093
v36	1095.94	36.4342	1159.03	47.637
v37	1108.91	0.0179	1174.91	269.8673

v38	1117.51	1251.742	1196.76	334.0389
v39	1171.46	0.0845	1202.03	462.5264
v40	1186.92	193.2214	1213.40	243.8459
v41	1213.09	0.0099	1229.39	455.6074
v42	1223.95	0.2758	1254.46	765.7997
v43	1224.59	8.0293	1269.86	50.4677
v44	1229.33	32.6305	1272.80	271.2435
v45	1263.33	5.0074	1282.69	191.0414
v46	1267.52	0.5716	1289.33	50.8383
v47	1289.24	0.6485	1303.18	1451.1853
v48	1295.07	0.1574	1321.43	209.7029
v49	1313.98	0.6872	1324.52	235.7564
v50	1320.17	0.4244	1327.40	370.3159
v51	1326.31	1.1007	1331.81	356.4206
v52	1341.82	5.1984	1345.92	321.2419
v53	1353.67	24.3743	1360.32	8.1924
v54	1364.21	3.1226	1383.78	994.652
v55	1365.94	0.0549	1384.72	1190.3273
v56	1389.90	10.0203	1416.71	3487.3534
v57	1390.45	0.2554	1516.89	21.0592
v58	1510.95	1494.6697	1522.43	10.2418
v59	1523.24	2.4372	1528.22	209.784
v60	1528.10	2.0157	1532.79	137.8874
v61	1530.97	361.8546	1545.77	584.9517
v62	1545.45	1.8476	1557.89	531.1511
v63	1552.39	405.8417	1652.19	15293.0443
v64	3066.91	2.8737	3056.45	42.7945
v65	3067.45	37.3536	3069.70	30.2766
v66	3077.66	26.2161	3076.86	65.7653
v67	3081.73	33.3565	3077.93	44.8423
v68	3087.42	117.1475	3082.03	55.2483
v69	3090.65	58.8987	3082.44	5.0722
v70	3092.87	24.4094	3089.83	118.7236
v71	3104.51	47.56	3109.58	101.34
v72	3120.35	67.126	3118.97	101.964
v73	3123.41	20.9848	3127.31	28.5861
v74	3124.54	31.8643	3130.74	37.9382
v75	3128.90	3.928	3134.39	62.2284
v76	3148.05	54.4735	3141.98	107.5308
v77	3153.90	9.1335	3147.84	39.9404

v78	3158.81	41.3255	3167.72	164.6999
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Normal modes	TS5		TS6	
	Frequencies(cm^{-1})	IR Inten	Frequencies(cm^{-1})	IR Inten
v1	-1158.72	3759.1881	-946.56	18912.2857
v2	17.75	0.9297	33.83	0.497
v3	45.37	1.0388	35.14	0.5439
v4	67.38	1.9308	41.11	0.0512
v5	97.74	1.4812	160.11	20.6319
v6	140.30	1.8842	251.06	0.0274
v7	179.42	0.2945	258.11	3.6134
v8	257.15	3.5586	320.24	0.5154
v9	321.59	4.6389	382.37	107.5092
v10	326.20	2.5158	477.83	47.0846
v11	401.94	0.6938	490.96	2.7515
v12	490.26	5.8516	573.23	665.8624
v13	526.47	5.7613	589.75	152.6882
v14	550.95	13.3442	603.77	744.5175
v15	660.26	35.5498	741.03	26.4033
v16	735.92	211.9555	742.19	472.618
v17	751.56	0.2469	761.29	36.3075
v18	768.00	0.3473	790.15	0.5968
v19	811.36	4.7742	816.97	7.1642
v20	832.17	322.8392	823.60	11.9444
v21	847.06	82.6983	855.76	1.5017
v22	878.59	0.6895	881.92	25.407
v23	883.44	2.9533	912.19	13.8276
v24	918.41	0.2124	919.06	1.6695
v25	919.92	8.5765	943.78	18.9403
v26	940.15	0.1357	945.61	3.1107
v27	952.95	1.4584	955.82	3.5664
v28	968.12	26.2915	982.59	22.8298
v29	985.67	3.6016	985.20	0.007
v30	992.31	46.4635	1013.11	24.8285
v31	1021.84	3.174	1043.75	11.5583
v32	1035.98	24.3536	1053.64	3.7777
v33	1063.30	0.1935	1061.95	32.5282
v34	1071.03	6.953	1086.36	37.6049
v35	1075.45	0.2809	1100.78	39.3276
v36	1094.82	1.3242	1121.16	7.4585
v37	1129.45	101.804	1135.16	5.1841

v38	1151.19	0.0461	1156.62	0.0105
v39	1163.34	0.6913	1165.20	4.6154
v40	1184.57	3.5788	1179.99	0.0629
v41	1217.07	13.4337	1218.11	23.0516
v42	1217.99	24.7971	1227.11	0.2106
v43	1233.35	115.0117	1239.78	40.6947
v44	1245.15	29.3118	1267.91	0.3671
v45	1269.51	1.6024	1291.99	0.4979
v46	1282.23	118.0556	1293.15	839.8128
v47	1291.12	2.1482	1303.38	8.6148
v48	1299.12	18.8512	1305.58	0.7029
v49	1312.12	3.3056	1309.69	0.1947
v50	1323.35	1.3616	1325.97	0.3836
v51	1332.99	5.1105	1334.26	2.895
v52	1339.45	3.8294	1335.36	934.7217
v53	1341.81	13.0719	1352.02	7.4466
v54	1356.44	29.6278	1360.78	3073.7504
v55	1359.17	3.9005	1369.12	642.2788
v56	1381.46	18.7961	1387.20	2.7069
v57	1389.95	33.3653	1402.36	3829.5869
v58	1421.58	232.3392	1426.48	304.7077
v59	1523.57	1.2818	1515.59	8.1047
v60	1525.84	1.6271	1525.58	2.1125
v61	1532.88	10.0424	1530.59	68.5448
v62	1541.35	15.2491	1534.69	50.0592
v63	1556.09	3.4104	1555.94	5.8715
v64	3077.01	20.9239	3070.22	9.4759
v65	3080.35	2.2236	3073.96	5.8631
v66	3081.87	14.051	3077.92	8.5322
v67	3087.42	38.9896	3081.33	62.4011
v68	3088.19	10.7391	3087.06	25.0069
v69	3090.47	64.2169	3087.71	62.9136
v70	3093.93	11.9225	3093.33	49.8249
v71	3102.29	60.8173	3111.24	84.109
v72	3107.65	22.1968	3113.71	35.0188
v73	3117.76	29.3077	3117.16	13.3744
v74	3132.38	0.1737	3128.24	0.6156
v75	3137.45	34.1107	3130.82	17.222
v76	3149.91	8.2963	3139.01	62.7915
v77	3152.17	56.63	3147.99	71.3039

v78	3156.09	40.3093	3172.80	35.7949
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Normal modes	vdW2 Site 1 JP-10/AlO		vdW2 Site 2 JP-10/AlO	
	Frequencies(cm ⁻¹)	IR Inten	Frequencies(cm ⁻¹)	IR Inten
v1	14.50	0.4438	15.38	0.5811
v2	28.71	0.8293	30.35	0.8934
v3	49.16	3.3197	57.26	2.8778
v4	83.98	1.9209	70.31	1.9007
v5	85.82	1.0702	84.81	0.2598
v6	154.52	1.3146	137.52	0.3932
v7	184.93	1.2473	177.97	0.3268
v8	290.84	2.282	263.57	0.6714
v9	322.30	2.3938	316.96	0.1404
v10	330.75	2.7654	328.94	0.511
v11	396.64	6.5069	401.78	7.1358
v12	424.80	124.8752	412.58	130.1957
v13	496.67	16.3606	495.54	3.2553
v14	528.13	8.077	519.82	7.1771
v15	554.88	9.1029	555.03	3.8743
v16	569.01	253.0468	561.28	304.9999
v17	622.78	96.6667	661.10	1.1614
v18	668.61	0.6924	731.21	0.2935
v19	758.30	2.1696	763.79	0.5796
v20	781.20	0.8691	801.70	1.2223
v21	815.48	2.1641	838.84	0.5841
v22	868.05	119.8005	857.77	25.1437
v23	880.24	0.3171	871.12	98.9828
v24	884.61	2.1525	878.19	0.3358
v25	915.25	0.326	898.92	0.2642
v26	924.00	0.8407	914.57	0.4327
v27	930.17	1.5938	934.53	0.0898
v28	941.10	1.0605	940.05	1.6672
v29	956.53	0.0937	957.74	1.1416
v30	961.14	0.1039	974.92	1.34
v31	987.50	4.7214	996.88	0.4599
v32	1009.52	0.8099	1023.12	0.873
v33	1024.89	1.5222	1026.67	2.5587
v34	1037.24	4.6087	1062.49	0.2051
v35	1057.01	0.5526	1071.01	0.0475
v36	1064.25	0.187	1081.09	0.3044
v37	1075.33	0.1719	1107.81	0.2303

v38	1100.11	0.8551	1129.71	0.1352
v39	1151.06	1.1643	1159.70	1.3217
v40	1166.71	0.0904	1183.79	1.1865
v41	1173.91	0.7617	1212.72	0.388
v42	1201.97	0.9991	1215.97	0.6502
v43	1215.99	0.2165	1226.14	6.017
v44	1231.72	0.5295	1238.31	2.0005
v45	1254.69	2.7897	1252.58	3.5195
v46	1271.92	0.6198	1275.87	0.674
v47	1286.45	1.1441	1283.84	0.8316
v48	1297.24	1.8561	1301.97	3.7351
v49	1306.27	0.773	1316.49	2.1636
v50	1319.37	0.3827	1323.40	2.5604
v51	1333.04	1.3297	1328.25	1.8784
v52	1342.42	1.6305	1334.95	2.9426
v53	1350.73	3.4632	1349.90	0.9687
v54	1357.90	0.9821	1363.93	0.3006
v55	1362.69	0.7806	1376.49	0.4667
v56	1376.50	2.1353	1392.87	0.485
v57	1385.56	0.649	1520.62	2.4956
v58	1512.03	6.6184	1522.90	0.4724
v59	1526.18	5.6075	1530.26	5.6419
v60	1527.78	3.854	1532.74	11.4116
v61	1539.68	3.5376	1545.70	11.3645
v62	1558.13	10.7005	1557.71	13.9771
v63	3046.46	22.4845	3075.83	34.0972
v64	3075.35	24.7163	3077.02	20.7292
v65	3076.08	35.0363	3080.06	4.5443
v66	3076.69	7.8626	3085.35	26.8912
v67	3077.81	14.683	3094.95	17.2787
v68	3092.47	26.5145	3096.36	29.7478
v69	3101.12	26.7645	3099.06	48.5599
v70	3107.42	13.62	3106.29	24.7099
v71	3121.45	50.8805	3115.21	29.8274
v72	3126.28	7.2878	3132.83	25.8844
v73	3131.48	30.7653	3140.55	6.485
v74	3137.17	27.5649	3141.23	28.2929
v75	3146.43	58.3402	3154.67	28.8077
v76	3171.04	16.2888	3161.17	45.1915
v77	3211.00	19.8519	3182.03	16.8376

v78	3829.35	517.3454	3832.03	497.0561
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Normal modes	vdW2 Site 3 JP-10/AlO		vdW2 Site 4 JP-10/AlO	
	Frequencies(cm ⁻¹)	IR Inten	Frequencies(cm ⁻¹)	IR Inten
v1	22.85	1.8074	16.04	0.2555
v2	33.25	0.0127	22.06	1.6762
v3	46.46	3.9092	45.13	3.1994
v4	69.91	0.8148	72.23	0.8824
v5	102.74	1.8402	88.61	0.4484
v6	125.39	0.8564	117.39	0.4828
v7	187.28	0.814	174.33	1.6412
v8	247.52	0.1899	244.51	3.1036
v9	315.56	2.7301	301.12	0.3371
v10	328.22	2.1775	317.06	1.6639
v11	379.10	10.2494	392.56	0.3735
v12	380.25	119.7963	469.83	130.4129
v13	456.06	32.0656	487.09	1.2211
v14	531.35	1.635	540.73	4.3416
v15	542.38	55.5414	555.07	58.2908
v16	557.50	98.4691	558.18	172.239
v17	667.49	0.0016	635.65	12.5175
v18	743.84	1.2305	730.36	0.3412
v19	766.56	14.2776	754.47	0.648
v20	798.42	7.9257	812.02	1.99
v21	808.77	3.3219	839.79	6.8955
v22	852.01	0.5198	865.76	0.2884
v23	863.64	145.0037	869.70	120.5194
v24	876.69	0.7453	896.49	1.9442
v25	887.46	0.1637	902.36	0.2877
v26	904.89	0.2699	916.33	0.7775
v27	931.95	0.1096	921.16	0.4257
v28	944.01	2.3859	933.76	0.3464
v29	947.14	0.3047	947.07	1.2835
v30	971.67	0.9748	981.38	2.3953
v31	976.20	2.6045	983.65	2.0246
v32	1018.72	1.6824	1021.22	1.7741
v33	1024.01	1.3765	1037.30	1.8759
v34	1040.51	0.1201	1062.02	0.6446
v35	1066.45	0.1816	1070.71	0.1404
v36	1071.32	0.091	1080.00	0.0795
v37	1076.39	0.1953	1113.06	1.9771

v38	1096.56	0.8159	1145.48	0.4244
v39	1173.41	1.6252	1148.18	0.3583
v40	1182.74	1.8898	1174.32	0.2448
v41	1209.69	0.5277	1179.61	0.7034
v42	1214.39	0.1922	1208.67	1.5663
v43	1223.91	0.2955	1231.02	1.1657
v44	1224.67	1.5325	1246.74	2.7825
v45	1248.19	1.4233	1250.11	0.0977
v46	1263.42	0.2341	1268.40	0.0664
v47	1286.20	4.2162	1277.97	0.7467
v48	1286.27	0.1945	1289.96	0.9533
v49	1311.62	0.0067	1322.42	0.0945
v50	1319.62	0.0397	1323.50	0.3995
v51	1325.03	0.5484	1331.22	3.8402
v52	1344.46	3.2325	1334.70	4.2951
v53	1348.80	0.3153	1356.47	1.2905
v54	1363.58	0.5017	1359.16	0.2039
v55	1363.71	0.3836	1370.10	0.7192
v56	1381.53	4.4837	1384.60	0.9923
v57	1383.07	0.1273	1505.93	7.1635
v58	1523.06	3.1338	1521.49	1.447
v59	1526.38	2.0034	1526.15	2.907
v60	1527.50	10.3457	1531.38	6.653
v61	1543.66	2.0939	1541.15	12.3028
v62	1545.74	4.5482	1555.98	6.0946
v63	3073.80	31.4969	3026.47	25.0339
v64	3076.71	1.4939	3057.94	9.8296
v65	3081.95	27.2288	3075.76	12.5853
v66	3086.41	36.4234	3082.39	42.2395
v67	3087.25	8.228	3083.37	16.7104
v68	3090.17	19.6697	3085.98	19.6542
v69	3092.91	71.3293	3096.50	46.1853
v70	3129.99	22.0899	3100.11	27.3039
v71	3131.90	23.2237	3120.90	48.5908
v72	3135.50	0.1993	3131.79	26.0739
v73	3136.40	27.1875	3137.84	34.3841
v74	3144.15	19.6173	3143.55	9.1872
v75	3150.64	36.6547	3145.92	11.305
v76	3153.14	60.144	3151.02	46.3075
v77	3190.45	18.3199	3166.33	29.4946

v78	3861.54	448.7079	3769.73	596.8993
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Normal modes	vdW2 Site 5 JP-10/AlO		vdW2 Site 6 JP-10/AlO	
	Frequencies(cm ⁻¹)	IR Inten	Frequencies(cm ⁻¹)	IR Inten
v1	7.05	0.1182	14.12	0.758
v2	12.61	0.7093	29.20	0.2424
v3	40.89	1.009	45.26	3.5525
v4	62.69	3.9369	71.45	0.1727
v5	91.22	2.3488	87.38	1.577
v6	124.63	1.1393	120.09	0.2363
v7	138.93	8.6535	160.36	5.7919
v8	256.01	1.9826	253.09	0.5596
v9	281.12	3.9451	284.85	1.9617
v10	313.28	3.3422	323.98	2.7344
v11	352.42	32.5757	402.37	1.9801
v12	380.08	267.2557	434.58	119.7852
v13	403.87	22.5437	461.85	20.7013
v14	473.62	187.9611	500.46	20.1988
v15	499.38	1.0409	532.69	0.0356
v16	535.94	0.2863	552.99	316.9114
v17	632.14	3.6395	697.28	0.9507
v18	745.68	0.5377	700.59	4.4179
v19	761.27	3.7474	745.98	0.431
v20	770.52	0.0051	789.42	0.3052
v21	814.37	0.7192	811.09	0.8662
v22	847.23	2.1336	841.62	2.0316
v23	852.93	2.5354	862.77	1.0313
v24	862.90	126.4786	868.93	120.7525
v25	887.86	2.0407	913.56	1.8624
v26	918.55	0.5427	920.64	0.3778
v27	936.22	0.216	935.57	0.9232
v28	950.26	0.1624	949.61	0.3984
v29	954.36	1.6827	952.36	1.6662
v30	976.92	2.3123	971.79	1.3146
v31	985.95	0.4987	986.96	0.548
v32	1003.82	1.8962	991.87	2.2688
v33	1033.40	0.7936	1037.56	3.0623
v34	1043.02	0.6496	1055.06	0.2724
v35	1065.10	0.434	1066.84	0.5769
v36	1073.54	0.0109	1075.82	0.1256
v37	1097.50	0.4465	1087.08	0.0537

v38	1103.43	1.3938	1097.67	0.0329
v39	1138.74	0.1942	1149.63	0.7467
v40	1156.37	0.1821	1161.60	0.0346
v41	1178.40	0.755	1170.80	0.7427
v42	1207.46	0.2862	1206.34	0.1685
v43	1228.57	5.1441	1218.74	0.029
v44	1239.91	1.5266	1232.37	3.6319
v45	1257.03	0.1804	1255.38	2.7196
v46	1265.21	0.2436	1267.33	0.1171
v47	1291.15	2.0579	1286.12	1.1349
v48	1297.77	0.3451	1295.75	0.3102
v49	1316.07	0.7717	1311.84	0.117
v50	1321.02	0.3035	1325.38	0.0274
v51	1329.95	0.0949	1329.58	0.464
v52	1333.38	2.9746	1334.84	5.9386
v53	1339.26	1.8571	1336.09	0.3018
v54	1348.33	5.2465	1363.45	0.3423
v55	1370.14	2.8716	1368.27	7.5949
v56	1378.01	2.6491	1381.68	0.6564
v57	1389.45	1.3475	1393.33	0.655
v58	1515.07	3.0322	1506.54	10.5987
v59	1524.86	2.3341	1509.58	4.2552
v60	1527.77	4.161	1525.17	1.6738
v61	1544.22	18.26	1534.94	18.8879
v62	1555.19	4.6603	1554.91	5.6066
v63	3030.04	23.2447	3004.88	21.4429
v64	3033.47	23.8624	3005.98	22.6578
v65	3080.00	21.2361	3080.04	19.5436
v66	3084.28	15.3115	3082.58	23.397
v67	3088.74	24.6959	3089.58	58.3059
v68	3089.61	50.3149	3090.11	11.5354
v69	3096.84	28.1373	3090.59	8.3503
v70	3103.82	21.7177	3109.37	2.6276
v71	3115.15	66.3084	3112.93	82.4087
v72	3122.76	15.4141	3115.61	29.4235
v73	3130.20	0.8461	3123.94	14.701
v74	3144.36	24.4747	3131.04	0.0045
v75	3149.58	64.4202	3142.61	27.2062
v76	3151.52	23.5965	3150.57	60.97
v77	3221.03	16.5974	3213.20	25.9556

v78	3914.16	288.6037	3834.67	430.6408
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Normal modes	vdW1 Site 1 JP-10/BO		vdW1 Site2 JP-10/BO	
	Frequencies(cm ⁻¹)	IR Inten	Frequencies(cm ⁻¹)	IR Inten
v1	25.22	10.2391	24.97	10.4206
v2	28.20	11.4026	27.95	11.5301
v3	41.87	8.1567	41.75	7.9755
v4	47.01	6.1212	46.93	5.9934
v5	64.05	0.3342	64.06	0.3339
v6	135.43	0.0037	135.44	0.0037
v7	179.85	0.0551	179.85	0.0551
v8	261.57	0.0464	261.57	0.0464
v9	318.68	0.0704	318.68	0.0704
v10	332.36	0.4163	332.36	0.4164
v11	404.33	0.0015	404.34	0.0015
v12	496.04	0.4426	496.04	0.4426
v13	533.01	0.2006	533.01	0.2006
v14	556.37	1.5602	556.37	1.5603
v15	668.85	0.83	668.85	0.8301
v16	752.97	0.3057	752.97	0.3057
v17	766.82	0.7247	766.82	0.7247
v18	811.44	0.9058	811.43	0.906
v19	843.38	0.8878	843.38	0.8877
v20	881.79	1.0874	881.79	1.0875
v21	883.10	2.134	883.11	2.134
v22	916.33	0.0836	916.33	0.0836
v23	918.54	0.9404	918.54	0.9408
v24	941.19	0.082	941.19	0.082
v25	942.64	1.5478	942.64	1.5473
v26	952.36	1.4747	952.34	1.4751
v27	985.14	2.321	985.15	2.3208
v28	985.59	0.3338	985.58	0.3341
v29	1020.62	2.0434	1020.62	2.043
v30	1028.53	1.4684	1028.53	1.4685
v31	1066.23	0.0209	1066.24	0.0209
v32	1069.03	0.2564	1069.03	0.2564
v33	1075.24	0.0453	1075.24	0.0453
v34	1076.52	0.0612	1076.53	0.0612
v35	1095.19	0.8207	1095.19	0.8207
v36	1155.16	0.1692	1155.16	0.1692
v37	1170.51	0.2051	1170.51	0.205

v38	1183.65	1.6119	1183.65	1.6117
v39	1215.19	0.1902	1215.19	0.1901
v40	1221.52	0.0875	1221.52	0.0876
v41	1227.43	2.3231	1227.43	2.3231
v42	1245.21	1.3384	1245.21	1.3386
v43	1270.57	0.022	1270.57	0.0219
v44	1287.39	3.0543	1287.39	3.055
v45	1294.04	0.772	1294.04	0.7725
v46	1307.14	0.0025	1307.14	0.0024
v47	1319.85	0.0501	1319.85	0.0501
v48	1326.67	0.3669	1326.67	0.3669
v49	1334.36	0.2285	1334.36	0.2295
v50	1342.10	5.7713	1342.10	5.7694
v51	1345.50	0.0122	1345.50	0.0122
v52	1363.09	0.283	1363.09	0.283
v53	1364.93	2.1026	1364.93	2.1027
v54	1384.20	3.3768	1384.20	3.3774
v55	1387.91	0.1504	1387.91	0.1504
v56	1522.93	1.3486	1522.93	1.3468
v57	1524.98	2.6419	1524.98	2.6413
v58	1529.17	2.8968	1529.17	2.8972
v59	1533.93	8.6982	1533.93	8.7018
v60	1547.80	9.8715	1547.80	9.8705
v61	1561.58	5.5372	1561.58	5.5366
v62	1912.39	143.8264	1912.43	143.8168
v63	3067.19	3.1441	3067.19	3.1412
v64	3070.54	37.068	3070.54	37.0687
v65	3076.32	23.1088	3076.32	23.1088
v66	3081.66	31.672	3081.66	31.6419
v67	3083.60	45.5786	3083.60	45.5826
v68	3083.90	28.7317	3083.90	28.7855
v69	3086.32	69.1679	3086.32	69.1636
v70	3087.53	3.5902	3087.53	3.5741
v71	3109.53	87.9166	3109.53	87.9197
v72	3115.32	10.3538	3115.31	10.3542
v73	3126.21	0.2346	3126.21	0.2332
v74	3129.36	28.9422	3129.35	28.9439
v75	3139.90	20.663	3139.90	20.6566
v76	3145.71	15.8866	3145.71	15.8678
v77	3147.62	99.8338	3147.62	99.8489

v78	3165.12	11.9748	3165.12	11.9752
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Normal modes	vdW1 Site3 JP-10/BO		vdW1 Site4 JP-10/BO	
	Frequencies(cm ⁻¹)	IR Inten	Frequencies(cm ⁻¹)	IR Inten
v1	25.01	10.4022	27.76	8.8529
v2	28.00	11.5204	29.79	7.5264
v3	41.77	7.9948	33.53	0.7163
v4	46.94	6.0032	42.94	42.7611
v5	64.05	0.3331	55.95	1.9084
v6	135.45	0.0037	128.21	0.0162
v7	179.86	0.055	187.85	0.2858
v8	261.58	0.0464	262.06	0.1114
v9	318.68	0.0704	318.97	0.0705
v10	332.37	0.4163	330.55	0.0201
v11	404.34	0.0015	403.79	0.0599
v12	496.04	0.4425	492.75	0.4325
v13	533.01	0.2006	532.80	0.228
v14	556.38	1.5601	557.69	1.0373
v15	668.86	0.8299	669.81	0.8783
v16	752.97	0.3057	753.19	0.3022
v17	766.82	0.7244	765.81	0.6634
v18	811.44	0.9059	810.27	1.5409
v19	843.38	0.8877	841.09	0.9672
v20	881.78	1.0873	881.85	1.9589
v21	883.10	2.134	882.77	0.6132
v22	916.33	0.0837	913.96	0.2055
v23	918.53	0.9403	918.06	0.5606
v24	941.18	0.0819	941.04	0.0333
v25	942.64	1.5474	941.19	1.0092
v26	952.35	1.4747	952.17	1.2621
v27	985.14	2.3203	980.35	3.2247
v28	985.58	0.3339	986.15	0.3965
v29	1020.62	2.0433	1021.61	2.0061
v30	1028.52	1.4683	1025.25	1.1128
v31	1066.24	0.0209	1063.95	0.0056
v32	1069.03	0.2565	1068.00	0.1429
v33	1075.24	0.0453	1074.37	0.0326
v34	1076.52	0.0612	1078.78	0.1377
v35	1095.19	0.8208	1095.78	0.7191
v36	1155.16	0.1692	1150.17	0.2554
v37	1170.51	0.2051	1168.50	0.0679

v38	1183.65	1.6119	1183.11	1.1836
v39	1215.19	0.1903	1217.11	0.3799
v40	1221.53	0.0875	1221.45	0.0594
v41	1227.43	2.3233	1226.57	3.7636
v42	1245.21	1.3383	1244.32	1.3509
v43	1270.57	0.022	1270.01	0.0383
v44	1287.39	3.0537	1282.57	0.8493
v45	1294.04	0.7719	1291.74	1.4175
v46	1307.14	0.0025	1305.02	0.0011
v47	1319.85	0.0501	1317.35	0.1921
v48	1326.67	0.3669	1324.64	0.3111
v49	1334.37	0.2287	1331.12	0.9038
v50	1342.10	5.7711	1341.09	5.5236
v51	1345.50	0.0122	1341.80	0.353
v52	1363.09	0.283	1364.87	1.0352
v53	1364.93	2.1027	1373.41	0.3437
v54	1384.20	3.3765	1377.23	2.9754
v55	1387.91	0.1504	1380.13	0.3432
v56	1522.93	1.3474	1523.98	0.107
v57	1524.98	2.642	1525.14	4.6663
v58	1529.17	2.8966	1526.82	1.9742
v59	1533.93	8.6984	1536.87	9.136
v60	1547.80	9.8724	1547.60	16.9774
v61	1561.58	5.5376	1557.81	6.0959
v62	1912.43	143.8152	1914.12	72.1057
v63	3067.19	3.1403	3054.60	6.0678
v64	3070.53	37.0701	3070.51	57.631
v65	3076.30	23.1113	3072.68	28.1118
v66	3081.66	31.5678	3073.16	38.3365
v67	3083.58	45.566	3077.45	24.1082
v68	3083.90	28.7217	3087.39	64.9358
v69	3086.31	69.2393	3088.58	25.933
v70	3087.54	3.6115	3090.13	26.3741
v71	3109.52	87.9164	3113.51	71.4722
v72	3115.30	10.3601	3119.03	7.8932
v73	3126.19	0.2336	3126.51	1.4997
v74	3129.34	28.9391	3132.06	34.4639
v75	3139.88	20.677	3134.51	25.672
v76	3145.70	15.8691	3146.25	55.5298
v77	3147.60	99.8642	3151.14	28.813

v78	3165.10	11.9742	3155.33	43.8505
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Normal modes	vdW1 Site5 JP-10/BO		vdW1 Site6 JP-10/BO	
	Frequencies(cm ⁻¹)	IR Inten	Frequencies(cm ⁻¹)	IR Inten
v1	16.32	4.7766	25.22	10.239
v2	31.83	8.8446	28.20	11.3984
v3	46.61	2.4556	41.87	8.1581
v4	55.42	40.045	47.00	6.1256
v5	60.91	4.9459	64.04	0.3345
v6	131.47	0.021	135.43	0.0037
v7	180.22	0.0019	179.85	0.0551
v8	261.98	0.0167	261.57	0.0464
v9	319.24	0.0857	318.68	0.0704
v10	332.25	0.0609	332.36	0.4163
v11	403.18	0.059	404.33	0.0015
v12	492.59	0.351	496.04	0.4427
v13	532.41	0.2932	533.01	0.2006
v14	556.82	0.5982	556.37	1.5598
v15	668.73	0.9191	668.85	0.83
v16	751.91	0.4196	752.97	0.3058
v17	766.29	0.5512	766.82	0.7243
v18	811.31	0.8836	811.44	0.9059
v19	844.97	0.8828	843.38	0.8877
v20	881.58	2.0695	881.78	1.0872
v21	882.66	1.0606	883.10	2.1341
v22	913.85	0.142	916.33	0.0836
v23	918.38	0.5651	918.53	0.9404
v24	939.25	0.0405	941.18	0.0819
v25	941.89	1.541	942.64	1.5476
v26	955.36	1.6284	952.36	1.4742
v27	980.72	3.0369	985.13	2.3208
v28	986.92	0.9147	985.58	0.3339
v29	1019.90	2.1362	1020.61	2.0433
v30	1028.42	1.1878	1028.52	1.4681
v31	1063.41	0.0737	1066.23	0.0209
v32	1069.73	0.2694	1069.03	0.2565
v33	1075.96	0.077	1075.24	0.0453
v34	1079.10	0.0545	1076.52	0.0612
v35	1094.24	0.6561	1095.19	0.8205
v36	1149.74	0.14	1155.15	0.1692
v37	1166.88	0.0555	1170.51	0.2051

v38	1185.99	2.2576	1183.65	1.6121
v39	1217.66	0.05	1215.19	0.1902
v40	1219.59	0.0091	1221.52	0.0874
v41	1227.93	3.2541	1227.43	2.3233
v42	1244.58	2.428	1245.21	1.3382
v43	1269.96	0.0072	1270.57	0.022
v44	1285.21	1.5747	1287.39	3.0534
v45	1291.27	0.9021	1294.04	0.7717
v46	1307.71	0.0672	1307.14	0.0024
v47	1320.69	0.0825	1319.85	0.0501
v48	1326.41	0.5504	1326.67	0.3669
v49	1330.24	0.9209	1334.36	0.2283
v50	1340.55	4.2151	1342.10	5.7714
v51	1342.21	1.899	1345.50	0.0121
v52	1361.93	0.884	1363.09	0.2831
v53	1363.41	2.2728	1364.93	2.1023
v54	1384.43	1.8569	1384.20	3.3757
v55	1389.02	0.5162	1387.91	0.1506
v56	1523.41	0.1357	1522.93	1.3483
v57	1523.82	2.1706	1524.98	2.6418
v58	1528.72	2.7789	1529.17	2.8966
v59	1533.32	10.4657	1533.93	8.6978
v60	1547.08	13.6939	1547.80	9.8723
v61	1557.54	5.9277	1561.58	5.5387
v62	1913.15	73.6334	1912.40	143.8216
v63	3071.47	17.8843	3067.20	3.1392
v64	3072.62	10.6228	3070.54	37.0656
v65	3073.58	25.164	3076.31	23.112
v66	3075.95	37.6267	3081.67	31.6052
v67	3076.74	6.2658	3083.60	45.5824
v68	3085.69	39.5679	3083.91	28.745
v69	3087.27	48.5005	3086.32	69.2064
v70	3096.53	55.3004	3087.54	3.5952
v71	3101.79	62.7507	3109.53	87.9156
v72	3115.71	26.9262	3115.32	10.3572
v73	3124.94	3.1015	3126.20	0.2337
v74	3130.40	31.0599	3129.36	28.9492
v75	3138.37	29.4067	3139.89	20.6622
v76	3145.73	2.197	3145.71	15.9342
v77	3147.38	90.2866	3147.62	99.7907

v78	3154.53	32.6233	3165.13	11.9697
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Normal modes	TS1 JP-10/BO		TS2 JP-10/BO	
	Frequencies(cm ⁻¹)	IR Inten	Frequencies(cm ⁻¹)	IR Inten
v1	-1403.20	168.5055	-1519.46	2.9098
v2	30.82	4.2171	33.27	2.9417
v3	31.71	4.1266	41.88	3.041
v4	114.58	2.0527	130.83	0.8193
v5	151.14	1.7476	165.00	2.9825
v6	162.42	0.616	184.36	1.0285
v7	186.72	0.5447	187.12	2.9685
v8	244.15	0.3902	267.66	0.1221
v9	305.22	0.2981	273.96	0.5572
v10	335.62	0.0522	326.27	0.2026
v11	378.85	0.1128	339.31	0.0794
v12	494.34	0.6457	403.81	0.1039
v13	502.54	5.1846	495.37	0.6331
v14	547.68	0.1101	529.41	0.446
v15	566.99	0.5367	556.32	0.6983
v16	670.14	1.742	663.96	1.1427
v17	755.57	0.9736	742.45	2.4972
v18	777.29	0.4746	767.72	6.2292
v19	815.53	1.2946	816.95	5.1316
v20	871.53	0.4167	841.70	1.4082
v21	882.88	0.2821	877.99	1.8481
v22	899.00	2.1405	881.39	2.6286
v23	915.67	0.7131	905.78	1.0488
v24	928.88	1.5409	925.48	1.12
v25	937.41	0.4008	938.06	0.5402
v26	941.71	0.959	940.59	1.6842
v27	953.21	0.5996	969.50	6.3433
v28	981.37	2.8485	978.73	1.973
v29	988.23	5.4582	1005.16	8.0328
v30	1017.70	2.3007	1022.19	1.0068
v31	1035.44	2.3098	1027.35	2.1113
v32	1056.25	2.7429	1063.65	0.2253
v33	1064.96	1.2842	1072.13	0.3864
v34	1069.48	0.271	1082.18	0.2487
v35	1077.05	0.1609	1092.12	4.3581
v36	1110.18	3.2893	1106.66	0.3755
v37	1149.58	0.3025	1152.67	2.8121

v38	1169.32	0.628	1166.20	3.5013
v39	1184.25	0.981	1174.95	1.1628
v40	1206.50	4.0002	1208.27	8.3286
v41	1216.86	0.1832	1215.09	0.1445
v42	1222.50	1.5948	1218.80	1.9036
v43	1242.35	0.4329	1237.72	8.0875
v44	1249.38	2.3393	1254.35	3.056
v45	1282.08	3.3128	1267.28	0.7909
v46	1287.79	1.9528	1284.79	1.375
v47	1298.88	1.4666	1290.86	0.8809
v48	1309.08	1.4284	1311.48	7.4323
v49	1322.19	0.5659	1319.42	3.5538
v50	1333.13	0.5739	1326.43	1.9677
v51	1337.94	4.9806	1333.85	3.3962
v52	1340.80	1.5645	1335.98	3.1496
v53	1358.38	1.912	1351.57	2.221
v54	1362.52	0.5659	1363.99	0.172
v55	1364.60	2.0331	1377.46	0.8924
v56	1380.46	2.4836	1387.78	0.4789
v57	1387.11	0.8399	1522.26	2.4123
v58	1520.97	4.5357	1522.72	0.3228
v59	1527.21	7.4976	1527.68	3.3689
v60	1528.18	3.2984	1532.94	11.4094
v61	1539.01	7.5204	1545.50	12.7036
v62	1555.52	15.9563	1556.92	9.4423
v63	1908.50	142.6126	1914.96	100.7352
v64	3066.21	24.6438	3076.56	19.768
v65	3075.46	24.4323	3078.59	27.845
v66	3076.89	10.1929	3080.19	18.1342
v67	3077.67	18.9904	3081.42	1.6148
v68	3078.00	20.9078	3085.06	19.5862
v69	3090.71	41.3083	3093.60	35.0389
v70	3093.38	8.4537	3097.66	40.9224
v71	3118.12	33.4145	3100.63	8.5607
v72	3122.63	18.409	3115.79	41.9722
v73	3126.67	11.471	3134.80	27.2253
v74	3133.45	34.2565	3139.37	6.3554
v75	3138.44	26.3505	3140.02	16.0135
v76	3143.04	17.7946	3149.06	38.7967
v77	3147.22	52.2843	3158.13	42.4141

v78	3159.61	28.4779	3168.90	20.7908
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Normal modes	TS3 JP-10/BO		TS4 JP-10/BO	
	Frequencies(cm ⁻¹)	IR Inten	Frequencies(cm ⁻¹)	IR Inten
v1	-1633.90	3.6622	-1260.83	83.202
v2	40.25	2.9962	27.22	3.5843
v3	43.92	3.4046	32.44	3.3641
v4	138.19	0.0004	109.89	0.9275
v5	158.07	2.1508	147.59	1.056
v6	185.94	3.5711	167.70	0.4069
v7	206.77	2.6338	194.12	1.5312
v8	262.74	0.1365	262.24	0.1205
v9	285.00	1.13	291.47	1.5511
v10	320.34	0.0744	321.49	0.039
v11	327.63	0.018	340.83	0.4303
v12	435.59	0.7685	401.58	0.1506
v13	534.78	0.6381	499.06	0.2289
v14	545.19	0.3383	536.27	0.2371
v15	599.55	5.4477	556.20	0.6342
v16	669.03	0.3644	684.14	0.8315
v17	739.03	1.5049	753.40	0.6877
v18	776.40	0.6683	767.42	5.9237
v19	811.30	1.6339	816.16	0.3454
v20	840.26	2.354	848.05	0.0678
v21	880.94	0.8076	878.19	1.5768
v22	881.23	1.0592	890.29	3.2153
v23	906.53	0.3934	911.21	0.8917
v24	926.21	0	916.97	0.2967
v25	942.13	1.8831	933.69	3.0381
v26	950.37	0.109	938.84	0.2882
v27	963.71	0.4176	950.05	2.1595
v28	976.84	0.4274	980.88	3.3916
v29	1019.53	0.1025	985.90	1.3306
v30	1023.46	2.6242	1022.87	3.6213
v31	1024.79	2.6189	1044.79	1.0582
v32	1065.87	4.3579	1061.90	0.3201
v33	1072.43	0.0726	1074.48	0.6189
v34	1075.99	0.4392	1081.65	0.9545
v35	1083.83	0.4878	1102.86	1.5222
v36	1095.57	0.8567	1113.30	0.8139
v37	1146.78	1.8672	1151.23	1.821

v38	1166.97	1.1748	1165.93	0.7194
v39	1185.34	12.7316	1186.98	1.6718
v40	1217.17	0.0437	1205.56	9.8409
v41	1220.19	0.7401	1213.15	1.3744
v42	1221.04	4.5668	1233.55	3.8621
v43	1224.96	1.5079	1242.37	0.0291
v44	1261.91	0.4713	1264.89	1.1298
v45	1266.90	0.1451	1271.58	0.9668
v46	1282.70	1.6829	1279.82	0.2142
v47	1293.50	0.0324	1290.26	1.8233
v48	1316.10	0.1664	1292.21	0.3492
v49	1322.52	0.0697	1322.34	0.2395
v50	1327.41	2.2152	1328.55	0.4962
v51	1337.01	0.4909	1332.04	2.8922
v52	1341.70	2.833	1339.48	5.9452
v53	1358.53	2.3769	1360.16	1.4573
v54	1363.15	0.9666	1362.33	1.0827
v55	1365.64	0.045	1367.80	1.3406
v56	1384.50	2.838	1379.67	0.7483
v57	1387.08	0.3327	1513.14	6.4575
v58	1524.25	3.6314	1523.12	2.4008
v59	1528.10	5.0402	1527.76	2.2827
v60	1528.12	5.3741	1532.84	12.4447
v61	1544.28	0.1761	1543.58	15.6225
v62	1545.85	11.5092	1556.48	4.8101
v63	1910.67	101.1099	1905.36	132.7458
v64	3076.47	3.993	3058.74	16.0321
v65	3077.39	28.7076	3059.40	13.4112
v66	3082.78	23.6819	3077.52	16.419
v67	3083.38	13.6448	3080.76	21.3382
v68	3084.00	27.2025	3085.99	20.7994
v69	3090.72	10.4046	3087.42	29.5822
v70	3093.49	75.1234	3095.58	36.1959
v71	3118.39	11.6096	3116.33	21.084
v72	3127.16	45.176	3120.94	46.6219
v73	3132.74	15.5608	3129.14	16.0643
v74	3134.86	15.612	3136.30	1.1119
v75	3136.18	4.2834	3138.13	28.5914
v76	3139.08	22.1071	3147.82	15.3983
v77	3149.30	46.0715	3152.42	35.297

v78	3154.66	53.6723	3155.07	46.3146
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Normal modes	TS5 JP-10/BO		TS6 JP-10/BO	
	Frequencies(cm ⁻¹)	IR Inten	Frequencies(cm ⁻¹)	IR Inten
v1	-1471.12	100.942	-1384.87	105.4313
v2	32.49	3.8424	22.84	3.4005
v3	38.74	3.5258	35.65	3.7634
v4	106.50	2.5144	115.16	3.407
v5	143.67	0.7238	115.92	1.0033
v6	169.14	2.3885	172.52	0.971
v7	190.54	0.8349	181.13	0.8875
v8	234.19	0.1508	263.79	0.0088
v9	292.03	0.0402	320.20	0.4977
v10	327.89	0.0902	325.44	0.153
v11	398.72	0.1502	408.37	0.314
v12	437.19	0.6801	450.34	2.0056
v13	504.33	0.2605	497.04	1.2432
v14	535.60	1.0319	535.52	0.2106
v15	598.72	3.7465	618.52	3.1422
v16	701.45	6.5642	676.83	0.4392
v17	755.66	0.2918	750.05	0.2892
v18	770.07	0.8768	775.95	0.833
v19	814.91	0.4749	810.25	1.7571
v20	848.60	1.1562	841.65	2.1557
v21	874.80	2.8571	876.62	1.0643
v22	888.07	0.7659	899.31	1.8768
v23	918.98	0.3918	916.90	1.6066
v24	931.30	1.3306	919.30	0.551
v25	942.00	0.6435	940.83	0.7043
v26	951.90	1.3903	944.72	0.5111
v27	966.27	2.1792	952.38	1.5034
v28	982.17	3.8294	979.82	2.1033
v29	986.92	0.2321	986.45	0.369
v30	1025.61	1.5665	1026.56	2.8935
v31	1028.19	1.5894	1027.46	1.9148
v32	1064.53	0.1258	1066.16	0.1377
v33	1072.10	0.4753	1069.13	2.2543
v34	1075.45	1.1218	1075.78	0.004
v35	1094.87	1.3885	1094.14	1.043
v36	1115.15	0.9585	1095.56	0.0089
v37	1150.50	0.0802	1151.35	0.5364

v38	1160.80	1.1004	1164.57	0.0057
v39	1181.71	3.4361	1183.50	0.4492
v40	1202.69	2.1681	1219.10	0.0134
v41	1218.55	1.822	1230.32	6.0972
v42	1221.02	1.2089	1232.51	0.0049
v43	1242.76	0.7786	1242.03	7.8002
v44	1257.00	1.3414	1268.93	0.2836
v45	1270.73	0.0837	1270.57	19.7531
v46	1292.46	1.3845	1291.64	2.2444
v47	1297.81	0.5649	1301.20	0.3653
v48	1312.62	1.2752	1310.49	0.0513
v49	1322.85	1.4772	1323.65	0.0722
v50	1329.80	1.4602	1326.57	4.2874
v51	1333.59	1.1551	1333.55	3.2241
v52	1338.87	3.2494	1334.87	0.487
v53	1341.93	2.5423	1349.62	2.9386
v54	1350.67	2.3897	1352.24	1.9151
v55	1362.81	1.8574	1368.45	6.1217
v56	1381.13	1.9849	1385.13	1.1584
v57	1389.39	0.5153	1386.92	0.5232
v58	1522.58	2.0515	1511.40	11.0875
v59	1526.57	2.0657	1517.44	1.1378
v60	1530.39	10.8322	1526.48	1.7271
v61	1541.60	15.2547	1539.00	20.9748
v62	1556.43	4.9296	1556.82	5.4228
v63	1911.02	137.2431	1909.21	128.45
v64	3061.03	8.6494	3053.11	15.8746
v65	3069.99	18.6669	3054.64	10.1655
v66	3080.34	17.143	3078.80	0.0865
v67	3082.92	19.4697	3082.69	20.8039
v68	3088.54	39.2683	3087.80	27.5572
v69	3089.59	3.793	3091.51	21.2279
v70	3092.34	54.7429	3092.49	45.9977
v71	3115.20	61.7967	3114.71	65.2964
v72	3120.50	5.3483	3120.20	11.9794
v73	3127.85	19.3165	3122.04	25.8958
v74	3133.10	0.3997	3122.85	14.0512
v75	3138.57	21.5642	3132.90	0.0257
v76	3147.74	4.88	3143.18	31.1123
v77	3152.17	57.4395	3147.31	23.4208

v78	3152.70	45.884	3152.34	55.2308
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Normal modes	vdW2 Site 1 JP-10/BO		vdW2 Site 2 JP-10/BO	
	Frequencies(cm ⁻¹)	IR Inten	Frequencies(cm ⁻¹)	IR Inten
v1	10.90	1.7423	8.04	0.5259
v2	19.15	1.9005	14.96	1.9442
v3	51.99	0.6205	50.43	0.2882
v4	78.71	13.2506	74.23	14.3083
v5	87.76	15.0544	90.02	15.7316
v6	153.12	0.1635	136.43	0.1699
v7	180.43	0.2086	179.27	0.0492
v8	284.39	1.0903	263.80	0.1989
v9	313.29	2.7867	317.34	0.4557
v10	330.22	0.0851	331.39	0.0694
v11	391.09	1.8314	402.37	0.0858
v12	491.75	2.3945	494.73	0.7179
v13	509.53	19.2379	521.59	0.6503
v14	551.78	0.3829	555.72	0.5677
v15	590.31	13.492	661.28	1.4542
v16	668.39	0.8488	730.91	0.171
v17	758.09	0.7355	764.03	0.3294
v18	780.41	0.5943	801.64	0.6994
v19	804.02	6.6028	808.67	7.0748
v20	811.65	7.3764	817.57	7.4708
v21	815.44	1.4534	838.61	0.7136
v22	880.13	0.2778	856.15	4.6048
v23	883.81	2.1453	879.04	0.5096
v24	914.68	0.3006	899.89	0.168
v25	923.43	0.7171	913.97	0.4276
v26	930.49	1.5998	935.57	0.1019
v27	941.19	1.2304	940.23	1.9179
v28	955.75	0.3167	957.42	2.0693
v29	960.19	0.1889	976.11	1.5435
v30	982.75	3.5599	995.82	0.4202
v31	1008.82	0.6915	1022.63	0.79
v32	1023.73	1.5915	1026.67	2.8781
v33	1037.42	3.3402	1062.74	0.1963
v34	1057.37	0.1764	1072.34	0.0481
v35	1064.76	0.1442	1079.50	0.2286
v36	1075.71	0.1466	1107.24	0.3734
v37	1096.46	1.1931	1126.73	0.3864

v38	1142.85	0.8794	1158.92	1.384
v39	1164.64	0.2243	1181.44	0.7918
v40	1170.69	0.5909	1212.56	0.2473
v41	1202.04	1.1471	1214.37	0.7338
v42	1216.16	0.2419	1226.06	5.2179
v43	1230.38	0.6329	1236.38	1.9939
v44	1254.85	1.718	1251.97	3.5809
v45	1272.34	1.6815	1275.65	0.6021
v46	1286.46	1.519	1283.91	1.4332
v47	1293.04	2.207	1302.20	2.7443
v48	1306.59	0.6186	1317.32	1.6662
v49	1318.21	0.4994	1321.80	1.2459
v50	1332.03	1.464	1327.30	2.1155
v51	1342.00	1.5703	1333.72	2.438
v52	1351.87	2.7494	1348.05	1.2017
v53	1358.10	1.0579	1363.91	0.1464
v54	1362.85	0.6981	1376.41	0.575
v55	1376.92	1.9478	1389.48	0.7402
v56	1385.27	0.5716	1521.05	2.3159
v57	1511.27	5.6874	1523.07	0.4551
v58	1525.37	3.3013	1528.17	4.5486
v59	1528.11	4.0104	1532.81	11.4186
v60	1537.25	7.5938	1545.03	12.0487
v61	1553.99	12.6563	1556.62	9.0366
v62	1811.96	45.2736	1810.69	46.8834
v63	2892.37	3.1071	2889.92	3.5118
v64	3034.60	35.0407	3076.07	21.2937
v65	3074.96	23.067	3077.65	31.1702
v66	3076.53	33.3633	3080.36	10.7315
v67	3077.08	20.0801	3081.34	15.4824
v68	3078.04	1.0983	3084.74	26.3672
v69	3093.02	6.9715	3095.16	28.2804
v70	3095.80	41.8828	3097.71	48.8118
v71	3097.15	28.8342	3102.53	20.2208
v72	3118.55	56.3976	3113.67	36.6237
v73	3122.87	13.1932	3133.24	25.8959
v74	3131.74	32.0241	3138.54	22.7906
v75	3137.07	27.6638	3139.58	6.2804
v76	3145.93	54.7583	3148.27	43.6475
v77	3160.52	27.7594	3159.39	44.4864

v78	3219.66	21.0165	3171.33	24.1231
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Normal modes	vdW2 Site 3 JP-10/BO		vdW2 Site 4 JP-10/BO	
	Frequencies(cm ⁻¹)	IR Inten	Frequencies(cm ⁻¹)	IR Inten
v1	12.46	2.3083	13.16	1.212
v2	18.96	1.7465	18.96	1.4963
v3	44.03	0.1734	55.11	1.2326
v4	76.72	12.7347	80.88	12.6277
v5	82.09	14.675	86.79	11.6648
v6	110.12	0.4675	121.77	1.2487
v7	184.13	0.4444	167.67	0.3609
v8	243.06	0.0605	238.59	0.3783
v9	316.94	0.0777	299.65	0.5982
v10	317.27	0.4832	316.21	0.1449
v11	369.47	4.138	390.17	0.032
v12	456.64	6.6157	486.20	0.767
v13	531.40	0.6856	540.56	0.236
v14	545.03	1.1894	557.08	0.8934
v15	666.72	0.25	630.57	3.5491
v16	743.30	17.5152	730.58	0.2398
v17	745.80	1.1748	752.91	0.4215
v18	786.79	2.9739	811.24	5.4244
v19	796.51	7.197	812.26	3.3856
v20	804.19	7.457	817.22	6.846
v21	809.16	0.8666	838.03	1.7176
v22	848.33	2.2939	864.68	0.7982
v23	875.77	0.9018	895.48	1.9243
v24	886.09	1.3137	902.01	0.8024
v25	905.47	0.6366	914.90	0.6505
v26	930.28	0.0056	919.59	0.4807
v27	943.94	2.3332	933.89	0.25
v28	946.84	0.2228	946.56	1.3287
v29	973.71	0.4926	981.54	1.5038
v30	975.40	2.4049	982.75	3.3917
v31	1018.64	2.2824	1020.92	1.5263
v32	1022.79	1.4667	1034.94	1.5789
v33	1039.57	0.127	1059.19	0.2001
v34	1065.35	0.0561	1069.14	0.0621
v35	1072.03	0.0343	1077.37	0.0947
v36	1076.00	0.5087	1113.83	2.1617
v37	1096.29	1.0037	1143.18	0.4684

v38	1170.96	0.8238	1147.49	0.1157
v39	1182.37	1.8269	1171.11	0.0653
v40	1208.70	1.2738	1177.28	0.6736
v41	1215.94	0.3039	1207.52	2.0357
v42	1222.78	0.7326	1230.18	1.3928
v43	1225.19	1.4818	1244.14	2.283
v44	1248.73	1.0625	1249.96	0.6586
v45	1263.22	0.655	1266.92	0.13
v46	1283.07	2.2761	1276.15	1.157
v47	1286.67	0.0322	1289.45	1.1039
v48	1310.78	0.0013	1320.63	0.3296
v49	1320.00	0.0246	1323.13	0.2706
v50	1324.59	0.4074	1329.75	2.0512
v51	1343.97	2.2717	1334.56	4.7091
v52	1344.37	0.012	1356.50	1.4581
v53	1363.38	0.4937	1357.69	0.4577
v54	1363.52	0.8201	1368.25	0.8157
v55	1378.88	2.9471	1384.03	0.7363
v56	1381.19	0.383	1509.16	6.9806
v57	1519.47	4.6966	1521.98	0.9165
v58	1523.37	1.3611	1525.30	2.1274
v59	1525.98	7.6344	1532.10	9.5236
v60	1540.91	2.1132	1541.60	14.1701
v61	1544.77	7.7065	1554.60	4.4979
v62	1813.21	40.7126	1810.16	51.4216
v63	2902.73	0.3053	2878.38	5.7793
v64	3074.48	30.0001	3025.78	24.5265
v65	3075.53	25.1619	3033.51	26.3864
v66	3076.10	22.7287	3076.21	12.5743
v67	3076.41	0.9433	3080.36	17.4293
v68	3080.77	30.1418	3082.32	34.7996
v69	3089.10	17.7803	3083.39	22.4228
v70	3091.99	69.4078	3093.46	53.7379
v71	3129.33	34.8252	3095.09	37.116
v72	3131.13	22.0736	3120.62	46.7307
v73	3132.67	0.8343	3132.04	24.7458
v74	3134.12	24.2827	3135.55	2.2268
v75	3136.46	24.514	3136.65	33.6631
v76	3145.64	53.8831	3145.42	8.3852
v77	3151.63	52.7262	3149.46	49.9838

v78	3200.49	23.8061	3155.75	48.1098
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Normal modes	vdW5 Site 5 JP-10/BO		vdW2 Site 6 JP-10/BO	
	Frequencies(cm ⁻¹)	IR Inten	Frequencies(cm ⁻¹)	IR Inten
v1	12.06	2.8851	20.48	11.9246
v2	16.32	2.9613	43.97	0.6539
v3	44.92	5.3304	65.21	5.2745
v4	61.45	8.4374	78.25	0.4795
v5	86.38	12.052	132.79	0.5041
v6	122.36	0.3061	142.47	7.5732
v7	139.81	0.7437	155.27	33.2842
v8	257.10	0.3972	256.59	0.0117
v9	292.19	2.9512	290.63	0.4948
v10	316.52	1.8189	328.18	0.019
v11	368.74	32.5124	403.33	0.0396
v12	402.28	0.4808	469.24	28.4758
v13	499.67	0.541	504.94	5.8117
v14	535.15	0.1299	532.91	0.0527
v15	620.57	0.7962	696.55	2.0634
v16	745.07	0.3963	700.22	2.0929
v17	763.32	2.6066	746.77	0.3362
v18	769.57	0.2419	770.45	29.0286
v19	794.28	7.8351	777.48	10.3227
v20	799.48	7.3839	789.48	0.3215
v21	813.70	0.7819	810.75	0.8614
v22	846.48	0.6128	841.19	1.3818
v23	861.27	0.7291	862.72	0.5729
v24	888.43	1.7767	914.30	2.3861
v25	918.59	0.5754	920.66	0.3921
v26	935.75	0.237	935.40	1.0768
v27	951.98	0.083	951.15	0.5175
v28	954.61	1.538	952.65	1.3993
v29	977.31	2.372	973.26	1.3255
v30	986.30	0.5351	987.23	0.4643
v31	1004.63	2.3979	991.72	2.3896
v32	1029.56	1.7672	1038.87	2.0464
v33	1045.30	0.2019	1054.19	0.0856
v34	1064.91	0.1669	1066.69	0.4797
v35	1072.10	0.0979	1075.14	0.2623
v36	1091.15	0.1097	1086.50	0.0085
v37	1098.21	0.8214	1099.97	0.0886

v38	1136.85	0.0402	1150.02	0.882
v39	1154.38	0.2962	1162.60	0.0054
v40	1177.44	1.0312	1169.10	1.2031
v41	1204.93	0.3439	1206.94	0.4009
v42	1226.89	4.4629	1219.51	0.1697
v43	1236.53	0.4794	1233.07	2.8481
v44	1252.41	0.5829	1255.49	2.9619
v45	1264.27	0.12	1267.84	0.1865
v46	1291.76	1.6305	1288.13	1.3028
v47	1297.70	0.4752	1297.47	0.2047
v48	1310.96	0.5947	1313.36	0.1162
v49	1317.00	0.5844	1323.70	0.1616
v50	1330.89	0.0795	1328.95	0.092
v51	1332.83	1.5882	1334.74	2.7386
v52	1338.53	1.6737	1335.45	3.6333
v53	1345.83	5.6809	1364.31	0.8069
v54	1365.11	1.2468	1369.90	5.2374
v55	1377.85	2.3669	1379.71	0.5773
v56	1388.29	0.7429	1390.95	0.6731
v57	1511.12	2.4593	1505.67	11.2548
v58	1525.37	2.566	1512.39	4.2738
v59	1527.13	5.3044	1525.20	1.58
v60	1543.39	16.0419	1535.33	17.7862
v61	1555.13	4.1319	1555.00	5.0743
v62	1814.64	40.6824	1803.89	22.2762
v63	2906.44	0.8494	2912.17	3.2033
v64	3001.15	42.4352	3002.83	23.1778
v65	3009.54	40.5198	3004.89	22.9136
v66	3080.47	21.2368	3073.93	10.4859
v67	3084.89	10.9704	3079.64	17.2548
v68	3086.99	33.5865	3083.14	21.9568
v69	3089.52	19.6049	3089.23	52.4256
v70	3090.17	52.4023	3090.96	44.4523
v71	3108.50	26.706	3101.89	9.9801
v72	3115.43	64.1346	3111.69	71.4728
v73	3123.42	14.9669	3116.32	20.9991
v74	3130.27	0.9723	3122.29	11.8443
v75	3143.40	26.8063	3130.35	0.137
v76	3149.57	56.7951	3143.48	26.0725
v77	3152.37	26.2656	3150.03	58.7599

v78	3223.87	19.4333	3210.44	29.9922
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Normal modes	vdW1 Site 1 JP-10/BO ₂		vdW1 Site 2 JP-10/BO ₂	
	Frequencies(cm ⁻¹)	IR Inten	Frequencies(cm ⁻¹)	IR Inten
v1	20.34	0.9436	15.97	0.7548
v2	25.81	0.2536	30.02	0.3814
v3	34.54	0.1153	50.28	0.0495
v4	40.03	2.1405	61.26	3.458
v5	53.31	0.9517	64.72	0.4665
v6	135.16	0.0658	132.15	0.024
v7	181.90	0.0045	179.79	0.0001
v8	265.84	0.196	261.80	0.0083
v9	321.48	0.1562	319.39	0.1815
v10	333.14	0.0447	331.76	0.0622
v11	405.53	0.095	402.93	0.4082
v12	445.13	63.2813	431.83	127.7401
v13	489.49	85.475	486.15	33.1337
v14	495.33	0.703	492.38	0.58
v15	533.64	0.4134	532.22	0.2073
v16	556.15	0.4819	556.73	0.5651
v17	668.11	0.852	668.43	1.108
v18	751.80	0.3454	751.66	0.4325
v19	766.05	0.605	765.95	0.5976
v20	811.05	1.0631	810.35	0.9188
v21	841.34	1.0934	843.69	0.824
v22	881.71	1.089	881.24	1.7024
v23	882.12	1.3627	882.74	1.1809
v24	913.00	0.0973	913.67	0.1785
v25	918.21	0.6032	918.58	0.4137
v26	939.30	0.0398	939.46	0.0592
v27	941.80	1.2317	942.62	1.4846
v28	952.12	1.4909	957.93	1.5389
v29	964.61	0.0319	964.74	0.3038
v30	982.50	3.5683	980.72	2.8328
v31	989.63	0.4577	989.08	1.0767
v32	1019.76	2.1287	1020.17	2.6677
v33	1026.56	1.6946	1029.21	1.2117
v34	1063.17	0.0578	1064.92	0.0042
v35	1069.03	0.2889	1069.60	0.1714
v36	1075.21	0.1913	1076.41	0.0389
v37	1077.00	0.0884	1079.53	0.0832

v38	1094.13	0.6224	1093.64	0.4283
v39	1155.02	0.3245	1149.25	0.3761
v40	1167.26	0.0251	1166.16	0.0608
v41	1183.64	1.3244	1189.78	2.221
v42	1215.86	0.2398	1218.02	0.0396
v43	1219.79	0.0453	1218.88	0.0333
v44	1226.69	1.8197	1227.92	2.9171
v45	1244.08	2.6267	1244.95	2.9157
v46	1271.67	0.0503	1270.22	0.1194
v47	1284.60	1.3151	1286.13	1.7269
v48	1293.80	0.9986	1292.60	0.9689
v49	1306.39	0.0051	1309.67	0.0534
v50	1320.80	0.2284	1320.78	0.0524
v51	1327.15	0.6269	1326.34	0.4692
v52	1331.16	1.299	1331.04	0.6854
v53	1341.80	2.3669	1340.59	2.629
v54	1343.98	2.3484	1343.24	3.4067
v55	1362.27	0.6019	1362.68	0.8232
v56	1364.92	1.7016	1363.65	2.3338
v57	1383.54	1.7043	1383.65	1.9874
v58	1388.02	0.4773	1388.36	0.2657
v59	1523.17	1.8977	1522.96	0.6025
v60	1524.23	2.084	1523.76	2.2274
v61	1527.47	2.9108	1528.34	2.6657
v62	1533.95	9.4502	1533.26	10.9987
v63	1546.52	12.8554	1546.76	14.206
v64	1558.22	4.9139	1557.35	5.4252
v65	2196.34	562.7852	2065.91	182.342
v66	3070.20	9.5855	3070.81	0.7691
v67	3074.08	22.4667	3072.01	32.7965
v68	3074.28	17.5108	3073.47	17.4838
v69	3074.40	28.958	3076.52	19.1837
v70	3079.80	30.2366	3076.91	20.2004
v71	3085.30	31.2378	3081.87	75.2233
v72	3090.01	62.667	3089.08	47.1133
v73	3096.98	20.1872	3091.90	42.4844
v74	3110.84	72.7232	3096.57	52.6157
v75	3119.08	11.7421	3116.24	30.579
v76	3128.97	3.5331	3128.91	0.5242
v77	3129.43	35.132	3131.28	29.9857

v78	3134.23	29.871	3137.88	26.0005
v79	3143.56	44.4937	3145.58	21.3804
v80	3149.82	68.6737	3149.02	71.1596
v81	3158.71	27.4565	3155.51	31.5835

Normal modes	vdW1 Site 3 JP-10/BO ₂		vdW1 Site 4 JP-10/BO ₂	
	Frequencies(cm ⁻¹)	IR Inten	Frequencies(cm ⁻¹)	IR Inten
v1	20.75	0.9219	9.61	1.1432
v2	32.04	0.3783	31.62	0.0745
v3	47.01	0.4521	43.81	0.01
v4	59.87	2.7667	52.00	1.3046
v5	65.88	0.491	62.73	2.1252
v6	134.27	0.014	127.55	0.0073
v7	179.73	0.0352	186.99	0.4162
v8	262.52	0.079	263.35	0.1054
v9	318.45	0.1115	319.87	0.0639
v10	332.85	0.2036	331.21	0.0048
v11	403.75	0.2404	404.23	0.2542
v12	427.00	131.9233	429.06	124.0241
v13	484.41	34.0021	482.47	35.1324
v14	496.25	0.951	492.61	0.4981
v15	533.68	0.3977	533.05	0.3263
v16	557.21	0.5167	557.12	0.513
v17	668.88	0.9533	669.63	0.7824
v18	751.16	0.2907	754.07	0.2707
v19	766.89	0.8621	765.06	0.837
v20	812.09	1.3837	809.07	1.1988
v21	843.23	0.8264	840.44	0.887
v22	881.41	1.0391	882.11	1.835
v23	883.08	1.6915	882.76	0.9389
v24	914.74	0.1387	913.39	0.17
v25	919.61	0.4796	918.69	0.5518
v26	939.53	0.2061	940.72	1.1034
v27	942.34	1.0807	941.99	0.0721
v28	949.76	2.6601	952.20	1.0666
v29	964.02	0.5064	963.32	0.353
v30	984.38	2.2775	980.11	3.0123
v31	988.44	1.5579	986.37	0.4545
v32	1021.19	2.4364	1021.86	2.1949
v33	1028.53	1.3895	1023.06	1.5685
v34	1067.82	0.017	1064.29	0.0153
v35	1069.93	0.1903	1067.23	0.1364
v36	1076.54	0.1044	1075.71	0.4149
v37	1078.35	0.0997	1078.36	0.148

v38	1094.60	0.4939	1095.17	0.7105
v39	1154.91	0.6665	1149.99	0.3521
v40	1169.12	0.044	1168.42	0.0639
v41	1186.24	1.5116	1184.56	1.6216
v42	1216.32	0.2817	1216.58	0.404
v43	1219.99	0.5929	1221.00	0.0733
v44	1227.41	2.6813	1228.01	3.0626
v45	1244.59	1.86	1244.05	1.2218
v46	1268.44	0.051	1269.67	0.1423
v47	1285.76	1.3419	1282.17	1.0875
v48	1291.65	1.7949	1292.31	1.4734
v49	1307.55	0.0383	1306.89	0.0887
v50	1320.45	0.2725	1316.42	0.1326
v51	1326.66	0.621	1323.32	0.3379
v52	1332.30	1.6759	1331.67	0.7194
v53	1339.66	4.2663	1341.28	4.1862
v54	1346.33	1.3667	1341.73	1.7961
v55	1362.86	0.6915	1365.29	0.6058
v56	1364.65	1.1055	1369.37	0.3915
v57	1384.20	1.0007	1373.25	2.0629
v58	1387.61	0.2709	1377.75	1.406
v59	1523.81	0.864	1523.90	0.244
v60	1525.47	2.7656	1525.45	5.7573
v61	1529.94	3.2396	1526.72	1.0896
v62	1533.96	8.6776	1536.47	9.6943
v63	1548.12	14.8715	1547.37	17.9668
v64	1559.89	7.1918	1557.89	6.4064
v65	2041.91	139.756	2069.23	193.6789
v66	3070.95	9.6552	3034.34	71.4523
v67	3072.76	7.671	3073.75	21.8116
v68	3075.01	19.1269	3074.34	11.6274
v69	3075.37	40.3906	3079.71	34.1822
v70	3079.76	24.7243	3080.75	46.5685
v71	3080.88	5.0037	3085.66	27.1662
v72	3087.34	35.3116	3089.34	36.3946
v73	3088.86	68.4693	3089.64	42.7428
v74	3102.45	82.0789	3114.40	71.6393
v75	3117.25	25.6752	3119.83	8.5764
v76	3130.58	0.2555	3130.39	0.6074
v77	3131.35	31.6708	3131.80	32.7056

v78	3135.89	29.0988	3136.00	25.4265
v79	3144.13	20.2967	3147.95	2.8309
v80	3150.11	73.0009	3149.89	87.2264
v81	3150.37	22.3482	3154.08	39.1543

Normal modes	vdW1 Site 5 JP-10/BO ₂		vdW1 Site 6 JP-10/BO ₂	
	Frequencies(cm ⁻¹)	IR Inten	Frequencies(cm ⁻¹)	IR Inten
v1	28.53	1.0958	20.83	0.8052
v2	33.30	0.4644	34.81	1.555
v3	45.43	0.208	42.08	0.5998
v4	51.26	0.936	45.05	0.1373
v5	63.05	1.407	69.76	1.3065
v6	68.07	1.0311	135.21	0.0014
v7	225.10	0.052	191.92	0.1202
v8	260.17	0.1567	261.35	0.0627
v9	265.39	0.1535	319.34	0.085
v10	326.59	0.1457	334.50	0.3934
v11	408.17	0.2338	405.10	0.0066
v12	433.03	127.2996	443.53	60.0162
v13	484.65	1.335	487.66	78.3564
v14	488.11	37.1899	496.42	0.8031
v15	493.96	0.1551	532.96	0.1993
v16	630.31	0.7425	555.32	0.4621
v17	722.74	0.0601	669.04	0.854
v18	752.76	0.2587	752.82	0.3453
v19	793.66	1.1491	766.75	0.4933
v20	815.55	0.3097	811.58	0.8921
v21	817.40	0.6498	843.39	0.9864
v22	853.01	1.4504	881.96	0.7472
v23	858.05	1.5324	883.19	2.3177
v24	908.37	2.3451	915.48	0.1763
v25	915.43	0.6345	918.53	0.908
v26	930.87	0.2049	938.36	0.0062
v27	946.03	0.6611	940.65	1.5308
v28	955.10	1.0999	951.90	1.2808
v29	964.39	0.1458	965.52	0.0175
v30	973.15	3.5959	983.52	2.1468
v31	985.22	0.3729	985.88	0.5098
v32	1012.62	0.8548	1016.96	2.7075
v33	1016.89	1.986	1028.92	1.3904
v34	1051.25	0.4794	1066.13	0.0293
v35	1064.63	0.22	1068.83	0.2018
v36	1093.11	0.8416	1075.04	0.0263
v37	1107.69	0.6968	1076.19	0.0614

v38	1121.12	0.15	1096.51	0.8308
v39	1134.09	0.2608	1155.59	0.2016
v40	1155.57	0.2553	1170.15	0.0436
v41	1168.44	0.7361	1184.11	1.3152
v42	1216.22	1.8523	1212.97	0.3971
v43	1221.25	2.2181	1221.92	0.0697
v44	1228.54	0.7912	1227.54	2.5199
v45	1242.23	0.4178	1245.27	1.0985
v46	1270.20	0.4428	1270.73	0.0969
v47	1293.20	0.6644	1287.05	2.4318
v48	1303.61	0.0728	1294.86	0.8647
v49	1310.27	0.4857	1307.83	0.0042
v50	1312.73	0.708	1319.38	0.1818
v51	1327.95	1.6773	1327.19	0.3867
v52	1331.89	1.2402	1335.14	0.256
v53	1342.38	0.0233	1342.88	6.2826
v54	1350.20	3.7335	1346.58	0.0783
v55	1354.93	0.4854	1363.35	0.5669
v56	1371.25	5.4997	1365.69	2.2094
v57	1382.84	0.0802	1384.88	3.1248
v58	1392.39	0.1539	1388.87	0.2703
v59	1519.20	7.6039	1524.80	0.9225
v60	1524.27	0.3686	1525.26	3.2556
v61	1529.14	3.4855	1527.61	1.6554
v62	1533.71	6.5998	1536.06	10.2764
v63	1552.56	14.5963	1547.60	10.4087
v64	1566.65	9.1657	1561.56	6.8159
v65	2078.03	198.9796	2164.86	517.1047
v66	3033.27	81.8614	3069.73	3.2967
v67	3073.51	26.7473	3071.10	37.9625
v68	3074.28	27.2619	3077.88	22.8263
v69	3078.77	56.0982	3081.27	40.5674
v70	3089.88	24.2537	3081.62	11.4192
v71	3090.47	44.6014	3084.65	33.6558
v72	3098.22	41.6082	3087.76	71.5806
v73	3103.54	9.0607	3089.50	10.2259
v74	3113.79	67.2654	3110.84	82.5749
v75	3119.57	8.8337	3116.59	10.8463
v76	3123.08	16.2387	3123.01	31.4826
v77	3127.87	18.8486	3127.62	0.3539

v78	3129.03	14.6061	3138.43	23.0962
v79	3150.51	19.488	3144.31	32.824
v80	3153.64	88.903	3147.61	84.4018
v81	3183.04	21.8969	3162.23	13.3377

Normal modes	TS1 JP-10/BO ₂		TS2 JP-10/BO ₂	
	Frequencies(cm ⁻¹)	IR Inten	Frequencies(cm ⁻¹)	IR Inten
v1	-353.57	714.269	-431.02	1140.5985
v2	13.52	1.0207	20.52	1.0231
v3	37.21	0	45.02	0.0167
v4	57.56	0.8058	60.90	0.4577
v5	101.49	3.0469	114.35	2.7941
v6	141.47	0.5212	139.18	0.7622
v7	177.86	0.75	180.09	0.2268
v8	265.60	10.4215	264.12	0.3117
v9	323.07	7.6397	319.95	2.1071
v10	335.92	0.2924	331.80	0.0653
v11	395.28	7.4443	402.58	0.0366
v12	487.80	20.9243	459.76	1.2351
v13	494.64	22.6648	491.38	0.9338
v14	499.41	28.8995	498.69	34.9528
v15	535.55	2.2899	527.87	1.5856
v16	556.27	1.8574	557.25	0.6991
v17	668.26	2.2303	665.98	1.1949
v18	751.39	0.6726	743.54	16.8205
v19	760.19	14.2664	761.74	48.2176
v20	804.47	24.5623	805.93	78.4909
v21	826.23	27.5526	840.64	42.7678
v22	881.52	0.8154	872.64	135.4473
v23	882.84	2.5587	880.85	12.7064
v24	913.99	0.2618	906.47	189.1266
v25	922.82	4.666	912.93	34.4594
v26	934.28	0.4549	921.88	384.0394
v27	941.66	0.4547	939.69	13.1949
v28	952.47	3.6548	943.72	24.6921
v29	977.64	4.4193	967.61	24.5471
v30	984.09	20.6829	975.70	9.4493
v31	988.96	11.0702	992.82	0.7745
v32	1016.90	1.9514	1008.33	58.3312
v33	1027.45	3.3068	1022.92	6.9488
v34	1051.76	23.1099	1037.63	15.1515
v35	1064.48	0.8541	1061.72	14.4307
v36	1066.93	9.2612	1071.53	8.1175
v37	1077.36	0.2073	1074.15	4.0294

v38	1091.87	17.2044	1088.11	0.5302
v39	1147.44	4.9641	1125.53	2.7254
v40	1169.38	0.0376	1131.12	42.4255
v41	1170.44	5.2325	1173.02	11.1223
v42	1203.59	6.6443	1208.78	5.2765
v43	1215.89	28.5209	1214.31	5.9926
v44	1216.91	8.8248	1217.71	0.5286
v45	1239.72	1.2848	1235.78	5.9751
v46	1252.77	8.0154	1259.16	4.945
v47	1282.70	13.7213	1271.10	25.5491
v48	1288.15	2.1518	1284.94	2.2464
v49	1299.20	13.9827	1297.56	14.1615
v50	1310.22	9.2674	1313.22	0.3465
v51	1324.91	0.5909	1321.44	10.3123
v52	1330.61	11.2958	1327.45	0.7616
v53	1337.94	8.6617	1330.84	3.5531
v54	1340.30	45.318	1336.59	4.3799
v55	1361.62	0.7148	1352.69	12.6513
v56	1362.94	2.4903	1364.25	0.1106
v57	1380.80	18.5303	1380.07	2.1113
v58	1384.76	17.3225	1388.39	2.3199
v59	1418.79	149.2531	1522.50	7.6343
v60	1524.08	0.6195	1524.55	6.6636
v61	1527.75	5.1645	1528.69	1.1822
v62	1532.05	13.1338	1533.01	12.9986
v63	1540.92	4.9099	1546.57	25.6779
v64	1555.42	14.4521	1555.41	44.7476
v65	1911.37	2734.1216	1825.19	4518.8553
v66	2140.48	3502.3698	2036.45	1070.0888
v67	3074.57	19.5082	3075.66	23.9627
v68	3076.56	11.8509	3076.34	10.0893
v69	3076.96	15.0436	3079.87	32.1671
v70	3077.43	29.0116	3083.92	5.6226
v71	3083.61	10.5153	3087.74	25.2329
v72	3089.63	42.2216	3097.55	33.378
v73	3095.07	14.0073	3102.75	26.8312
v74	3121.74	20.4028	3104.33	9.4098
v75	3122.90	35.7665	3119.24	40.0308
v76	3129.19	9.5282	3134.71	27.8202
v77	3133.10	31.921	3140.78	3.3096

v78	3138.03	27.3972	3141.55	20.0422
v79	3140.95	19.5693	3150.23	34.15
v80	3146.87	55.5337	3160.18	36.2589
v81	3159.50	30.0649	3171.91	21.8838

Normal modes	TS3 JP-10/BO ₂		TS4 JP-10/BO ₂	
	Frequencies(cm ⁻¹)	IR Inten	Frequencies(cm ⁻¹)	IR Inten
v1	-598.46	2613.3736	-1193.49	7068.8658
v2	4.01	1.2498	48.67	1.9946
v3	52.96	0.7753	90.94	0.8584
v4	68.94	0.0217	115.25	0.747
v5	98.45	2.3663	139.35	0.7877
v6	138.10	0.0243	164.13	0.7787
v7	191.05	1.9696	185.94	0.1585
v8	262.25	0.2443	273.70	3.638
v9	318.14	0.0022	300.23	172.7633
v10	333.97	1.4222	319.31	0.2176
v11	404.89	21.3434	330.97	0.7069
v12	440.47	9.975	399.66	3.4039
v13	501.87	32.6751	485.01	13.8318
v14	532.02	0.3529	537.73	0.8758
v15	548.69	2.5257	544.70	21.217
v16	575.59	1.3343	552.79	7.5925
v17	666.40	1.223	635.46	46.8972
v18	741.35	0.9027	659.91	473.203
v19	761.59	237.1344	728.81	18.1062
v20	808.09	18.2843	756.08	6.6702
v21	839.88	44.9816	806.91	4.8924
v22	868.79	516.3801	842.27	4.4096
v23	874.08	3.849	867.92	22.8953
v24	894.98	292.656	895.29	19.1843
v25	911.52	0.7225	899.99	9.4882
v26	922.47	244.1108	911.88	7.8363
v27	939.62	0.4702	919.42	1.7442
v28	943.93	17.1511	935.15	0.8504
v29	969.72	106.8948	950.18	4.9465
v30	977.80	0.5366	976.79	6.5681
v31	998.52	19.2268	987.83	2.6951
v32	1006.33	3.1212	1022.56	16.6795
v33	1028.24	0.9917	1032.87	34.4613
v34	1034.68	0.7055	1053.47	8.1773
v35	1069.81	38.0198	1061.16	14.9356
v36	1073.48	39.6218	1077.34	4.5156
v37	1076.76	0.0539	1079.71	11.4647

v38	1095.77	1.7459	1101.72	3.2329
v39	1098.61	0.4759	1123.29	50.2939
v40	1156.66	1071.0841	1149.31	34.1829
v41	1167.01	0.1975	1152.27	49.2051
v42	1190.08	140.5386	1164.40	18.9625
v43	1215.72	0.0202	1180.30	117.3081
v44	1218.72	0.2615	1208.67	0.9236
v45	1226.88	17.4865	1223.32	80.2033
v46	1236.48	4.1513	1235.49	40.8791
v47	1252.44	3.9375	1245.58	3.2944
v48	1268.99	1.0826	1266.92	4.1175
v49	1287.02	3.6561	1273.24	0.9694
v50	1297.72	0.1574	1286.70	5.2659
v51	1315.10	0.7452	1296.67	3.1309
v52	1321.78	0.232	1324.29	6.942
v53	1328.57	0.1488	1327.09	0.1646
v54	1341.00	3.8714	1330.25	24.2915
v55	1349.92	12.3793	1341.93	7.7687
v56	1364.53	0.4329	1361.02	6.3394
v57	1365.83	1.4309	1364.33	3.0567
v58	1386.79	11.971	1367.29	2.3826
v59	1388.18	0.3474	1373.41	1.4958
v60	1524.53	3.061	1493.64	11.5595
v61	1528.44	2.3005	1523.01	2.1074
v62	1531.70	4.1626	1533.06	10.9166
v63	1546.28	7.5393	1534.29	6.7091
v64	1547.85	5.4064	1542.65	11.9074
v65	1823.62	3726.754	1559.52	6.443
v66	2018.89	269.7729	1905.65	1013.4951
v67	3076.18	33.1783	3049.70	5.2
v68	3077.78	2.8305	3064.83	4.0082
v69	3086.06	19.9062	3081.29	16.3308
v70	3088.72	38.6451	3093.70	30.8617
v71	3089.28	14.6822	3096.15	18.9003
v72	3092.56	14.9971	3096.82	14.478
v73	3095.39	63.465	3107.40	31.0499
v74	3120.46	5.2163	3133.35	29.2331
v75	3128.69	48.4081	3141.79	7.0105
v76	3133.17	7.6666	3145.98	25.0211
v77	3136.48	19.7368	3152.97	23.9547

v78	3138.49	1.4014	3156.77	6.2124
v79	3144.82	17.7647	3159.07	3.3032
v80	3153.08	37.8228	3163.25	16.746
v81	3157.07	48.3825	3177.76	11.0528

Normal modes	TS5 JP-10/BO ₂		TS6 JP-10/BO ₂	
	Frequencies(cm ⁻¹)	IR Inten	Frequencies(cm ⁻¹)	IR Inten
v1	-466.92	929.7386	-2114.01	15943.5411
v2	19.95	0.6479	49.41	2.393
v3	46.34	0.2416	67.38	0.7971
v4	63.44	1.1027	103.87	1.9112
v5	74.32	0.3607	126.60	0.6714
v6	122.41	1.1518	187.41	3.6182
v7	216.83	4.7075	224.29	5.8467
v8	249.79	0.1696	254.75	2.3392
v9	261.40	4.7222	295.66	5.8954
v10	313.76	3.0366	326.42	0.2172
v11	403.29	0.9551	346.57	66.6118
v12	467.26	12.0459	409.52	0.8072
v13	493.44	9.2232	491.85	0.5514
v14	497.09	37.1421	504.68	0.4628
v15	513.69	44.7684	535.81	40.2445
v16	624.93	14.0362	595.37	181.2974
v17	721.62	15.6516	704.92	8.2044
v18	753.43	0.3004	718.20	5.2556
v19	776.82	48.0554	737.11	5.4287
v20	807.97	8.2922	774.38	0.2441
v21	819.91	4.0948	813.94	0.2624
v22	844.43	9.2077	824.50	2.9318
v23	855.77	1.4974	846.51	7.974
v24	899.47	26.7708	863.85	4.9861
v25	917.51	0.6384	907.94	1.1967
v26	930.68	6.9754	919.39	2.0103
v27	936.92	10.236	923.40	41.4041
v28	955.77	1.3781	949.93	0.5785
v29	972.01	3.5037	955.90	0.4046
v30	984.02	3.3598	969.27	4.2155
v31	988.22	6.8578	988.25	0.712
v32	1010.27	3.4649	1004.89	16.9006
v33	1018.26	3.8354	1014.58	6.7097
v34	1049.86	4.482	1041.68	28.0866
v35	1065.13	12.9456	1064.74	14.1209
v36	1086.77	46.0536	1067.76	2.2345
v37	1092.25	3.6014	1077.21	15.2452

v38	1113.28	0.4101	1093.46	0.5111
v39	1129.17	0.0504	1110.57	0.5047
v40	1151.28	3.4359	1142.35	2.6469
v41	1167.08	11.2787	1160.31	5.5145
v42	1210.45	71.951	1172.27	1.7413
v43	1214.47	6.6378	1214.85	72.7411
v44	1222.64	4.2143	1226.67	1.4417
v45	1235.15	10.3687	1237.70	27.8998
v46	1254.51	6.5392	1242.96	21.7862
v47	1268.28	9.0582	1263.57	75.269
v48	1292.10	3.7722	1272.92	10.7697
v49	1304.70	3.6122	1288.36	13.7352
v50	1307.50	4.0491	1298.52	6.0486
v51	1327.15	5.1019	1310.19	4.3417
v52	1329.40	1.893	1318.80	6.2081
v53	1332.43	3.2515	1326.92	0.3671
v54	1342.46	0.433	1328.90	12.801
v55	1344.37	40.3078	1338.98	4.0004
v56	1370.03	2.8216	1344.10	1.8739
v57	1388.54	1.3038	1354.01	7.6422
v58	1392.49	0.4309	1373.36	6.7937
v59	1431.96	9.1013	1384.39	1.7097
v60	1521.26	3.6064	1394.83	0.2975
v61	1526.71	2.3065	1486.53	31.3514
v62	1530.14	18.4365	1497.01	6.8118
v63	1546.71	25.325	1527.36	2.483
v64	1561.55	6.8702	1541.14	12.1193
v65	1915.76	1683.2422	1562.60	2.9288
v66	2137.98	2740.6255	1919.70	569.444
v67	3079.67	22.4465	3037.01	10.1661
v68	3082.56	13.7615	3055.15	14.1249
v69	3088.61	14.0221	3083.31	19.8876
v70	3091.15	12.3689	3090.15	8.6556
v71	3091.88	50.7095	3092.71	46.1508
v72	3098.07	22.485	3101.47	18.6811
v73	3107.30	10.7894	3103.45	25.9844
v74	3112.57	5.9518	3110.69	6.4079
v75	3115.72	91.5297	3117.06	34.1603
v76	3121.11	9.4178	3118.53	9.7158
v77	3130.84	13.6385	3133.85	1.5096

v78	3134.53	0.1945	3140.59	5.2697
v79	3150.78	18.928	3150.09	16.3727
v80	3153.49	65.1627	3152.94	41.8261
v81	3176.90	19.9361	3187.62	14.0649

Normal modes	vdW2 Site 1 JP-10/BO ₂		vdW2 Site 2 JP-10/BO ₂	
	Frequencies(cm ⁻¹)	IR Inten	Frequencies(cm ⁻¹)	IR Inten
v1	20.50	2.3706	7.74	1.0856
v2	26.79	1.4865	21.55	1.2096
v3	62.53	0.2913	53.37	0.9811
v4	64.30	1.848	63.36	4.1443
v5	128.71	4.3932	133.04	6.1822
v6	160.09	2.8505	139.54	5.0262
v7	188.05	2.2894	178.87	0.1801
v8	293.91	2.442	263.65	0.3976
v9	326.48	3.6955	317.11	0.5325
v10	332.29	0.8125	331.72	0.057
v11	399.24	0.3028	401.57	0.0604
v12	489.66	27.9685	478.59	76.4358
v13	492.79	17.8878	486.27	29.2379
v14	510.17	81.2635	499.09	27.3207
v15	521.43	3.2436	516.56	17.3574
v16	552.90	7.4453	521.08	3.9195
v17	568.22	41.6398	557.16	0.6097
v18	668.56	1.2331	660.84	1.6425
v19	686.36	72.7748	725.87	0.2849
v20	758.95	3.5682	765.21	0.3382
v21	782.39	1.8365	800.88	1.0136
v22	816.86	1.7802	839.57	1.3396
v23	880.12	0.2213	859.24	3.5759
v24	882.01	4.6889	879.23	0.7243
v25	914.76	0.6505	900.44	0.4342
v26	922.32	0.9635	914.27	0.844
v27	930.86	1.3691	936.33	0.2399
v28	940.96	0.9506	942.21	2.325
v29	955.25	0.204	961.23	2.0639
v30	961.71	0.2359	976.14	1.5785
v31	982.71	4.6985	997.50	0.4824
v32	1010.26	0.4433	1022.91	1.1234
v33	1023.27	22.8335	1024.86	17.4262
v34	1026.41	1.8728	1028.12	2.5941
v35	1035.60	0.7364	1063.30	0.0504
v36	1053.98	7.1745	1072.48	0.7405
v37	1065.03	1.1539	1077.92	89.1786

v38	1073.72	46.435	1082.68	43.1928
v39	1079.25	32.7842	1108.96	0.4846
v40	1102.99	8.6332	1126.93	0.9603
v41	1150.04	3.0302	1159.16	2.782
v42	1167.80	0.3431	1183.56	1.4677
v43	1174.16	0.8513	1214.21	1.5716
v44	1203.29	0.9288	1216.39	0.2982
v45	1217.16	0.2388	1226.96	6.0983
v46	1231.05	0.5322	1237.46	2.1883
v47	1254.60	2.3723	1252.87	3.3616
v48	1276.54	2.3164	1276.41	0.4685
v49	1289.57	1.1751	1285.81	2.2081
v50	1295.90	2.8415	1303.58	3.4981
v51	1306.83	0.9057	1317.26	2.1279
v52	1319.05	0.5421	1322.18	0.7077
v53	1333.27	1.5956	1328.52	2.0981
v54	1343.28	1.3732	1335.78	2.845
v55	1348.99	3.9895	1350.10	1.8164
v56	1359.27	0.8176	1365.56	0.4439
v57	1363.48	0.6481	1376.46	0.614
v58	1377.43	2.302	1390.03	1.0674
v59	1386.00	0.8747	1520.56	2.7043
v60	1509.03	7.8306	1523.12	0.5812
v61	1526.34	4.0125	1530.70	6.2592
v62	1528.38	4.3549	1532.85	11.1794
v63	1539.14	6.8561	1545.65	10.5044
v64	1557.19	14.2639	1557.28	9.2041
v65	2062.07	333.1714	2058.76	298.2644
v66	3038.20	22.1868	3076.74	19.9313
v67	3076.77	22.2034	3080.17	15.7278
v68	3078.35	31.7121	3082.27	27.1933
v69	3079.32	8.7818	3086.06	2.1487
v70	3081.21	12.287	3089.17	23.6542
v71	3095.36	25.6074	3099.05	30.7729
v72	3103.91	1.9017	3104.84	25.9469
v73	3104.99	32.0258	3107.52	14.7123
v74	3123.06	29.5525	3117.94	36.7172
v75	3127.57	14.5785	3135.80	25.4349
v76	3134.54	29.6036	3144.92	20.277
v77	3140.37	25.0509	3145.65	8.1374

v78	3149.16	48.6414	3155.61	22.7291
v79	3168.35	19.783	3165.14	32.2116
v80	3198.84	18.0309	3179.00	18.6567
v81	3522.17	939.8796	3487.35	928.0309

Normal modes	vdW2 Site 3 JP-10/BO ₂		vdW1 Site 4 JP-10/BO ₂	
	Frequencies(cm ⁻¹)	IR Inten	Frequencies(cm ⁻¹)	IR Inten
v1	12.1168	0.4315	30.41	1.5073
v2	49.6797	0.8641	50.56	1.8945
v3	59.289	3.3385	57.17	2.5573
v4	74.7655	0.0328	71.76	1.765
v5	115.244	6.587	123.52	1.0062
v6	125.2828	0.9894	138.89	5.76
v7	193.7937	0.4441	183.79	3.0695
v8	245.3831	0.0104	254.86	0.6036
v9	316.1639	0.4274	306.34	1.5376
v10	318.4052	0.1103	319.89	0.1568
v11	394.2835	2.2733	394.26	0.0361
v12	452.3282	90.2324	487.21	35.5508
v13	475.5891	53.4671	488.91	0.5968
v14	509.461	20.6341	517.11	48.165
v15	515.8287	10.5285	536.71	4.4233
v16	532.8848	2.6377	554.82	1.4027
v17	549.0566	1.4981	568.75	67.2147
v18	666.957	0.018	645.24	5.3149
v19	738.6039	1.5339	731.20	0.269
v20	774.1267	3.7796	755.27	0.8696
v21	807.1504	0.2074	810.93	2.494
v22	818.7799	11.9918	840.70	2.9125
v23	863.1253	10.1696	866.17	0.2896
v24	872.8306	0.6075	897.06	2.4924
v25	884.5734	4.8868	901.86	1.0059
v26	903.9749	0.1917	914.08	0.8858
v27	927.178	0.0358	920.15	0.5292
v28	943.5852	1.8465	934.00	0.2371
v29	949.1392	0.3332	947.42	1.7036
v30	968.4874	1.1937	979.67	3.9548
v31	975.6283	3.9225	985.07	2.2087
v32	1020.213	0.7266	1022.38	0.7131
v33	1022.797	43.8685	1024.36	18.0678
v34	1023.24	4.7183	1036.56	5.9431
v35	1041.697	3.4352	1059.58	1.0741
v36	1057.218	96.7339	1071.99	0.8556
v37	1067.001	0.0597	1077.99	5.1316

v38	1072.108	0.3235	1090.98	86.7918
v39	1080.11	0.6462	1111.27	4.8182
v40	1096.973	2.8208	1146.54	3.4955
v41	1167.701	0.9671	1150.35	1.3787
v42	1183.156	2.1185	1174.46	0.5519
v43	1208.8	0.5052	1182.47	0.5706
v44	1219.588	0.272	1206.35	3.9115
v45	1222.979	0.8852	1230.86	1.2784
v46	1225.47	1.5527	1247.09	1.634
v47	1247.918	1.7171	1253.90	0.3748
v48	1262.791	0.3915	1269.55	0.0308
v49	1278.604	2.777	1278.52	1.7188
v50	1287.105	0.0081	1291.87	1.7618
v51	1312.581	0.0028	1321.94	0.3022
v52	1323.327	0.1132	1324.12	0.2453
v53	1325.89	0.7342	1330.97	3.2922
v54	1340.032	0.0947	1339.16	4.3833
v55	1345.056	2.8246	1358.49	1.342
v56	1363.668	1.2661	1359.77	0.2758
v57	1364.432	0.2928	1369.01	0.9709
v58	1377.423	2.2829	1378.52	1.6303
v59	1380.473	0.257	1505.73	8.6751
v60	1523.474	3.4713	1522.26	1.3351
v61	1526.141	4.0334	1532.79	9.5566
v62	1528.758	13.771	1533.50	4.8621
v63	1543.467	0.3833	1542.63	14.3953
v64	1545.071	7.3029	1560.09	5.3042
v65	2063.051	298.9734	2055.32	286.2429
v66	3076.225	20.5125	3031.28	18.697
v67	3080.695	16.185	3051.85	6.3082
v68	3081.82	3.4178	3079.16	11.0008
v69	3084.158	30.9515	3084.77	15.927
v70	3085.221	26.6547	3086.51	34.6799
v71	3093.467	25.3843	3089.71	15.7452
v72	3096.666	52.8194	3099.12	39.4447
v73	3134.469	29.2062	3101.38	21.065
v74	3136.564	1.628	3126.07	39.1885
v75	3137.628	34.2155	3134.91	21.1375
v76	3139.047	12.1862	3142.66	29.1259
v77	3139.851	29.0367	3143.32	3.5653

v78	3156.055	27.1853	3149.33	7.008
v79	3156.724	37.5725	3154.18	36.9329
v80	3173.306	20.87	3161.13	33.0417
v81	3605.203	840.4576	3412.31	856.9246

Normal modes	vdW2 Site 5 JP-10/BO ₂		vdW2 Site 6 JP-10/BO ₂	
	Frequencies(cm ⁻¹)	IR Inten	Frequencies(cm ⁻¹)	IR Inten
v1	27.40	1.0546	28.35	1.5453
v2	45.09	0.8708	44.57	1.2241
v3	51.58	0.3489	53.95	5.8144
v4	68.84	6.7314	83.08	0.5329
v5	104.21	0.4027	93.65	1.6806
v6	141.22	5.7408	125.31	3.9177
v7	175.29	5.2943	198.11	5.7278
v8	248.17	0.1633	250.89	0.0104
v9	280.97	0.9841	269.57	0.0978
v10	334.43	0.664	328.17	0.0892
v11	401.33	1.3043	403.75	0.4322
v12	481.18	38.6487	472.27	44.1407
v13	492.57	6.6547	480.19	41.5306
v14	511.08	44.4692	504.25	42.1724
v15	515.39	40.1264	509.13	58.6732
v16	535.40	38.3458	520.77	3.9243
v17	587.15	24.1459	610.44	30.3889
v18	707.74	2.0404	723.29	0.4437
v19	740.38	0.3705	743.27	1.1704
v20	756.58	0.5993	773.29	1.9214
v21	791.40	2.1718	779.92	2.2165
v22	816.46	0.9598	814.68	0.9549
v23	827.09	0.7141	827.11	0.8195
v24	853.10	2.9196	850.26	1.0435
v25	887.54	2.5107	910.39	1.7039
v26	919.45	0.4369	916.91	0.7932
v27	931.50	0.5963	931.60	1.0522
v28	939.22	0.5357	949.38	0.0796
v29	955.82	1.6401	952.20	0.3439
v30	970.15	1.3644	957.11	4.1573
v31	986.01	0.1588	987.77	1.8083
v32	1003.77	2.4258	994.51	1.5029
v33	1020.24	2.1783	1021.22	22.9115
v34	1024.51	22.0734	1024.19	4.8425
v35	1044.35	2.0014	1056.33	4.3807
v36	1064.89	33.3195	1061.03	114.0015
v37	1070.34	5.2737	1064.37	4.0765

v38	1072.74	112.2041	1070.35	0.4138
v39	1093.20	3.1353	1092.70	0.2109
v40	1111.23	0.3612	1109.47	4.1366
v41	1139.29	0.3054	1137.56	1.1965
v42	1160.23	1.3404	1159.94	0.3378
v43	1170.52	0.6394	1169.90	2.3742
v44	1201.97	0.4935	1207.56	1.2055
v45	1226.17	5.3337	1223.43	0.6613
v46	1238.61	1.2298	1234.44	2.2658
v47	1258.91	0.2411	1259.01	0.0785
v48	1271.52	0.4298	1269.42	0.4317
v49	1292.68	1.5302	1283.06	0.202
v50	1306.45	2.3412	1294.68	1.2759
v51	1312.32	0.0613	1312.92	0.1761
v52	1321.21	1.2255	1317.21	0.3763
v53	1327.63	1.4725	1324.82	0.6806
v54	1333.27	3.5467	1336.00	5.2306
v55	1341.83	0.198	1343.52	0.756
v56	1349.67	4.734	1359.04	0.4358
v57	1368.32	1.5112	1371.34	7.1499
v58	1378.60	4.2658	1383.80	0.2417
v59	1395.34	0.8608	1395.15	0.3342
v60	1512.88	5.3279	1500.17	14.6164
v61	1525.86	2.5165	1507.88	4.3073
v62	1534.19	12.6938	1526.49	2.1516
v63	1544.59	19.7558	1531.17	11.711
v64	1555.69	4.245	1554.94	4.4804
v65	2058.66	255.2814	2059.75	256.1781
v66	3031.52	18.0839	3013.63	20.0173
v67	3050.84	14.8272	3031.21	22.9476
v68	3082.62	13.2513	3075.95	7.9398
v69	3083.13	21.2073	3082.11	19.4837
v70	3089.98	26.7757	3088.17	13.9358
v71	3092.47	38.6218	3091.43	39.7169
v72	3094.24	25.6923	3092.49	11.9807
v73	3109.09	7.6225	3097.52	19.2275
v74	3119.67	66.9521	3105.04	48.7384
v75	3124.75	7.7386	3116.28	45.7013
v76	3133.92	0.4968	3130.74	7.5596
v77	3149.71	9.632	3132.44	2.2648

v78	3152.82	46.7784	3151.44	47.2067
v79	3155.65	29.5014	3170.02	33.8499
v80	3192.13	15.9397	3179.16	22.0342
v81	3541.12	712.0001	3609.41	589.4182

Table S7: B3LYP/cc-pVTZ cartesian coordinates and vibrational frequencies of van-der-Waals complexes (vdW), transition states (TS), and products of the reactions of atomic and molecular oxygen with JP-10; the vdW R2-O₂H, vdW R4-O₂H, and tsR4-O₂H are obtained at the MP2/cc-pVDZ level.

Atom	X	Y	Z	Atom	X	Y	Z
JP-10							
C	0.221599	-0.586778	0.787828				
C	0.221599	-0.586778	-0.787828				
C	0.221599	0.917698	1.132164				
C	0.221599	0.917698	-1.132164				
C	-0.640430	1.510860	0.000000				
C	1.610944	1.491910	0.780878				
C	1.610944	1.491910	-0.780878				
C	-1.025973	-1.391810	1.205692				
C	-1.025973	-1.391810	-1.205692				
C	-1.332464	-2.291529	0.000000				
H	1.116767	-1.067916	1.185227				
H	1.116767	-1.067916	-1.185227				
H	-0.101929	1.137231	2.149267				
H	-0.101929	1.137231	-2.149267				
H	-1.670972	1.157614	0.000000				
H	-0.652613	2.601951	0.000000				
H	2.418876	0.892255	1.201430				
H	1.721563	2.504095	1.171744				
H	1.721563	2.504095	-1.171744				
H	2.418876	0.892255	-1.201430				
H	-1.869551	-0.719955	1.384894				
H	-0.867295	-1.953863	2.126671				
H	-0.867295	-1.953863	-2.126671				
H	-1.869551	-0.719955	-1.384894				
H	-0.660917	-3.154606	0.000000				
H	-2.353016	-2.676881	0				

R1				R2			
C	0.356808	0.791831	-0.530988	C	-0.367857	-0.853431	-0.460482
C	0.306839	-0.781831	-0.511081	C	-0.341184	0.739732	-0.549712
C	-0.909247	1.179987	0.296881	C	0.873855	-1.094842	0.366479
C	-0.950367	-1.087387	0.336458	C	0.915189	1.110978	0.277478
C	-0.928521	0.060642	1.365959	C	0.898150	0.026865	1.392021
C	-2.099939	0.789000	-0.524269	C	2.140895	-0.885474	-0.434481
C	-2.198711	-0.711808	-0.499849	C	2.174627	0.690305	-0.520471
C	1.723928	1.179859	0.070428	C	-1.735623	-1.205494	0.158285
C	1.657420	-1.233391	0.082264	C	-1.699702	1.204189	0.010152
C	2.609570	-0.053165	-0.161268	C	-2.633182	-0.002263	-0.164079
H	0.277473	1.180997	-1.545990	H	-0.276890	-1.304312	-1.448923
H	0.194274	-1.187244	-1.517718	H	-0.231081	1.070387	-1.583457
H	-0.975840	-2.097827	0.742262	H	0.931206	2.149093	0.610262
H	-0.050345	0.054299	2.010286	H	0.023426	0.075124	2.037162
H	-1.820111	0.091397	1.992398	H	1.795616	0.039603	2.010162
H	-2.609640	1.433385	-1.225666	H	2.103959	-1.357978	-1.415330
H	-3.117591	-1.057909	-0.008343	H	3.021517	-1.262225	0.086782
H	-2.192756	-1.167349	-1.495715	H	3.078576	1.085558	-0.056182
H	1.630318	1.369333	1.142746	H	2.148392	1.049337	-1.549613
H	2.130629	2.086527	-0.378501	H	-1.643581	-1.320204	1.240408
H	2.014041	-2.164103	-0.360161	H	-2.128945	-2.145937	-0.227922
H	1.560276	-1.409704	1.156724	H	-2.066351	2.100800	-0.491105
H	2.961562	-0.067230	-1.196427	H	-1.609675	1.447883	1.071824
H	3.492062	-0.074574	0.479762	H	-2.975105	-0.060414	-1.201185
H	-0.901028	2.207591	0.657136	H	-3.522067	0.049889	0.465979

R3				R4			
C	0.357220	0.789040	-0.493336	C	0.386982	0.745511	-0.346332
C	0.357220	-0.789040	-0.493336	C	0.373830	-0.771908	-0.459568
C	-0.884615	1.136071	0.364225	C	-0.882722	1.142475	0.353113
C	-0.884615	-1.136071	0.364225	C	-0.932601	-1.131885	0.291198
C	-0.889656	0.000000	1.351703	C	-1.004469	-0.029734	1.370591
C	-2.149542	0.781904	-0.472582	C	-2.081289	0.833922	-0.582121
C	-2.149542	-0.781904	-0.472582	C	-2.113919	-0.726898	-0.619452
C	1.718837	1.202758	0.098313	C	1.771233	1.247046	-0.055594
C	1.718837	-1.202758	0.098313	C	1.734374	-1.182593	0.141857
C	2.637239	0.000000	-0.155561	C	2.661917	-0.006477	-0.217693
H	0.250809	1.189074	-1.502976	H	0.323691	-1.125168	-1.496125
H	0.250809	-1.189074	-1.502976	H	-0.889255	2.147470	0.770822
H	-0.886695	2.148385	0.763180	H	-0.980092	-2.160334	0.646722
H	-0.886694	-2.148385	0.763181	H	-0.185759	-0.060090	2.089497
H	-1.356771	0.000000	2.326702	H	-1.949387	-0.027044	1.917823
H	-2.101546	1.204921	-1.477358	H	-1.947358	1.275129	-1.568627
H	-3.048160	1.172421	0.004885	H	-3.004351	1.236430	-0.162412
H	-3.048160	-1.172421	0.004885	H	-3.055338	-1.107766	-0.221885
H	-2.101546	-1.204922	-1.477358	H	-2.004011	-1.123002	-1.629252
H	1.620652	1.362626	1.175268	H	1.831302	1.635067	0.971050
H	2.097249	2.129779	-0.334168	H	2.086103	2.070038	-0.704088
H	2.097249	-2.129779	-0.334168	H	2.095703	-2.139750	-0.236205
H	1.620652	-1.362626	1.175268	H	1.653818	-1.271026	1.228535
H	2.976297	0.000000	-1.195430	H	2.982869	-0.097348	-1.257985
H	3.527560	0.000000	0.474775	H	3.562062	0.030623	0.396137

R5				R6			
C	0.354822	0.825549	-0.527558	C	0.378264	0.788215	-0.592492
C	0.398518	-0.747160	-0.568349	C	0.378264	-0.788214	-0.592493
C	-0.875036	1.119032	0.379462	C	-0.814966	1.129964	0.326439
C	-0.826934	-1.141531	0.283694	C	-0.814967	-1.129965	0.326436
C	-0.822960	-0.052455	1.375750	C	-0.746245	-0.000002	1.372604
C	-2.145412	0.778215	-0.425799	C	-2.120891	0.780262	-0.416516
C	-2.107161	-0.780851	-0.500026	C	-2.120892	-0.780260	-0.416518
C	1.692891	1.232101	-0.018594	C	1.763975	1.241534	-0.071369
C	1.768750	-1.159745	0.021685	C	1.763974	-1.241534	-0.071369
C	2.661012	0.099699	-0.024271	C	2.569660	0.000000	0.088275
H	0.171613	1.258958	-1.519951	H	0.211684	1.187054	-1.593210
H	0.298379	-1.124448	-1.586799	H	0.211685	-1.187052	-1.593212
H	-0.871702	2.120148	0.807533	H	-0.788334	2.148027	0.713501
H	-0.801317	-2.173347	0.633018	H	-0.788336	-2.148030	0.713494
H	0.073615	-0.050865	1.994937	H	0.174143	-0.000004	1.956924
H	-1.696761	-0.099638	2.027529	H	-1.592580	-0.000003	2.061282
H	-2.144533	1.246699	-1.410624	H	-2.143788	1.201565	-1.422132
H	-3.038112	1.123638	0.096950	H	-2.986955	1.172048	0.118245
H	-2.986862	-1.216972	-0.025396	H	-2.986957	-1.172046	0.118240
H	-2.075452	-1.151923	-1.525102	H	-2.143788	-1.201559	-1.422136
H	1.979056	2.263338	0.140529	H	1.664983	1.785478	0.880045
H	2.207755	-1.998306	-0.519133	H	2.237746	1.955603	-0.755016
H	1.647388	-1.481567	1.057547	H	2.237744	-1.955605	-0.755014
H	3.265714	0.106438	-0.945315	H	1.664980	-1.785477	0.880046
H	3.380277	0.140731	0.798313	H	3.610716	0.000001	0.380962

vdW R1-OH				vdW R2-OH			
C	-0.772810	-0.657213	-0.692403	C	0.273851	0.423926	-0.757221
C	-1.019410	0.859983	-0.354834	C	1.043481	-0.895272	-0.292165
C	0.648642	-0.912862	-0.094862	C	-1.056529	0.195484	-0.076934
C	0.272106	1.270509	0.388679	C	-0.001553	-1.614043	0.598023
C	0.621563	-0.015376	1.164488	C	-0.725898	-0.417084	1.275696
C	1.608738	-0.148799	-0.958924	C	-1.887978	-0.861903	-0.771596
C	1.424137	1.315865	-0.645727	C	-1.130254	-2.166033	-0.308156
C	-1.936338	-1.432605	-0.039277	C	1.149336	1.600354	-0.280725
C	-2.324308	0.896014	0.466896	C	2.321732	-0.395011	0.407607
C	-3.062600	-0.396545	0.089088	C	2.561466	1.010267	-0.161615
H	-0.770848	-0.833952	-1.768052	H	0.160592	0.453004	-1.840705
H	-1.141337	1.452805	-1.262561	H	1.304806	-1.513630	-1.151724
H	0.175723	2.178962	0.980969	H	-2.010427	1.915653	0.153441
H	-0.135557	-0.307968	1.889868	H	0.428925	-2.357868	1.268121
H	1.586704	0.033014	1.667746	H	-0.078905	0.189382	1.905051
H	1.974006	-0.514306	-1.910731	H	-1.601854	-0.718344	1.848857
H	2.324605	1.761112	-0.205062	H	-1.900634	-0.744536	-1.854034
H	1.185059	1.915315	-1.529002	H	-2.919725	-0.867514	-0.420465
H	-1.648901	-1.788689	0.952964	H	-1.796232	-2.820077	0.254608
H	-2.226343	-2.308201	-0.620409	H	-0.739735	-2.736708	-1.150619
H	-2.912037	1.793057	0.270530	H	0.811268	1.957100	0.694086
H	-2.100411	0.891002	1.536662	H	1.096323	2.449626	-0.961174
H	-3.562805	-0.270976	-0.874963	H	3.165061	-1.067970	0.248903
H	-3.825960	-0.682015	0.813950	H	2.164100	-0.331839	1.487216
H	0.878226	-1.967343	0.049546	H	3.019226	0.937044	-1.151907
O	4.250659	-0.681646	0.513332	H	3.225736	1.614584	0.456925
H	3.436283	-0.572466	-0.036847	O	-2.451806	2.794748	0.301992

vdW R3-OH				vdW R4-OH			
C	-0.923025	0.789747	0.528084	C	0.389887	0.318598	0.458269
C	-0.923016	-0.789583	0.528334	C	0.286425	-0.491632	-0.832623
C	0.529605	1.137831	0.088002	C	-0.920893	0.153746	1.181134
C	0.529620	-1.137790	0.088369	C	-1.108701	-1.146934	-0.678421
C	0.808682	-0.000132	-0.860509	C	-1.209594	-1.340425	0.850235
C	1.472666	0.781470	1.264380	C	-2.043210	0.847851	0.365997
C	1.472676	-0.781033	1.264633	C	-2.168784	-0.046656	-0.907322
C	-2.048635	1.204540	-0.439484	C	1.757830	0.164010	1.067663
C	-2.048623	-1.204694	-0.439103	C	1.547684	-1.381273	-0.798337
C	-2.999478	-0.000086	-0.469911	C	2.581000	-0.530378	-0.037756
H	-1.118872	1.191483	1.523482	H	0.576047	2.230282	-0.216202
H	-1.118863	-1.191005	1.523858	H	0.315381	0.129843	-1.734202
H	0.645418	2.149171	-0.295539	H	-0.902743	0.420444	2.235852
H	0.645451	-2.149253	-0.294843	H	-1.253925	-2.036979	-1.288689
H	0.592296	-0.000306	-1.921180	H	-0.467066	-2.024374	1.260772
H	2.858315	-0.000202	-1.287534	H	-2.199305	-1.662413	1.178729
H	1.119327	1.203949	2.205086	H	-1.799293	1.882150	0.130641
H	2.475971	1.165849	1.084947	H	-2.971938	0.850405	0.937375
H	2.475987	-1.165457	1.085328	H	-3.165499	-0.482119	-0.982652
H	1.119338	-1.203209	2.205475	H	-1.987609	0.509647	-1.827049
H	-1.643359	1.374232	-1.440607	H	1.695920	-0.469823	1.962842
H	-2.539061	2.128795	-0.133213	H	2.203529	1.105846	1.397959
H	-2.539040	-2.128855	-0.132535	H	1.885102	-1.671384	-1.793491
H	-1.643348	-1.374702	-1.440172	H	1.343749	-2.300287	-0.242827
H	-3.630759	0.000053	0.422829	H	3.003794	0.222381	-0.706647
H	-3.663345	-0.000226	-1.335189	H	3.410329	-1.116740	0.357268
O	3.842715	-0.000242	-1.385870	O	0.705457	3.141460	-0.585339

vdW R5-OH				vdW R6-OH			
C	0.000263	-0.204620	1.048616	C	0.124857	0.241986	0.782553
C	0.302265	-1.241672	-0.095180	C	0.124164	0.207567	-0.793329
C	0.777390	1.062675	0.586286	C	-1.319409	-0.172185	1.135305
C	1.247730	-0.454323	-1.026855	C	-1.320431	-0.220775	-1.126335
C	0.665407	0.970953	-0.946793	C	-1.641121	-1.193511	0.026150
C	2.280484	0.786618	0.795788	C	-2.261901	0.990436	0.760073
C	2.601843	-0.270060	-0.308035	C	-2.262410	0.957058	-0.800475
C	-1.487970	-0.130462	1.122979	C	1.234000	-0.731744	1.246385
C	-1.068034	-1.618958	-0.705775	C	1.231868	-0.786562	-1.215284
C	-2.125839	-1.237982	0.349812	C	2.023799	-1.051580	0.021402
H	0.399903	-0.526444	2.018616	H	0.340317	1.242605	1.155671
H	0.795906	-2.132248	0.295655	H	0.340169	1.190797	-1.209865
H	0.425644	1.984819	1.046306	H	-1.436564	-0.520699	2.160880
H	1.333422	-0.882952	-2.024630	H	-1.438952	-0.612978	-2.135847
H	-0.354296	1.056434	-1.319637	H	-1.003992	-2.078218	0.044829
H	1.281311	1.710695	-1.460041	H	-2.681619	-1.521099	0.033641
H	2.496291	0.425204	1.801685	H	-1.914496	1.943054	1.160709
H	2.861166	1.697399	0.646862	H	-3.263385	0.818250	1.155670
H	3.358204	0.103647	-0.998701	H	-3.264214	0.768616	-1.187756
H	2.975811	-1.207679	0.104701	H	-1.914988	1.891621	-1.241580
H	-2.337894	1.488424	-0.044277	H	0.796973	-1.649635	1.668517
H	-2.000446	0.394610	1.921212	H	1.845496	-0.312482	2.050522
H	-1.117171	-2.672898	-0.978152	H	1.842209	-0.403957	-2.038469
H	-1.244034	-1.046793	-1.617973	H	0.793328	-1.722141	-1.595189
H	-2.328828	-2.090347	1.016819	H	3.227865	0.678377	-0.013078
H	-3.091907	-0.972347	-0.087232	H	2.888687	-1.703653	0.035098
O	-2.826790	2.087183	-0.655784	O	3.655333	1.568425	-0.032803

tsR1-OH				tsR2-OH			
C	-0.684089	-0.703386	-0.616337	C	0.331526	0.442619	-0.731374
C	-0.958984	0.834603	-0.427124	C	0.872733	-0.993399	-0.322555
C	0.674291	-0.904512	0.109609	C	-1.023046	0.440877	-0.032312
C	0.280553	1.312267	0.359347	C	-0.264922	-1.559740	0.560298
C	0.576788	0.104798	1.271023	C	-0.773575	-0.290671	1.288043
C	1.734756	-0.241588	-0.760640	C	-2.012059	-0.469710	-0.754693
C	1.494421	1.269002	-0.598647	C	-1.474870	-1.887625	-0.346104
C	-1.895102	-1.429452	0.006931	C	1.393846	1.444216	-0.237735
C	-2.316600	0.928363	0.298526	C	2.224745	-0.738143	0.372356
C	-3.027030	-0.392582	-0.030110	C	2.689769	0.625422	-0.157438
H	-0.600127	-0.969084	-1.670830	H	0.207601	0.528806	-1.810748
H	-1.022134	1.347562	-1.388008	H	1.019965	-1.618808	-1.203989
H	0.150530	2.271937	0.857315	H	-1.500812	1.649109	0.129038
H	-0.221593	-0.118071	1.976706	H	0.044059	-2.385892	1.199869
H	1.512602	0.198809	1.821171	H	-0.030397	0.180877	1.926989
H	1.841097	-0.620935	-1.775786	H	-1.681139	-0.461384	1.865917
H	2.360352	1.761845	-0.151373	H	-2.010655	-0.310434	-1.832023
H	1.301723	1.763272	-1.552241	H	-3.028525	-0.314460	-0.395047
H	-1.682270	-1.703861	1.043006	H	-2.233549	-2.443653	0.204633
H	-2.141573	-2.350190	-0.522147	H	-1.189748	-2.487236	-1.210515
H	-2.888188	1.805521	-0.005688	H	1.129629	1.822417	0.751804
H	-2.166822	1.005358	1.378408	H	1.473880	2.311013	-0.892756
H	-3.454741	-0.344888	-1.035195	H	2.941383	-1.537303	0.180200
H	-3.841741	-0.624597	0.656857	H	2.090974	-0.684718	1.455776
H	0.885155	-1.939751	0.371519	H	3.119969	0.509260	-1.155936
O	3.981481	-0.705651	0.322641	H	3.450856	1.090995	0.469530
H	2.841851	-0.502800	-0.260298	O	-1.948547	2.758541	0.310792

tsR3-OH				tsR4-OH			
C	-0.840475	-0.791620	-0.551145	C	0.380817	0.519905	0.332603
C	-0.840477	0.786740	-0.558175	C	0.316396	-0.508174	-0.834191
C	0.600522	-1.138254	-0.091165	C	-0.909509	0.298551	1.120995
C	0.600598	1.137423	-0.101506	C	-1.007210	-1.250104	-0.538720
C	0.860385	0.004029	0.884249	C	-1.045494	-1.241107	1.003570
C	1.568017	-0.786425	-1.243172	C	-2.110092	0.766186	0.267261
C	1.567986	0.775023	-1.250327	C	-2.175973	-0.298297	-0.872695
C	-1.988422	-1.204466	0.391344	C	1.737820	0.364724	1.016465
C	-1.988310	1.207901	0.380781	C	1.631061	-1.308695	-0.723658
C	-2.938282	0.001820	0.398753	C	2.609889	-0.350500	-0.026606
H	-1.016333	-1.195830	-1.549058	H	0.374165	1.651203	-0.148962
H	-1.016508	1.182059	-1.559615	H	0.270959	-0.015255	-1.807238
H	0.709887	-2.148360	0.298416	H	-0.891416	0.707425	2.129539
H	0.710095	2.151020	0.278864	H	-1.079329	-2.225971	-1.017053
H	0.339117	0.008374	1.838602	H	-0.228535	-1.790385	1.470248
H	2.102962	0.005699	1.259828	H	-1.987619	-1.608299	1.413025
H	1.236889	-1.213201	-2.189825	H	-1.968109	1.777240	-0.108544
H	2.566394	-1.169047	-1.036929	H	-3.021613	0.756987	0.865152
H	2.566369	1.159566	-1.047724	H	-3.125518	-0.834018	-0.854735
H	1.236741	1.193078	-2.200825	H	-2.071622	0.144304	-1.863363
H	-1.608991	-1.378390	1.401592	H	1.625411	-0.258723	1.909963
H	-2.473732	-2.126995	0.072181	H	2.153234	1.317226	1.345959
H	-2.473539	2.127677	0.053650	H	1.989039	-1.650862	-1.694636
H	-1.608765	1.390528	1.389444	H	1.480552	-2.196940	-0.104588
H	-3.551738	-0.002116	-0.506276	H	2.992968	0.377922	-0.744801
H	-3.619416	0.005579	1.250385	H	3.468281	-0.859308	0.412444
O	3.286415	0.007166	1.586185	O	0.431614	2.844065	-0.709070

tsR5-OH				tsR6-OH			
C	-0.141546	-0.013232	0.995418	C	0.116043	0.787808	-0.261506
C	0.110400	-1.220595	0.017834	C	0.116052	-0.787840	-0.261303
C	0.820266	1.076382	0.460971	C	-1.305058	1.131923	0.232088
C	1.197700	-0.671969	-0.929761	C	-1.305032	-1.131855	0.232404
C	0.799108	0.811585	-1.057003	C	-1.581426	0.000170	1.241958
C	2.258747	0.646981	0.818970	C	-2.302098	0.780538	-0.892590
C	2.518070	-0.560736	-0.136779	C	-2.302082	-0.780822	-0.892377
C	-1.639728	0.255379	0.932400	C	1.278020	1.215526	0.659048
C	-1.258769	-1.537743	-0.620749	C	1.278005	-1.215318	0.659368
C	-2.298006	-0.990719	0.369509	C	2.180872	0.000111	0.749377
H	0.118175	-0.258148	2.029336	H	0.283494	1.182594	-1.263143
H	0.475648	-2.095413	0.558098	H	0.283495	-1.182884	-1.262839
H	0.561564	2.084798	0.777465	H	-1.406126	2.149369	0.608513
H	1.288076	-1.228403	-1.861829	H	-1.406063	-2.149199	0.609114
H	-0.174039	0.972983	-1.520611	H	-0.908732	0.000293	2.099800
H	1.536367	1.406518	-1.597882	H	-2.607029	0.000209	1.613708
H	2.359449	0.380782	1.871624	H	-1.999926	1.201117	-1.851968
H	2.959455	1.458787	0.622319	H	-3.294196	1.171739	-0.665025
H	3.354525	-0.357193	-0.805912	H	-3.294172	-1.171984	-0.664713
H	2.750446	-1.480491	0.401158	H	-1.999890	-1.201657	-1.851637
H	-1.846134	1.160738	0.102932	H	0.911778	1.456412	1.664230
H	-2.088391	0.686968	1.826443	H	1.795915	2.105412	0.299605
H	-1.386261	-2.602028	-0.817567	H	1.795892	-2.105317	0.300197
H	-1.363171	-1.019348	-1.575788	H	0.911727	-1.455897	1.664612
H	-2.459976	-1.705134	1.185774	H	2.867379	-0.000034	-0.288136
H	-3.271696	-0.797377	-0.081143	H	2.941121	0.000206	1.529326
O	-2.126435	2.077495	-0.777411	O	3.510695	-0.000229	-1.417556

vdW R1-O ₂ H				vdW R2-O ₂ H			
C	-0.507452	-0.708164	0.321538	C	-0.043276	0.434461	-0.505791
C	-1.057497	0.138299	-0.886946	C	1.524169	0.152366	-0.527007
C	0.173582	0.370962	1.215553	C	-0.506924	-0.764630	0.301938
C	-0.661835	1.585133	-0.513900	C	1.663893	-1.151591	0.298297
C	-0.793229	1.572269	1.022573	C	0.556036	-0.970806	1.375816
C	1.377584	0.877793	0.470581	C	-0.471955	-2.047167	-0.513372
C	0.870275	1.730960	-0.669368	C	1.080190	-2.322193	-0.534678
C	-1.730262	-1.427786	0.925665	C	-0.199768	1.829624	0.135655
C	-2.570047	-0.160204	-0.949303	C	2.167090	1.415425	0.085417
C	-2.735631	-1.507922	-0.232117	C	1.135881	2.526741	-0.166945
H	0.220882	-1.449330	-0.006086	H	-0.480677	0.423418	-1.517080
H	-0.585253	-0.156492	-1.825026	H	1.883981	0.001416	-1.560441
H	-1.231453	2.349139	-1.040204	H	-2.229504	-0.219789	0.652761
H	-1.802794	1.374668	1.379937	H	2.685201	-1.332722	0.673759
H	-0.432158	2.487665	1.491678	H	0.716442	-0.105221	2.036456
H	1.183543	2.773638	-0.543350	H	0.399384	-1.877273	1.983914
H	1.231311	1.419018	-1.654161	H	-0.902078	-1.914620	-1.518351
H	-2.156406	-0.841845	1.743635	H	-1.009560	-2.867527	-0.009296
H	-1.471917	-2.404634	1.334577	H	1.310815	-3.291663	-0.061602
H	-2.947036	-0.174414	-1.972125	H	1.487342	-2.339907	-1.559497
H	-3.131009	0.610980	-0.414892	H	-0.327955	1.736766	1.229960
H	-2.460977	-2.324037	-0.905559	H	-1.080513	2.363245	-0.254820
H	-3.757526	-1.693638	0.100446	H	3.158655	1.629448	-0.347699
H	0.362450	0.048288	2.236959	H	2.304465	1.282051	1.174682
H	2.348749	1.022533	0.930683	H	1.165233	2.827377	-1.230920
O	4.182935	-0.957603	0.035916	H	1.306740	3.430271	0.442432
O	3.071306	-1.208722	-0.634159	O	-3.318509	0.545029	-0.609785
H	2.402742	-0.538975	-0.296214	O	-3.158989	0.160140	0.631006

vdW R3-O ₂ H				vdW R4-O ₂ H			
C	0.708905	1.027648	0.788596	C	0.369232	-0.123234	0.648194
C	0.708905	1.027648	-0.788596	C	0.301841	-0.427834	-0.857101
C	-0.757361	0.684935	1.138550	C	-0.959654	-0.540218	1.238432
C	-0.757361	0.684935	-1.138550	C	-1.094994	-1.081618	-0.975105
C	-1.155265	-0.223373	0.000000	C	-1.229387	-1.811717	0.381154
C	-1.632611	1.923427	0.782384	C	-2.062176	0.407999	0.701205
C	-1.632611	1.923427	-0.782384	C	-2.141727	0.047145	-0.817046
C	1.772024	-0.008460	1.204902	C	1.723133	-0.527584	1.195050
C	1.772024	-0.008460	-1.204902	C	1.557369	-1.296980	-1.089974
C	2.718018	-0.101909	0.000000	C	2.571450	-0.731165	-0.077649
H	0.972233	2.008243	1.186685	H	0.498062	1.717812	0.565156
H	0.972233	2.008243	-1.186685	H	0.362109	0.484020	-1.480358
H	-0.909171	0.313321	2.149423	H	-0.959989	-0.674011	2.331619
H	-0.909171	0.313321	-2.149423	H	-1.228696	-1.698523	-1.878723
H	-0.472640	-1.906370	0.000000	H	-0.480515	-2.607002	0.536819
H	-2.076459	-0.801631	0.000000	H	-2.238133	-2.228924	0.551291
H	-1.218187	2.838379	1.207084	H	-1.818786	1.467810	0.875398
H	-2.642910	1.807588	1.173362	H	-3.017105	0.195412	1.211288
H	-2.642910	1.807588	-1.173362	H	-3.148602	-0.316270	-1.083522
H	-1.218187	2.838379	-1.207084	H	-1.909935	0.909624	-1.462874
H	1.307147	-0.981881	1.381246	H	1.619847	-1.483835	1.749693
H	2.282055	0.269309	2.127640	H	2.154326	0.203070	1.902806
H	2.282055	0.269309	-2.127640	H	1.913667	-1.259419	-2.132774
H	1.307147	-0.981881	-1.381246	H	1.339097	-2.353033	-0.843752
H	3.407688	0.746600	0.000000	H	2.938792	0.248464	-0.434674
H	3.321456	-1.009919	0.000000	H	3.446225	-1.382881	0.082533
O	-0.296075	-2.909153	0.000000	O	0.583738	2.713608	0.455240
O	-1.482722	-3.480537	0.000000	O	0.206151	2.947507	-0.776852

vdW R5-O ₂ H				vdW R6-O ₂ H			
C	-0.265931	0.180784	0.982522	C	0.102029	-0.542138	0.411286
C	-1.104927	1.184990	0.109529	C	0.309471	0.487352	-0.764462
C	-0.605528	-1.201198	0.351366	C	1.526335	-0.698270	0.984972
C	-1.848639	0.248632	-0.866123	C	1.824216	0.777248	-0.703880
C	-0.792096	-0.841466	-1.134071	C	2.101805	0.721369	0.811617
C	-2.051133	-1.553800	0.757963	C	2.372120	-1.494315	-0.030818
C	-2.907630	-0.545005	-0.070830	C	2.576737	-0.476575	-1.196570
C	1.143234	0.669213	0.896101	C	-0.942047	0.080163	1.366855
C	-0.081942	2.146112	-0.540054	C	-0.613965	1.691076	-0.465058
C	1.197109	2.045147	0.314343	C	-1.533070	1.233419	0.621867
H	-0.581883	0.174348	2.032879	H	-0.271224	-1.496908	0.042797
H	-1.811179	1.748516	0.720262	H	0.041044	0.051692	-1.726666
H	0.122962	-1.977952	0.576416	H	1.548669	-1.108368	1.993950
H	-2.246458	0.758553	-1.742618	H	2.115175	1.694612	-1.214595
H	0.112215	-0.471340	-1.616298	H	1.573160	1.483617	1.384812
H	-1.177244	-1.672883	-1.725466	H	3.163174	0.786270	1.054876
H	-2.210510	-1.460203	1.832432	H	1.871088	-2.407670	-0.352092
H	-2.284330	-2.583008	0.484166	H	3.327550	-1.785382	0.406700
H	-3.585004	-1.068983	-0.745522	H	3.634691	-0.257926	-1.344552
H	-3.516565	0.104993	0.558277	H	2.185410	-0.840624	-2.146876
H	2.224761	-0.404771	-0.295186	H	-0.467650	0.437393	2.293436
H	1.921138	0.290967	1.552895	H	-1.693545	-0.647111	1.684819
H	-0.460019	3.166229	-0.599357	H	-1.143453	2.044186	-1.354197
H	0.136016	1.830361	-1.561869	H	-0.029113	2.556024	-0.117443
H	1.175848	2.787626	1.126884	H	-2.869887	0.305674	-0.283227
H	2.111928	2.251365	-0.246447	H	-2.252550	1.903429	1.080916
O	2.925179	-0.932384	-0.781539	O	-3.576674	-0.240775	-0.758740
O	3.821474	-1.251899	0.137049	O	-3.557618	-1.433585	-0.193449

tsR1-O ₂ H				tsR2-O ₂ H			
C	-0.495616	-0.721972	0.281931	C	-0.033601	-0.457722	-0.577851
C	-1.050496	0.182051	-0.881492	C	-1.548604	0.018249	-0.475686
C	0.235132	0.300902	1.197450	C	0.642594	0.658162	0.201858
C	-0.600814	1.601054	-0.468777	C	-1.460242	1.314773	0.367472
C	-0.695605	1.539558	1.069280	C	-0.306707	0.979534	1.354403
C	1.448394	0.807421	0.454666	C	0.700697	1.950431	-0.601831
C	0.930320	1.705855	-0.656832	C	-0.799653	2.416804	-0.499795
C	-1.723725	-1.428222	0.890681	C	-0.004059	-1.871197	0.040796
C	-2.572515	-0.068935	-0.914223	C	-2.297082	-1.164603	0.176234
C	-2.759882	-1.436883	-0.242466	C	-1.435565	-2.391804	-0.161264
H	0.202670	-1.470198	-0.090442	H	0.323843	-0.484011	-1.620163
H	-0.611268	-0.093384	-1.841171	H	-1.964904	0.230724	-1.476594
H	-1.157865	2.400414	-0.954728	H	2.022283	0.132363	0.537187
H	-1.701305	1.360388	1.446882	H	-2.418865	1.615394	0.822939
H	-0.294474	2.426675	1.559906	H	-0.522603	0.129512	2.019525
H	1.278851	2.733233	-0.512092	H	0.009483	1.848655	1.955191
H	1.257647	1.404729	-1.655742	H	1.032916	1.780371	-1.637938
H	-2.112476	-0.861387	1.740257	H	1.376052	2.687946	-0.136952
H	-1.484230	-2.426528	1.257053	H	-0.869122	3.399300	-0.003097
H	-2.975917	-0.033778	-1.926419	H	-1.279181	2.502891	-1.489214
H	-3.095946	0.697841	-0.337034	H	0.219144	-1.810994	1.121941
H	-2.526383	-2.234983	-0.952031	H	0.772581	-2.502171	-0.418744
H	-3.778102	-1.605474	0.109862	H	-3.337505	-1.245873	-0.180873
H	0.432815	-0.062976	2.203247	H	-2.334183	-1.032296	1.273629
H	2.362047	1.060083	0.986568	H	-1.583734	-2.670667	-1.221273
O	4.059961	-1.049384	-0.037079	H	-1.671622	-3.275911	0.454796
O	2.895433	-1.171758	-0.614016	O	3.190166	-0.931244	-0.495426
H	2.269621	-0.410494	-0.206676	O	2.994677	-0.321381	0.627129

tsR3-O ₂ H				tsR4-O ₂ H			
C	0.752162	0.978413	0.788471	C	0.359874	-0.027627	0.619729
C	0.752162	0.978413	-0.788471	C	0.276664	-0.440477	-0.864324
C	-0.728701	0.708246	1.138575	C	-0.983137	-0.379265	1.236379
C	-0.728701	0.708246	-1.138575	C	-1.135100	-1.066756	-0.933677
C	-1.175437	-0.179715	0.000000	C	-1.277344	-1.700476	0.469204
C	-1.542086	1.987998	0.782436	C	-2.070070	0.548782	0.639713
C	-1.542086	1.987998	-0.782436	C	-2.157655	0.091258	-0.851442
C	1.765533	-0.106447	1.205086	C	1.683493	-0.508327	1.195575
C	1.765533	-0.106447	-1.205086	C	1.503649	-1.359690	-1.052092
C	2.706073	-0.243658	0.000000	C	2.532966	-0.790663	-0.058381
H	1.062252	1.945438	1.186081	H	0.509983	1.428784	0.552775
H	1.062252	1.945438	-1.186081	H	0.356776	0.432550	-1.538805
H	-0.898791	0.344851	2.149556	H	-0.981402	-0.437824	2.336372
H	-0.898791	0.344851	-2.149556	H	-1.284100	-1.741095	-1.792896
H	-0.586732	-1.793564	0.000000	H	-0.542904	-2.497568	0.675314
H	-2.143664	-0.677107	0.000000	H	-2.292465	-2.085995	0.672740
H	-1.083026	2.881350	1.207158	H	-1.810286	1.613437	0.745078
H	-2.556847	1.922115	1.173472	H	-3.026981	0.382705	1.162871
H	-2.556847	1.922115	-1.173472	H	-3.172024	-0.267051	-1.095553
H	-1.083026	2.881350	-1.207158	H	-1.907020	0.904108	-1.552443
H	1.256571	-1.057251	1.381720	H	1.509585	-1.445931	1.762807
H	2.288164	0.147996	2.127507	H	2.144757	0.210202	1.895891
H	2.288164	0.147996	-2.127507	H	1.864052	-1.375858	-2.093939
H	1.256571	-1.057251	-1.381720	H	1.248627	-2.397373	-0.766030
H	3.434435	0.571888	0.000000	H	2.936337	0.161136	-0.449986
H	3.266444	-1.178833	0.000000	H	3.382523	-1.466718	0.133969
O	-0.422969	-2.817981	0.000000	O	0.652874	2.518676	0.429818
O	-1.608760	-3.378228	0.000000	O	0.430188	2.779065	-0.811350

tsR5-O ₂ H				tsR6-O ₂ H			
C	0.237001	-0.165886	0.984433	C	0.098941	-0.585726	0.358764
C	0.969975	-1.220224	0.075475	C	0.302567	0.527286	-0.738603
C	0.694150	1.192704	0.381485	C	1.517324	-0.754457	0.943354
C	1.783905	-0.333088	-0.889514	C	1.810240	0.841123	-0.633807
C	0.829756	0.856133	-1.115513	C	2.067074	0.684239	0.878301
C	2.171206	1.399905	0.775661	C	2.393694	-1.461265	-0.111810
C	2.921516	0.339256	-0.090720	C	2.594684	-0.360841	-1.200641
C	-1.220301	-0.527853	0.919366	C	-0.972117	-0.051434	1.336303
C	-0.146177	-2.070928	-0.571204	C	-0.649199	1.687262	-0.368551
C	-1.373116	-1.907047	0.343658	C	-1.599032	1.122391	0.646093
H	0.564294	-0.217023	2.029175	H	-0.248954	-1.519519	-0.081510
H	1.629372	-1.859500	0.664017	H	0.056310	0.155625	-1.733065
H	0.043711	2.027790	0.634382	H	1.533235	-1.233538	1.921596
H	2.121870	-0.855482	-1.783590	H	2.090380	1.797365	-1.074471
H	-0.109695	0.587432	-1.596200	H	1.515634	1.394393	1.495135
H	1.285362	1.664539	-1.688616	H	3.123389	0.751659	1.142014
H	2.334879	1.264121	1.845017	H	1.916054	-2.359422	-0.503783
H	2.494650	2.410236	0.524242	H	3.348359	-1.763750	0.319594
H	3.635131	0.817063	-0.762330	H	3.650078	-0.112489	-1.316459
H	3.476834	-0.379505	0.512726	H	2.224228	-0.664932	-2.179933
H	-2.002689	0.416096	-0.089305	H	-0.518659	0.275782	2.283325
H	-1.901004	-0.184747	1.695956	H	-1.702280	-0.818381	1.606907
H	0.147864	-3.113433	-0.689001	H	-1.153854	2.110896	-1.240409
H	-0.381410	-1.693227	-1.568028	H	-0.091699	2.522696	0.079180
H	-1.341793	-2.642375	1.160833	H	-2.741548	0.354887	-0.227435
H	-2.324931	-2.067218	-0.166864	H	-2.290318	1.771699	1.176007
O	-2.648219	1.022840	-0.702810	O	-3.472964	-0.185555	-0.778342
O	-3.711774	1.283086	0.002664	O	-3.538963	-1.383750	-0.262046

JP-10				
Normal modes	Frequency(cm ⁻¹)	IR Inten	Frequency(cm ⁻¹)	IR Inten
v1	132.37	0.0112		
v2	175.83	0.0024		
v3	264.43	0.0613		
v4	314.4	0.0388		
v5	316.61	0.0535		
v6	394.96	0.0293		
v7	489.18	0.2313		
v8	532.92	0.1785		
v9	554.31	0.6264		
v10	671.91	0.6036		
v11	738.15	0.2999		
v12	752.67	0.3414		
v13	791.27	1.3181		
v14	829.07	0.5855		
v15	864.53	1.0142		
v16	865.08	0.0232		
v17	887.77	0.5934		
v18	891.04	0.0758		
v19	912.58	0.8196		
v20	917.25	0.0674		
v21	923.99	0.9959		
v22	955.67	1.8485		
v23	961.26	0.0214		
v24	990.79	1.6513		
v25	998.36	0.5391		
v26	1042.02	0.2663		
v27	1048.92	0.4814		
v28	1052.57	0.0513		
v29	1053.46	0.025		
v30	1073.39	0.6124		
v31	1137.02	0.1158		
v32	1151.23	0.0064		
v33	1169.34	1.0532		
v34	1194.09	0.198		
v35	1203.91	0.0851		

v36	1207.67	1.4543
v37	1226.44	1.2542
v38	1253.48	0.0104
v39	1262.65	0.7486
v40	1292.21	1.2505
v41	1305.31	0.0002
v42	1307.75	0.2664
v43	1314.54	0.4983
v44	1320.92	0.0042
v45	1326.65	0.0641
v46	1333.18	1.0454
v47	1344.57	0.7653
v48	1352.54	0.9778
v49	1367.11	0.8201
v50	1371.99	0.4778
v51	1493.72	0.1473
v52	1495.36	2.3993
v53	1496.43	1.1264
v54	1502.51	6.5608
v55	1513.53	8.926
v56	1524.14	3.8204
v57	3016.21	16.8227
v58	3021.07	29.0278
v59	3024.72	24.1971
v60	3029.55	1.3904
v61	3034.93	24.4597
v62	3042.89	17.3718
v63	3044.74	82.9402
v64	3046.88	34.4594
v65	3063	5.8434
v66	3067.74	45.6645
v67	3070.4	31.8506
v68	3072.12	109.9999
v69	3076.4	45.4314
v70	3079.32	11.4533
v71	3085.88	99.6687
v72	3090.62	39.6989

Normal modes	R1		R2	
	Frequency(cm ⁻¹)	IR Inten	Frequency(cm ⁻¹)	IR Inten
v1	144.14	0.0916	137.73	0.0767
v2	172.45	0.1305	173.99	0.0496
v3	267.5	7.2001	266.86	0.2483
v4	298	2.165	313.65	0.2096
v5	315.87	0.3488	316.41	0.2939
v6	366.1	5.5818	394.46	0.0744
v7	435.92	13.0759	492.3	0.599
v8	491.93	0.4299	522.52	0.7427
v9	547.4	0.0591	552.08	0.618
v10	566.54	3.3887	664.62	1.1613
v11	671.19	0.5024	713.45	0.1548
v12	743.93	0.6185	749.37	0.269
v13	763.34	0.2909	769.77	0.6977
v14	791.79	1.5729	824.04	0.4542
v15	861.88	0.2907	834.7	3.756
v16	863.91	0.3945	853.7	0.4236
v17	886.39	0.5003	871.01	0.181
v18	900.77	1.2501	882.7	0.3417
v19	907.54	0.486	908.99	1.6557
v20	912.59	0.8491	915.2	0.2637
v21	932.46	0.1256	928.22	1.3881
v22	935.22	0.2481	947.59	1.3123
v23	955.54	2.0572	966.65	0.5089
v24	978.33	0.7943	991.39	0.7622
v25	994.17	1.0163	1002.8	1.6883
v26	1008.42	1.4141	1037.72	0.4684
v27	1032.36	0.0319	1048.55	0.1456
v28	1040.72	0.7618	1059.42	0.1583
v29	1049.02	0.026	1083.87	0.1635
v30	1069.1	0.6036	1093.98	0.1091
v31	1119.32	0.4389	1140.49	1.0979
v32	1142.62	0.2572	1163.29	0.1783
v33	1154.7	0.6472	1190.06	0.1626
v34	1184.65	0.7262	1196.93	0.6595

v35	1193.68	0.3631	1207.64	4.6767
v36	1207.11	0.1274	1217.27	1.3779
v37	1231.32	1.2258	1233.13	1.5708
v38	1251.86	0.8086	1255.58	0.9227
v39	1272.11	0.402	1262.96	0.6151
v40	1283.04	1.9516	1292	1.6531
v41	1302.23	0.1749	1301.77	0.6656
v42	1306.89	0.1404	1308.57	0.2938
v43	1319.51	0.3661	1315.41	0.7123
v44	1324.17	0.3823	1321.25	1.0947
v45	1336.03	1.3279	1335.26	0.4959
v46	1343.25	0.9062	1343.39	0.3136
v47	1345.69	0.5726	1358.6	0.4468
v48	1359.53	1.1246	1372.6	0.762
v49	1366.83	0.4175	1490.52	1.0101
v50	1473.74	3.8526	1492.99	0.0972
v51	1494.17	1.621	1496.24	2.5589
v52	1495.91	2.5165	1500.85	7.364
v53	1505.73	5.1738	1511.11	6.8655
v54	1518.41	7.6693	1522.39	5.5066
v55	2962.7	47.8864	3017.6	23.3304
v56	3005.25	27.6022	3024.99	27.5936
v57	3017.44	18.3495	3034.22	16.5652
v58	3023.01	31.5333	3036.72	13.5793
v59	3026.27	24.7536	3038.81	18.3207
v60	3036.08	8.3388	3047.68	47.047
v61	3051.88	48.6339	3052.82	49.4094
v62	3053.71	10.7873	3057.79	27.5609
v63	3067.94	38.65	3067.8	42.5488
v64	3072.11	42.4071	3071.04	33.7399
v65	3078.2	81.4318	3073.07	56.3947
v66	3079.83	96.0844	3074.57	13.1348
v67	3083.68	6.6638	3083.2	53.6511
v68	3096.52	33.3638	3094.52	74.4557
v69	3192.55	22.4166	3108.19	32.335

Normal modes	R3		R4	
	Frequency(cm ⁻¹)	IR Inten	Frequency(cm ⁻¹)	IR Inten
v1	112.75	0.0013	118.71	0.0982
v2	178.4	0.1225	156.58	0.1601
v3	251.42	0.037	234.82	0.4595
v4	300.12	1.3246	281.27	0.2846
v5	314.22	0.0548	314.04	0.0844
v6	333.29	8.0965	383.13	0.0241
v7	423.63	5.0365	482.08	0.6028
v8	532.05	0.5301	538.75	0.2116
v9	544.12	0.9831	560.16	1.0979
v10	665.9	13.1529	620.83	3.3064
v11	671.51	0.2193	719.6	0.077
v12	737.38	1.3347	737.1	0.2361
v13	762.63	0.6053	795.28	1.9847
v14	791.98	0.8512	825.7	0.7923
v15	831.42	1.563	843.08	0.17
v16	850.8	0.3443	872.27	0.7838
v17	867.47	0.0807	878.75	0.5798
v18	872.88	1.1343	886.89	0.3659
v19	909	0.0569	891.39	0.6118
v20	915.01	1.9186	903.4	0.2422
v21	921.14	0.0378	915.97	0.8334
v22	947.82	1.3689	954.23	0.079
v23	947.98	0.134	957.47	2.9678
v24	987.98	1.5697	987.35	1.1165
v25	990.03	0.0979	1014.5	0.2568
v26	992.66	0.997	1036.96	0.0286
v27	1036.21	0.1587	1043.09	1.0385
v28	1048.32	0.092	1058.67	0.1445
v29	1055.38	0.1271	1090.39	1.1632
v30	1072.28	0.6894	1122.98	0.4735
v31	1152.62	0.3515	1131.23	0.137
v32	1163.64	1.0785	1148.93	0.1773
v33	1187.04	0.9747	1165.15	0.6424
v34	1191.49	0.2726	1189.63	1.8604

v35	1203.2	0.3981	1205.61	1.3702
v36	1205.53	0.3846	1221.96	1.0038
v37	1237.15	1.1689	1230.18	0.3143
v38	1246.11	0.0073	1249.07	0.3255
v39	1260.48	1.5996	1252.11	0.5066
v40	1277.88	0.0043	1285.64	1.1026
v41	1301.24	0.0147	1303.8	0.6094
v42	1308.16	0.3664	1309.86	0.2144
v43	1316.38	0.007	1312.03	0.1984
v44	1328.09	0.1424	1324.56	1.122
v45	1332.26	0.4739	1337.28	0.5783
v46	1345.31	0.5263	1341.01	1.2093
v47	1346.75	0.3768	1350.3	0.0196
v48	1363.3	2.1732	1363.06	0.3218
v49	1366.74	0.4244	1474.48	3.1552
v50	1489.61	3.0274	1491.73	0.3539
v51	1492.68	0.6336	1493.77	1.4779
v52	1494.24	5.2637	1499.83	5.8859
v53	1508.07	0.7402	1507.59	7.0511
v54	1509.95	6.5107	1520.41	2.1935
v55	3014.87	20.9594	2955.29	36.2429
v56	3020.93	32.1861	2976.34	27.4842
v57	3024.68	22.8561	3011.5	21.9143
v58	3029.64	7.1275	3023.08	14.2887
v59	3033.54	28.0222	3033.31	52.8643
v60	3041.28	15.2047	3036.15	26.4074
v61	3046.42	88.4567	3036.66	41.546
v62	3065.25	0.0936	3047.21	64.4467
v63	3067.92	38.5508	3069.7	13.186
v64	3070.38	50.0545	3070.4	54.6294
v65	3077.91	61.4707	3079.35	61.0943
v66	3086.04	65.1896	3079.7	37.7455
v67	3090.49	74.4246	3084.8	44.56
v68	3093.56	14.3785	3090.44	22.6704
v69	3185.75	18.6547	3093.15	61.0325

Normal modes	R5		R6	
	Frequency(cm ⁻¹)	IR Inten	Frequency(cm ⁻¹)	IR Inten
v1	117.54	0.078	44.39	0.9717
v2	130.03	0.2488	105.48	0.001
v3	260.81	0.2589	256.3	0.017
v4	278.81	0.4121	257.55	0.7199
v5	314.66	0.4143	323.58	0
v6	393.11	0.5897	389.9	17.5186
v7	423.72	19.2794	395.34	6.8536
v8	497.02	1.0396	494.33	0.1102
v9	534	0.1252	527.9	0.0025
v10	627.67	0.5817	693.96	0.3037
v11	737.25	0.0973	718.94	0.4832
v12	749.56	1.4282	729.5	0.1642
v13	765.25	0.9295	764.56	0.0285
v14	795.78	0.7469	796.61	1.0192
v15	830.66	0.3578	829.04	0.7482
v16	845.15	0.4212	835.9	0.4135
v17	869.45	0.9338	887.43	0.4564
v18	886.7	0.658	889.07	0.812
v19	904.13	0.2894	908.77	0.7099
v20	921.91	0.0814	924.6	1.0064
v21	924.93	1.3023	936.59	0.4479
v22	947.98	1.3356	941.94	0.9111
v23	960.55	0.1525	962.31	0.0613
v24	977.33	1.585	964.3	1.2647
v25	1000.35	0.8711	1012.62	1.6014
v26	1018.04	0.38	1019.76	0.0168
v27	1046.88	0.4199	1043.6	0.5475
v28	1050.01	0.1124	1055.13	0.7413
v29	1063.81	0.3506	1059.14	0.3877
v30	1073.9	1.1094	1082.78	0.0481
v31	1118.89	0.0402	1127.43	0.478
v32	1141.4	0.2253	1139.44	0.6212
v33	1159.52	0.7048	1146.52	0.1233
v34	1183.37	0.2825	1174.32	0.6634

v35	1206.14	2.6552	1199.12	0.0617
v36	1217	0.8212	1210.9	1.252
v37	1229.67	0.5063	1230.86	1.4038
v38	1246.93	0.0596	1251.82	0.0033
v39	1278.47	0.3802	1267.67	0.0054
v40	1286.32	1.0909	1293.03	1.0358
v41	1295.15	0.122	1301.71	0.1589
v42	1299.97	0.3742	1305.94	0.1114
v43	1311.11	0.3983	1309.85	0.4764
v44	1319.79	0.968	1322.05	0.3622
v45	1322.92	1.3454	1328.56	2.0577
v46	1334.76	2.2571	1347.86	0.085
v47	1348.15	0.7248	1354.3	2.4838
v48	1361.49	1.0143	1364.48	0.0572
v49	1370.92	1.212	1377.57	1.3146
v50	1472.81	1.8999	1471.5	5.5625
v51	1494.92	1.0556	1474.42	1.8097
v52	1496.09	3.1172	1494.93	1.0178
v53	1507.38	10.2599	1503.57	8.3837
v54	1520.71	2.8065	1522.32	3.4532
v55	2915.82	48.3636	2932.28	37.7165
v56	2948.9	37.5495	2934.23	29.0825
v57	3022.4	28.5809	2983.45	37.9977
v58	3034.74	26.2904	2983.63	26.3922
v59	3040.46	24.6668	3034.46	20.1696
v60	3043.34	20.5903	3043.05	46.2238
v61	3044.25	74.3395	3044.88	17.4481
v62	3046.6	30.0892	3045.28	45.6163
v63	3062.85	4.5672	3060.42	53.313
v64	3074.43	62.3167	3063.07	9.496
v65	3077.52	56.994	3073.14	86.2422
v66	3083.26	25.8908	3079.75	4.2022
v67	3086.63	73.6727	3084.8	46.3141
v68	3090.17	31.1567	3086.94	69.297
v69	3173.89	24.6839	3179.57	31.2055

Normal modes	vdW R1-OH		vdW R2-OH	
	Frequency(cm ⁻¹)	IR Inten	Frequency(cm ⁻¹)	IR Inten
v1	34.67	2.2341	29.5	1.6018
v2	49.18	2.7602	33.41	1.9271
v3	110.54	0.3226	117.35	0.0673
v4	147.99	0.7535	136.44	0.0516
v5	178.8	0.5656	174.92	0.0433
v6	292.87	1.1954	265.13	0.3102
v7	314.18	0.9586	312.68	0.1121
v8	320.57	2.5221	315.88	0.1015
v9	388.71	0.4457	394.28	0.0995
v10	476.03	60.2942	489.65	3.2687
v11	489.42	36.4313	513.19	25.0076
v12	499.34	29.1939	537.77	40.8873
v13	542.39	35.179	549.79	29.0164
v14	552.08	4.7228	556	29.8317
v15	618.08	31.9418	662.57	1.2422
v16	671.79	0.5105	710.26	0.3886
v17	743.73	1.5346	749.83	0.2754
v18	766.09	0.3978	770.46	0.9756
v19	793.9	1.7245	825.14	0.7536
v20	861	1.6552	837.86	1.5367
v21	863.48	0.3244	855.16	0.5558
v22	887.56	0.591	870.69	0.3188
v23	901.62	1.2749	884.07	0.3658
v24	907.25	0.4466	909.19	1.7766
v25	912.21	0.4658	914.52	0.1815
v26	931.41	0.3592	930	1.448
v27	933.55	0.3333	949.06	0.7645
v28	954.94	3.9593	968.1	0.2518
v29	980.61	0.7543	991.2	0.7287
v30	998.21	1.6943	1003.84	1.7231
v31	1009.34	1.6054	1037.64	0.5651
v32	1032.76	0.0488	1048.3	0.1524
v33	1041.18	1.0015	1061.28	0.1915
v34	1049.8	0.0157	1084.85	0.2919
v35	1073.16	1.7395	1094.16	0.1141
v36	1126.29	0.8699	1142.1	1.8982

v37	1147.79	0.1996	1165.49	1.0857
v38	1156.86	0.777	1191.36	0.3022
v39	1185.42	0.5803	1198.09	0.9587
v40	1194.79	0.3792	1207.56	6.0398
v41	1207.92	0.2427	1219.36	1.4835
v42	1232.08	1.5779	1236.19	1.8953
v43	1253.23	1.0518	1256.96	0.9031
v44	1272.75	0.3841	1263.91	0.424
v45	1285.66	2.3056	1293.21	2.069
v46	1302.57	0.2267	1302.32	1.0444
v47	1308.45	0.4104	1310.44	0.3604
v48	1320.84	0.6729	1317.12	0.5485
v49	1325.59	0.6556	1323.45	0.9846
v50	1334.04	1.8021	1336.73	0.5393
v51	1343.37	0.7713	1344.22	0.314
v52	1346.71	0.4965	1359.45	0.632
v53	1360.97	1.2283	1374.18	0.3956
v54	1368.12	0.6324	1491.14	1.3246
v55	1469	5.1656	1493.64	0.23
v56	1495.34	1.9362	1495.39	2.7309
v57	1496.68	2.804	1501.61	7.6312
v58	1507.89	3.3919	1511.24	6.4151
v59	1522.33	9.5702	1523.31	6.9196
v60	2977.92	30.7494	3019.74	21.4966
v61	3019.46	19.1784	3027.02	27.6727
v62	3023.32	14.6018	3039.54	13.3643
v63	3025.67	31.3902	3041.82	7.3922
v64	3029.54	24.3785	3044.53	22.649
v65	3037.12	8.4382	3054.15	32.5557
v66	3052.33	37.4339	3058.96	42.6635
v67	3062.04	11.9571	3064.53	17.7147
v68	3071.04	38.6185	3072.64	30.0775
v69	3075.12	41.8223	3076.27	48.2444
v70	3082.76	75.6567	3077.27	48.0084
v71	3082.98	69.6326	3081.03	11.4474
v72	3087.83	10.1442	3089.09	47.5226
v73	3106.56	24.638	3101.57	57.0882
v74	3162.29	20.1079	3116.67	26.0955
v75	3386.25	299.2574	3243.95	297.4061

Normal modes	vdW R3-OH		vdW R4-OH	
	Frequency(cm ⁻¹)	IR Inten	Frequency(cm ⁻¹)	IR Inten
v1	31.96	1.9521	33.58	1.6595
v2	51.24	2.627	49.67	2.363
v3	102.34	0.1827	116.68	0.0735
v4	117.05	0.2951	124.83	0.1713
v5	184.08	0.7473	167.07	0.6637
v6	257.78	0.0129	249.65	1.196
v7	309.33	0.8064	284.58	0.3864
v8	314.58	0.1619	314.04	0.5603
v9	391.74	2.6605	385.75	0.0127
v10	426.24	9.925	484.43	0.7529
v11	452.62	54.6468	515.3	58.2087
v12	506.86	86.4264	531.36	29.4202
v13	531.47	0.2534	548.53	41.024
v14	553.1	2.0794	558.26	1.9571
v15	664.35	1.8755	636.23	5.0957
v16	717.92	12.7592	719.4	0.1844
v17	740.53	0.5144	738.18	0.5997
v18	766.2	12.6196	793.6	2.3261
v19	789.45	0.8442	827.39	1.0255
v20	840.48	2.5554	847.23	0.1073
v21	846.05	0.6727	872.92	0.8435
v22	867.19	0.5757	877.67	0.9114
v23	883.39	0.9571	887.11	0.5044
v24	893.08	0.804	893.91	0.4327
v25	914.53	0.0446	903.92	0.08
v26	914.65	2.2032	916.92	0.8357
v27	943.14	1.4322	955.09	0.9419
v28	980.9	0.4579	958.24	2.4491
v29	982.74	1.4369	988.9	1.1862
v30	985.12	0.0233	1014.62	0.4707
v31	1010.62	0.9248	1038.58	0.0252
v32	1035.86	0.4501	1045.09	1.2739
v33	1045.36	0.1284	1059.48	0.0296
v34	1056.27	0.1295	1087.59	1.1826
v35	1072.79	0.7356	1122.81	0.2192

v36	1151.31	1.0893	1134.46	0.2442
v37	1171.35	1.8807	1154.85	0.6179
v38	1180.95	0.6504	1163.01	1.027
v39	1192.01	0.4109	1187.1	2.6156
v40	1201.91	0.3459	1205.6	1.6855
v41	1217.08	0.2159	1223.6	1.4885
v42	1234.72	0.1017	1231.16	0.2773
v43	1253.37	2.2294	1250.68	0.2709
v44	1260.49	0.9991	1254.25	1.1011
v45	1275.92	0.1441	1286.71	1.1869
v46	1301.5	0.0205	1303.46	0.2171
v47	1305.51	0.4978	1310.4	0.2546
v48	1317.15	0.1382	1313.08	0.0976
v49	1327.21	0.241	1326.43	1.3336
v50	1334.73	0.5237	1340.01	0.6236
v51	1344.52	0.6845	1341.49	0.5137
v52	1344.88	0.4008	1350.04	0.4063
v53	1360.96	0.2253	1358.03	0.3873
v54	1365.76	2.5	1470.22	6.5338
v55	1475.63	0.0938	1492.38	0.8626
v56	1493.92	2.8922	1497.97	1.7781
v57	1496.33	5.1057	1501.44	5.4227
v58	1510.91	2.7605	1508.57	8.0771
v59	1514.85	7.0096	1522.89	2.4138
v60	3017.49	13.9449	2964.96	26.208
v61	3020.97	28.8017	2987.99	17.0751
v62	3026.64	31.4963	3024.59	21.394
v63	3032.42	0.0662	3027.62	3.4462
v64	3043.82	31.5081	3040.08	40.4197
v65	3045.44	22.3587	3041.84	27.6185
v66	3054.7	64.9224	3042.55	35.6
v67	3071.91	38.2749	3052.44	51.1791
v68	3074.3	30.9074	3075.86	3.4809
v69	3075.53	15.3445	3077.12	58.084
v70	3081.37	60.0786	3083.84	59.7234
v71	3095.09	62.2718	3085.3	25.8482
v72	3095.56	18.4366	3089.08	39.1889
v73	3099.19	33.1865	3094.7	24.5872
v74	3169.4	13.605	3100.58	36.8133
v75	3372.37	275.5598	3324.28	281.8576

Normal modes	vdW R5-OH		vdW R6-OH	
	Frequency(cm ⁻¹)	IR Inten	Frequency(cm ⁻¹)	IR Inten
v1	31.84	1.7789	29.17	2.2935
v2	48.34	1.8513	31.16	2.3311
v3	95.14	0.2494	98.34	0.2037
v4	132.81	0.2407	119.72	0.1593
v5	159.09	2.5202	172.36	5.4222
v6	264.03	0.2642	258	0.2089
v7	296.12	1.736	274.79	1.2496
v8	315.19	1.4068	320.35	1.0875
v9	394.75	1.1806	393.65	4.338
v10	431.82	85.1826	441.63	56.5173
v11	438.28	59.2958	452.62	47.1751
v12	495.22	11.1572	489.47	10.2232
v13	533.15	6.5314	533.41	0.0637
v14	541.69	21.7777	534.42	62.0755
v15	636.4	3.8224	691.22	1.6782
v16	737.16	0.2874	691.5	1.3417
v17	746.34	0.96	731.46	0.2608
v18	775.61	2.856	775.96	0.4837
v19	797.64	0.4546	796.32	0.6349
v20	829.98	0.3954	828.32	0.7722
v21	848.68	0.3419	844.53	0.6844
v22	869.84	1.7206	886.48	0.5198
v23	887.03	0.6403	888.23	0.4033
v24	903.65	0.2831	912.2	0.6834
v25	920.65	0.4237	923.44	1.1716
v26	924.38	1.4443	927.01	0.7851
v27	947.71	1.0358	950.21	1.2157
v28	960.99	0.1207	961.99	0.0178
v29	980.49	1.177	965.07	1.1607
v30	998.75	1.0993	1007.23	3.8437
v31	1016.82	1.0084	1023.74	0.0027
v32	1046	0.1423	1043.88	0.6649
v33	1050.24	0.1047	1052.74	0.5806
v34	1060.42	0.8123	1058.12	0.3018
v35	1071.54	1.821	1068.42	0.4481

v36	1122.22	0.203	1129.98	0.7868
v37	1143.88	0.4023	1145.37	0.0085
v38	1161.3	0.5363	1150.8	1.0968
v39	1184.8	1.1546	1182.97	0.4464
v40	1204.93	2.8879	1196.81	0.1123
v41	1217.82	0.4363	1211.93	1.3274
v42	1227.86	0.3336	1232.95	1.6353
v43	1247.74	0.1595	1249.9	0.1381
v44	1277.56	0.8224	1263.47	0.5344
v45	1288.37	1.4109	1292.83	0.8666
v46	1295.44	1.4265	1307.18	0.0641
v47	1300.99	0.3541	1307.58	0.1685
v48	1313.69	0.6619	1307.69	0.1179
v49	1318.98	1.3908	1322.19	0.7117
v50	1323.81	0.1712	1326.87	2.7391
v51	1335.53	2.5229	1343.71	0.0073
v52	1348.64	1.7499	1353.14	3.22
v53	1362.39	0.5999	1366.28	0.0893
v54	1368.95	0.9293	1373.46	0.6594
v55	1468.43	5.5208	1463.06	5.0912
v56	1495.16	1.2143	1471.13	2.7258
v57	1498.47	2.1661	1495.65	1.0964
v58	1508.6	12.202	1504.23	9.7094
v59	1523.49	2.7833	1523.12	3.7739
v60	2929.3	32.48	2932.18	16.6271
v61	2963.89	28.3246	2934.89	27.634
v62	3029.3	16.1912	3018.03	28.1619
v63	3037.41	24.8631	3019.06	16.7718
v64	3045.16	21.156	3037.45	19.9857
v65	3045.5	6.9261	3044.5	39.0211
v66	3047.78	94.6336	3047.81	49.3061
v67	3050.2	12.5271	3053.62	16.5938
v68	3065.7	4.1386	3066.9	15.2941
v69	3078.25	69.9068	3069.02	33.317
v70	3082.63	24.9538	3074.01	80.3611
v71	3085.14	18.7127	3081.54	2.2359
v72	3088.8	80.0611	3084.64	33.2568
v73	3093.58	32.2448	3089.31	81.8036
v74	3149.72	21.6937	3160.63	27.4172
v75	3456.42	189.3358	3411.42	236.6912

Normal modes	tsR1-OH		tsR2-OH	
	Frequency(cm ⁻¹)	IR Inten	Frequency(cm ⁻¹)	IR Inten
v1	-932.5	891.971	-1274.16	562.6168
v2	70.7	2.332	72.87	2.411
v3	78.81	2.6707	84.1	1.767
v4	146.04	0.7486	144.95	0.2605
v5	178.37	0.6195	175.14	0.0211
v6	269.32	4.9218	268.37	0.2518
v7	306.58	1.2243	309.06	0.5869
v8	322.16	0.7114	316.56	0.1363
v9	375.06	1.143	377.68	2.2338
v10	493.41	0.3357	398.88	0.6269
v11	539.95	3.519	490.43	0.1806
v12	558.36	1.3247	530.84	1.2352
v13	631.8	82.1758	553.38	0.9572
v14	681.26	24.3216	666.82	0.9409
v15	746.63	11.746	722.66	1.147
v16	757.58	2.9913	753.34	1.8528
v17	794.22	1.5093	790.7	3.2541
v18	842.54	8.9397	827.47	1.5875
v19	864.64	0.2246	858.99	0.138
v20	868.74	1.5064	867.8	1.2016
v21	889.83	1.0304	878.87	0.6124
v22	898.86	4.2587	894.99	2.4254
v23	911.81	0.0576	910.18	2.2615
v24	913.79	1.3419	915.62	0.2206
v25	926.56	0.9301	936.8	3.4974
v26	953.35	7.569	954.16	0.6611
v27	956.2	1.4766	971.33	11.1644
v28	987.35	2.9066	991.28	4.8185
v29	1006.42	4.7284	995.74	8.0401
v30	1032.25	2.7951	1004.28	7.3196
v31	1035.93	2.4614	1039.9	0.4124
v32	1041.62	1.4192	1048.14	3.5134
v33	1051.29	0.006	1050.55	2.079
v34	1079.33	0.6731	1062.7	0.2715
v35	1136.12	6.1294	1091.93	2.416
v36	1137.11	3.347	1118.88	3.3018

v37	1154.01	0.5803	1148.21	3.9525
v38	1174.46	6.7857	1178.95	7.1977
v39	1192.74	1.1719	1193.09	0.5238
v40	1196.21	1.2977	1201.14	0.6267
v41	1213.99	0.6269	1212.24	4.8875
v42	1225.96	4.2398	1230.02	3.2782
v43	1249.36	8.5277	1251.3	3.0854
v44	1261.03	2.0505	1260.76	0.5367
v45	1288.42	1.2536	1271.8	1.2113
v46	1291.83	1.2551	1298.9	1.9059
v47	1304.31	0.3851	1306.61	3.5262
v48	1312.48	0.2264	1314.11	0.6568
v49	1320.93	0.3974	1320.16	0.2144
v50	1325.16	1.3528	1326.91	1.7673
v51	1328.86	1.7959	1338.23	1.36
v52	1343.12	0.747	1344.08	0.456
v53	1349.14	0.5234	1360.65	1.1517
v54	1363.19	1.814	1371.09	0.2161
v55	1370.15	0.4695	1493.23	0.6478
v56	1482.32	6.0591	1493.93	1.1189
v57	1495.35	2.1346	1496.47	2.0157
v58	1496.83	2.726	1502.15	7.1454
v59	1507.49	3.9428	1512.43	7.269
v60	1521.1	9.8328	1524.61	6.2709
v61	3019.55	21.3664	3019.65	21.5207
v62	3025.86	28.2259	3026.81	28.3738
v63	3029.44	19.9982	3038.97	12.1392
v64	3030.67	26.5356	3041.02	5.8513
v65	3034.45	3.069	3045.17	29.4561
v66	3048.11	34.6066	3056.6	5.0664
v67	3062.45	12.6764	3059.38	67.8769
v68	3062.97	14.7917	3065.19	14.1679
v69	3071.6	43.053	3072.89	29.6595
v70	3075.27	42.8529	3077.22	25.7547
v71	3082.4	66.29	3077.87	54.9347
v72	3083.28	55.2831	3080.85	27.1755
v73	3087.05	43.0799	3089.7	46.8997
v74	3094.29	17.7348	3102.22	53.1647
v75	3106.81	24.8145	3115.32	26.9397

Normal modes	tsR3-OH		tsR4-OH	
	Frequency(cm ⁻¹)	IR Inten	Frequency(cm ⁻¹)	IR Inten
v1	-1301.13	599.9046	-655.93	619.5207
v2	85.89	2.0128	79.03	1.7397
v3	88.77	2.2444	87.44	2.3239
v4	131.11	0.4323	146.12	0.5478
v5	174.21	0.569	172.36	1.1252
v6	263.5	0.282	268.07	0.584
v7	282.06	0.7367	307.71	2.3507
v8	315.04	0.0084	317.58	0.1673
v9	372	0.798	393.96	0.0327
v10	432.37	0.1411	479.17	22.4097
v11	535.37	0.087	532.7	4.2869
v12	553.85	3.2082	552.67	10.9825
v13	607.89	11.8973	568.08	138.4318
v14	665.43	1.4587	695.62	23.6959
v15	737.06	1.6311	741.94	3.3278
v16	752.01	1.574	767.67	46.6427
v17	789.15	2.0476	796.21	1.9947
v18	835.58	6.2237	832.73	0.5416
v19	854.29	0.5683	860.27	1.8152
v20	863.9	0.0815	868.53	3.7245
v21	885.23	0.2812	885.97	2.6278
v22	888.25	0.7461	889.93	0.6212
v23	911.11	0.5375	908.74	0.0651
v24	915.67	0.0063	913.49	1.237
v25	927.78	3.0971	924.57	9.8232
v26	947.56	5.7733	955.38	3.4549
v27	973.69	1.8093	960.19	1.1229
v28	987.44	2.1968	991.33	6.0706
v29	992.23	1.411	1010.22	1.3798
v30	1031.37	3.772	1046.18	0.9294
v31	1036.07	2.7023	1048.29	1.4758
v32	1039.33	0.1646	1052.78	1.9537
v33	1050.4	0.0408	1061.74	17.4861
v34	1074.32	0.6791	1076.51	2.0801
v35	1078.07	3.7279	1123.39	2.243
v36	1147.57	1.0357	1145.26	2.9123

v37	1163.56	17.3184	1152.18	4.6217
v38	1186.57	5.2459	1178.61	4.8426
v39	1193.51	0.4463	1190.77	1.6092
v40	1194.63	0.022	1198.35	5.8007
v41	1215.92	2.2093	1204.89	3.2327
v42	1232.14	2.2533	1224.46	0.2688
v43	1237.04	0.1604	1248.36	1.809
v44	1260.01	4.1101	1256.16	0.484
v45	1267.2	2.1424	1268.98	1.9735
v46	1287.15	0.0491	1291.31	1.123
v47	1303.31	0.0395	1307.92	0.2445
v48	1311.28	0.2544	1314.38	1.4222
v49	1318.15	0.16	1318.18	0.3237
v50	1327.63	0.3534	1331.21	1.2302
v51	1332.97	0.8895	1339.05	1.2264
v52	1342.95	0.5805	1345.22	1.2967
v53	1347.76	0.8957	1349.84	0.1563
v54	1361.98	0.1699	1358.61	0.4546
v55	1366.28	3.6244	1475.81	6.4612
v56	1469.2	0.0384	1493.72	1.3551
v57	1496.88	3.0291	1497.26	1.4702
v58	1497.29	4.7292	1501.8	6.0628
v59	1512.25	0.026	1509.71	9.4151
v60	1513.08	11.6834	1522	2.202
v61	3018.69	14.9679	3003.82	14.7823
v62	3023.46	28.0796	3022.95	14.3514
v63	3028.11	28.706	3034.12	21.4468
v64	3034.36	0.0053	3035.32	20.5331
v65	3046.29	29.4899	3042.26	28.2646
v66	3047.49	20.351	3047.98	29.1859
v67	3057.66	64.4634	3054.4	47.9652
v68	3072.86	37.2639	3072.78	23.5533
v69	3075	35.1829	3076.21	6.8386
v70	3077.3	10.6038	3077.66	55.7308
v71	3082	56.8219	3081.25	59.5346
v72	3091.96	62.5993	3084.35	38.2624
v73	3092.07	8.1117	3090.46	28.7693
v74	3102.08	37.0362	3093.52	33.7737
v75	3110.61	24.1379	3106.95	22.5549

Normal modes	tsR5-OH		tsR6-OH	
	Frequency(cm ⁻¹)	IR Inten	Frequency(cm ⁻¹)	IR Inten
v1	-946.34	595.9346	-922.56	745.9918
v2	64.73	1.3763	57.13	2.3371
v3	87.97	1.7397	75.08	2.0341
v4	142.37	0.6667	142.86	0.427
v5	195.92	0.8493	182.95	3.0993
v6	269.92	0.3515	263.26	0.1131
v7	310.69	2.2719	311.37	2.5877
v8	319.9	1.0452	320.25	0.4483
v9	396.96	0.3426	398.16	0.6244
v10	497.55	0.1428	490.21	0.0497
v11	529.65	3.6858	534.96	0.4385
v12	577.73	0.7433	579.94	10.924
v13	602.56	72.2332	639.19	96.7388
v14	697.35	2.973	672.68	0.9517
v15	738.3	0.7882	735.54	0.3537
v16	748.37	0.3382	758.78	5.7572
v17	792.12	3.3737	791.39	3.9104
v18	828.17	0.9957	828.64	1.5033
v19	857.73	2.7682	859.18	0.5428
v20	864.43	1.968	864.83	9.2874
v21	886.93	0.868	887.7	1.1158
v22	893.01	0.7778	887.92	0.1672
v23	910.35	1.1396	914.47	1.2901
v24	921.21	1.8638	915.25	0.5261
v25	925.13	0.9294	924.07	2.2371
v26	956.22	1.1111	954.56	0.9523
v27	960.94	0.0923	961.39	0.0034
v28	991.27	1.4005	992.87	2.7903
v29	997.89	2.4938	996.83	4.1753
v30	1034.85	0.3321	1037.81	2.6596
v31	1047.26	0.1999	1048.44	0.322
v32	1049.53	0.2236	1050.11	0.0393
v33	1053.55	0.0471	1062.01	0.8249
v34	1074.97	5.2227	1065.79	2.0044
v35	1112.13	8.8797	1133.9	0.254

v36	1140.3	0.8144	1141.18	2.0317
v37	1154.74	6.7027	1163.84	2.8746
v38	1167.81	1.4875	1169.41	3.2939
v39	1197.87	4.2131	1193.72	27.1512
v40	1204.49	2.1962	1200.93	0.2146
v41	1213.34	0.4806	1214.24	0.7013
v42	1225.02	2.6486	1233.29	2.0042
v43	1250.77	2.487	1239.77	0
v44	1276.39	1.8655	1258.38	0.0027
v45	1287.83	10.5341	1278.79	3.1371
v46	1293.49	0.728	1292.69	1.0688
v47	1301.58	3.8055	1306.67	0.0615
v48	1312.25	1.2006	1308	0.0007
v49	1316.34	0.5527	1312.59	2.3296
v50	1322.99	0.7779	1319.78	0.1982
v51	1331.88	0.9414	1326.37	0.4812
v52	1337.04	2.4507	1337.41	1.3539
v53	1348	4.9518	1353.01	3.2163
v54	1355.57	0.5492	1368.36	0.6661
v55	1368.35	0.4025	1371.22	0.1674
v56	1476.96	5.9225	1472.3	7.4279
v57	1495.71	1.2403	1482.17	2.0569
v58	1497.4	2.7705	1495.89	1.0462
v59	1508.23	10.8641	1505.5	11.3301
v60	1522.13	3.9041	1523.62	4.0251
v61	2988.67	18.0315	2988.62	7.3786
v62	3008.85	13.668	2992.57	15.2631
v63	3037.29	18.5197	3037.65	21.4573
v64	3039	33.0755	3046.02	44.9002
v65	3042.01	7.8687	3048.1	42.3535
v66	3043.91	42.5605	3049.96	0.4423
v67	3048.5	54.7978	3058.76	14.7804
v68	3065.7	2.2712	3066.62	0.5391
v69	3073.51	17.1549	3069.31	39.381
v70	3079.45	51.2641	3073.86	89.2775
v71	3081.36	40.5813	3073.86	28.7372
v72	3084.75	42.5557	3081.69	6.1464
v73	3087.01	13.9289	3086.31	39.2842
v74	3088.03	79.5672	3089.69	73.8952
v75	3094.96	28.825	3090.89	34.5264

Normal modes	vdW R1-O ₂ H		vdW R2-O ₂ H	
	Frequency(cm ⁻¹)	IR Inten	Frequency(cm ⁻¹)	IR Inten
v1	24.68	1.5639	24.01	1.3122
v2	32.33	1.3439	53.57	0.829
v3	57.27	0.0517	57.03	0.8597
v4	93.05	0.3479	99.18	0.9423
v5	130.73	4.3947	138.32	0.0056
v6	164.63	1.9729	179.49	0.9171
v7	186.66	2.1611	200.47	11.0995
v8	301	0.4818	261.96	0.4994
v9	316.55	0.1732	316.31	0.233
v10	353.05	0.5826	330.45	0.1032
v11	407.51	0.1103	397.38	0.0254
v12	490.84	1.2629	484.96	0.4098
v13	539.48	0.266	515.96	2.331
v14	549.57	1.0159	544.14	0.6776
v15	607.84	19.9738	622.3	75.2357
v16	627.88	53.744	652.71	0.6565
v17	674.58	0.4392	724.63	0.217
v18	746.62	0.38	758.23	0.184
v19	765.84	0.2468	800.71	0.7757
v20	791.83	1.9541	829.64	0.7453
v21	856.22	0.9074	855.68	1.9692
v22	863.48	0.0347	875.32	0.4134
v23	884.46	0.3421	891.23	0.1546
v24	897.56	0.3446	912.05	0.5392
v25	910.06	0.1087	923.8	0.253
v26	913.09	0.8231	938.38	1.3756
v27	930.07	0.1834	955.6	1.4649
v28	950.45	1.8406	967.46	0.8419
v29	958.01	3.6533	990.06	0.2337
v30	982.42	1.3846	1013.23	0.3991
v31	990.25	1.7006	1018.3	1.4902
v32	998.53	0.9648	1052.48	0.0654
v33	1039.53	0.371	1057.69	0.0664
v34	1049.15	0.1252	1068.18	0.5291
v35	1054.5	0.6244	1097.16	0.4192

v36	1067.31	1.1524	1119.43	0.3362
v37	1118.26	0.2743	1147.61	1.4395
v38	1141.06	0.2546	1167.94	1.9407
v39	1162.18	1.2372	1196.41	0.0724
v40	1178.33	15.0418	1198.6	1.4412
v41	1187.13	0.6067	1208.63	3.829
v42	1195.28	0.3186	1219.75	2.1416
v43	1209.01	0.3813	1233.04	3.0346
v44	1229.46	0.4533	1256.84	0.1331
v45	1254.95	1.3583	1262.08	23.56
v46	1279.95	1.5245	1267.51	36.5368
v47	1286.32	0.6502	1279.57	2.058
v48	1304.15	0.4802	1292.52	1.1092
v49	1309.09	0.1748	1308.86	0.3041
v50	1320.81	0.33	1312.03	1.0826
v51	1324.8	0.3647	1315.52	0.729
v52	1335.15	1.0473	1327.84	0.4506
v53	1344.71	0.746	1344.48	0.0141
v54	1348.12	0.7632	1353.83	0.4681
v55	1364.63	0.4836	1372.29	0.8754
v56	1370.76	0.4613	1470.95	1.2164
v57	1470.79	6.1704	1472.78	0.227
v58	1495.14	1.7565	1478.47	2.1214
v59	1497.25	3.0625	1483.76	10.4259
v60	1502.55	10.2434	1496.92	6.7809
v61	1507.33	9.6349	1506.17	6.9355
v62	1520.76	8.3029	1521.02	18.3033
v63	2951.94	304.6055	3071.88	406.3918
v64	2993.29	35.409	3080.52	24.5839
v65	3020.25	13.0456	3083.11	28.8543
v66	3020.64	19.4068	3087.07	25.162
v67	3024.91	29.7649	3092.82	20.2697
v68	3029.93	27.1104	3094.96	18.0435
v69	3040.49	8.862	3106.52	38.5109
v70	3055.2	42.5611	3112.72	20.2411
v71	3057.53	20.7549	3128.82	32.9195
v72	3072.99	34.3008	3131.84	6.6612
v73	3076.45	43.2845	3147.89	23.8241

v74	3084.23	81.8866	3154.98	11.1563
v75	3086.67	42.1779	3155.47	27.5404
v76	3098.68	18.9452	3169.85	19.6185
v77	3099.77	29.6955	3177.02	25.7186
v78	3150.07	7.9329	3186.6	18.3915

Normal modes	vdW R3-O ₂ H		vdW R4-O ₂ H	
	Frequency(cm ⁻¹)	IR Inten	Frequency(cm ⁻¹)	IR Inten
v1	32.31	1.2021	34.06	1.1821
v2	41.95	1.611	60.23	0.4826
v3	61.8	0.0183	68.18	0.7221
v4	74.33	0.2362	112.76	0.4758
v5	123.86	0.034	124.5	0.2239
v6	147.75	3.8694	179.81	0.2528
v7	199.68	1.9581	208.07	9.91
v8	256.19	0.2385	250.42	0.5524
v9	310.98	0.0396	305.02	1.2092
v10	314.8	0.0062	320.52	0.1278
v11	402.15	0.1989	389.11	0.0359
v12	532.38	0.1071	479.04	0.8115
v13	536.13	3.3212	533.7	0.5474
v14	551.36	2.2442	545.67	0.8747
v15	666.13	14.1625	633.46	3.8686
v16	691.41	30.5727	663.36	72.4388
v17	727.4	0.0473	726.92	0.6222
v18	757.82	0.597	751.21	1.1399
v19	787.31	0.1788	807.09	1.6468
v20	807.19	3.3968	829.83	2.4436
v21	840.54	2.348	862.54	0.2414
v22	851.93	0.0467	892.31	0.3084
v23	868.27	0.0652	894.82	1.78
v24	874.63	1.4551	912.66	0.6329
v25	912.25	0.0027	916.9	0.1949
v26	916.05	1.78	931.75	0.0157
v27	921.6	0.0187	944.26	0.9742
v28	942.86	0.1425	969.61	2.9124
v29	946.59	0.3523	976.09	0.8631
v30	990.82	1.7113	1015.06	0.5472
v31	992.97	1.7709	1024.1	2.2832
v32	1002.24	0.2645	1047.8	0.4499
v33	1040.77	0.1772	1061.61	0.2833
v34	1052.26	0.0001	1067.04	0.1104
v35	1057.62	0.1849	1102.54	1.4185

v36	1071.59	0.7993	1131.52	0.0405
v37	1151.43	0.535	1136.84	0.0774
v38	1159.41	12.0202	1162.3	0.3228
v39	1179	14.585	1165.8	1.4778
v40	1192.83	2.2258	1195.98	2.5647
v41	1193.87	0.1747	1217.44	0.2749
v42	1204.02	0.8886	1229.4	4.6784
v43	1205.31	0.6793	1237.26	0.8397
v44	1235.35	1.8726	1247.51	0.3911
v45	1246.92	0.0005	1260.15	12.1313
v46	1261.05	1.0162	1265.25	46.4701
v47	1282.39	0.005	1271.05	0.2201
v48	1304.51	0.003	1298.97	0.513
v49	1311.96	0.3051	1305.23	0.1953
v50	1317.51	0.0001	1315.15	1.3696
v51	1327.7	0.029	1323.15	1.3132
v52	1332.76	0.7873	1338.62	0.5028
v53	1346.48	0.7266	1341.03	0.0272
v54	1350.04	0.0272	1350.44	0.4724
v55	1364.49	0.6901	1368.67	0.6883
v56	1369.68	0.3149	1454.45	7.0352
v57	1492.96	1.5202	1472.05	1.0282
v58	1493.35	3.3813	1477.47	1.741
v59	1497.78	2.8542	1482.72	8.3521
v60	1503.21	14.5985	1492.6	6.9192
v61	1509.46	4.5426	1506.37	4.7108
v62	1519.96	6.0171	1525.89	8.2544
v63	2626.18	88.7933	3037.75	36.1291
v64	3018.71	15.6357	3069.86	407.6858
v65	3025.1	24.97	3078.88	19.4352
v66	3029.89	28.6808	3083.13	2.9793
v67	3037.61	4.3652	3088.61	23.5368
v68	3041.36	24.866	3090.15	16.2005
v69	3048.77	14.6564	3094.76	16.4375
v70	3053.32	76.5299	3105.67	44.6255
v71	3073.76	7.9575	3116.48	27.5166
v72	3074.96	38.4207	3138.03	38.2969
v73	3075.6	31.2517	3148.81	19.9863

v74	3082.98	65.9086	3153.27	33.2007
v75	3093.92	47.8054	3157.67	1.4761
v76	3097.28	55.5116	3157.88	7.0162
v77	3097.98	9.341	3162.8	34.743
v78	3117.4	12.9118	3175.07	26.5958

Normal modes	vdW R5-O ₂ H		vdW R6-O ₂ H	
	Frequency(cm ⁻¹)	IR Inten	Frequency(cm ⁻¹)	IR Inten
v1	18.45	1.524	19.36	1.3998
v2	36.34	1.2313	39.75	0.4617
v3	51.55	0.1552	52.97	1.0484
v4	90.82	0.2422	94.07	0.3113
v5	120.14	2.0982	126.86	0.3467
v6	144.51	0.3787	186.78	0.8231
v7	195.39	4.9313	201.96	8.7813
v8	269.86	0.2479	260.94	0.0168
v9	308.59	0.3787	281.01	1.0672
v10	333.41	1.2126	325.52	0.0796
v11	395.14	0.2343	395.98	0.5889
v12	491.83	0.4441	490.39	0.9203
v13	534.78	0.3398	533.32	0.4724
v14	581.91	11.2958	547.95	14.2294
v15	613.15	60.049	687.6	1.5465
v16	658.51	8.5592	692.59	40.7838
v17	736.94	0.3744	712.55	20.0851
v18	746.55	1.2586	732.12	0.4649
v19	781.84	4.004	778.3	0.938
v20	800.37	0.69	798.29	0.6912
v21	829.94	0.3486	828.37	1.0606
v22	850.08	0.5871	845.7	0.301
v23	870.39	1.5243	886.57	1.0281
v24	887.26	0.603	888.17	0.4948
v25	903.17	0.366	913.7	0.7071
v26	920.98	0.3723	923.75	1.0176
v27	924.63	1.2577	924.23	1.8734
v28	947.54	1.5656	948.65	0.5762
v29	961.36	0.2855	962.26	0.026
v30	981.28	1.1212	966.83	1.8278
v31	998.39	0.6324	1004.55	2.7674
v32	1017.42	0.9503	1024.47	0.5262
v33	1046.14	0.1196	1044.67	0.8787
v34	1049.67	0.1287	1051.82	0.8008
v35	1059.67	0.697	1058.67	0.4567

v36	1071.59	2.0018	1074.22	0.003
v37	1123.81	0.5861	1130.19	0.8499
v38	1143.55	0.1805	1145.54	0.101
v39	1161.82	0.7129	1153.01	0.4992
v40	1176.09	13.5192	1175.83	15.8454
v41	1186.53	2.2944	1192.01	3.7222
v42	1205.33	3.5316	1198.53	0.0185
v43	1218.65	0.3903	1213.09	1.2984
v44	1227.7	0.3719	1233.81	2.0236
v45	1248.21	0.2519	1249.71	0.4037
v46	1277.69	1.3171	1262.84	0.7614
v47	1288.05	1.3784	1292.65	1.0791
v48	1294.92	0.7951	1307.22	0.0509
v49	1301.66	0.4167	1308.93	0.6173
v50	1314.78	0.2572	1311.3	0.3579
v51	1319.8	1.6941	1321.91	1.201
v52	1324.06	0.4398	1327.06	1.6529
v53	1335.84	1.8757	1346.17	0.3133
v54	1349.17	1.6194	1354.71	4.0234
v55	1362.48	0.6573	1365.62	0.1477
v56	1368.91	1.0759	1370.71	0.8852
v57	1469.02	4.0518	1458.81	19.8817
v58	1492.55	14.3168	1468.63	4.2905
v59	1495.91	0.8417	1496.31	1.0858
v60	1497.7	3.8445	1504.17	9.2433
v61	1509.92	11.3912	1507.2	9.2372
v62	1522.78	1.6135	1523.21	3.9234
v63	2935.27	29.6311	2785.53	199.0387
v64	2971.51	30.7998	2938.86	13.6759
v65	2999.53	247.1953	2941.98	20.9887
v66	3034.28	26.2647	3024.6	16.6952
v67	3039.18	25.6884	3033.3	5.8841
v68	3046.41	12.3807	3038.25	19.7717
v69	3046.99	9.1826	3044.82	37.4833
v70	3049.21	107.1955	3048.46	48.8684
v71	3051.8	12.6307	3054.24	13.8542
v72	3067.75	3.5407	3067.56	14.5735
v73	3079.77	51.9366	3069	28.6668

v74	3084.27	43.1111	3074.65	75.1828
v75	3088.44	35.7434	3081.99	2.9094
v76	3091.98	47.0152	3084.57	33.5859
v77	3092.43	44.1936	3089.95	79.4418
v78	3132.18	7.9185	3140.56	28.4242

tsR1-O ₂ H				
Normal modes	Frequency(cm ⁻¹)	IR Inten	Frequency(cm ⁻¹)	IR Inten
v1	-507.33	87.3089		
v2	25.69	1.1685		
v3	41.71	1.2673		
v4	74.86	0.2723		
v5	138.03	1.246		
v6	164.3	0.4884		
v7	176.1	0.0733		
v8	299.18	0.7187		
v9	315.47	0.1615		
v10	328.88	3.536		
v11	400.28	2.7662		
v12	489.81	1.3566		
v13	533.85	0.4938		
v14	555.8	0.4071		
v15	623.93	8.2114		
v16	675.09	1.0007		
v17	744.11	1.557		
v18	760.35	6.8655		
v19	792.37	1.4527		
v20	844.45	8.0192		
v21	861.85	1.9815		
v22	871.58	22.3855		
v23	875.9	7.5775		
v24	895.48	5.334		
v25	909.97	1.5336		
v26	911.25	0.47		
v27	927.3	1.962		
v28	952.01	4.9997		
v29	957.91	5.0076		
v30	978.78	3.8228		
v31	991.49	1.7425		
v32	995.66	3.7744		
v33	1041.12	0.7253		
v34	1050.45	1.2523		
v35	1058.9	1.0805		

v36	1063.29	7.3434
v37	1105.33	14.6627
v38	1135.1	3.8423
v39	1156.54	8.1609
v40	1173.32	17.618
v41	1189.68	0.3909
v42	1195.71	0.3819
v43	1210.53	1.0375
v44	1227.82	0.3158
v45	1256.21	0.9646
v46	1279.23	1.0453
v47	1290.32	0.4718
v48	1305.17	0.4328
v49	1310.3	0.3509
v50	1320.58	0.2665
v51	1323.84	0.1224
v52	1330.83	1.6671
v53	1344.55	0.6303
v54	1349.15	1.2455
v55	1366.12	0.307
v56	1373.41	0.5273
v57	1469.78	3.2453
v58	1473.74	6.6858
v59	1495.2	1.815
v60	1497.07	2.9768
v61	1506.79	5.4828
v62	1520.53	8.3178
v63	1674.77	11.6324
v64	3007.99	26.5795
v65	3020.31	12.8411
v66	3024.51	27.7991
v67	3029.35	26.9983
v68	3033.56	7.9443
v69	3042.94	16.028
v70	3054.55	32.5081
v71	3062.5	20.4839
v72	3073.34	33.6736
v73	3076.72	42.6568

v74	3084.78	89.2472
v75	3085.77	31.5698
v76	3097.07	11.6038
v77	3098.87	36.0451
v78	3117.51	19.1249

Normal modes	tsR3-O ₂ H		tsR4-O ₂ H	
	Frequency(cm ⁻¹)	IR Inten	Frequency(cm ⁻¹)	IR Inten
v1	-114.09	3.999	-1429.39	350.373
v2	33.74	1.1147	36.26	1.5682
v3	51.04	1.3224	78.18	0.7212
v4	68.36	0.0567	96.27	0.9742
v5	125.15	0.0339	142.44	0.3441
v6	149.41	2.0056	161.25	0.6585
v7	197.94	0.8471	227.96	1.4425
v8	256.68	0.242	270.96	0.267
v9	311.91	0.0665	305.55	0.0754
v10	314.31	0.0049	328.99	0.0271
v11	399.23	1.2796	389.81	0.7861
v12	532.28	0.2078	421.1	3.1698
v13	548.11	0.4209	506.41	1.275
v14	556.9	7.5824	533.55	0.2969
v15	670.95	1.3091	546.07	1.3554
v16	722.8	7.4411	691.92	2.3131
v17	754.07	0.3711	750.7	0.9209
v18	767.5	29.9022	784.13	2.3903
v19	779.23	1.3504	813.64	1.198
v20	811.64	0.5118	848.6	4.1051
v21	834.69	4.5461	874.72	2.0878
v22	852.79	0.0008	893.56	2.3892
v23	868.77	0.1146	909.47	1.4507
v24	874.74	0.471	915.37	0.3906
v25	912.78	0.0022	930.05	1.181
v26	915.54	1.3656	934.52	0.5078
v27	922.87	0.1733	947.83	2.2671
v28	937.52	1.171	969.21	3.1675
v29	946.42	0.3309	977.09	1.712
v30	990.77	2.6082	1000.86	23.1104
v31	993.6	1.7226	1022.3	7.0845
v32	1003.78	0.4361	1031.23	3.536
v33	1041.17	0.2572	1051.62	2.0948
v34	1052.2	0.0016	1065.6	0.6757
v35	1058.57	0.1974	1070.76	0.1631

v36	1071.35	1.7521	1100.12	1.102
v37	1149.6	33.3973	1134.88	0.9068
v38	1151.2	0.4968	1144.52	2.208
v39	1179.08	11.7515	1160.9	1.2194
v40	1193.79	0.1579	1194.38	4.9277
v41	1195.81	4.2723	1197.31	2.5264
v42	1204.11	0.6797	1216.91	1.5411
v43	1205.51	0.6213	1232.74	2.3179
v44	1234.94	2.1293	1236.2	0.0935
v45	1246.76	0.0001	1250.23	0.5285
v46	1261.48	0.8613	1264.9	0.3631
v47	1283	0.005	1271.78	0.9724
v48	1304.76	0.0038	1300.55	0.2431
v49	1312.32	0.422	1305.81	0.9032
v50	1317.39	0.0017	1315.08	1.6782
v51	1327.89	0.0437	1323.92	1.3681
v52	1332.76	0.9229	1337.68	0.249
v53	1346.43	0.6953	1341.97	0.0574
v54	1350.35	0.0141	1349.68	1.0468
v55	1364.37	0.5752	1362.79	0.4603
v56	1369.75	0.3088	1417.39	19.2351
v57	1492.9	1.5094	1455.83	5.5837
v58	1494.68	2.0905	1472.41	1.2312
v59	1498.04	2.9327	1477.59	2.3304
v60	1505.09	11.7862	1483.52	8.2622
v61	1509.49	5.1595	1493.28	6.5137
v62	1522.64	5.8166	1507.92	3.4634
v63	2182.23	7.4846	1542.04	13.4645
v64	3019.37	19.5244	3046.74	16.6449
v65	3027.85	26.286	3078.08	10.0615
v66	3032	21.9442	3082.32	5.3467
v67	3037.46	4.6228	3089.24	21.936
v68	3041.36	24.9056	3090.79	28.1157
v69	3048.72	13.6604	3094.82	17.2205
v70	3053.19	79.6952	3106.59	38.6715
v71	3073.86	4.2216	3125.62	16.492
v72	3075.33	40.6523	3136.79	39.7446
v73	3075.75	31.606	3146.69	20.5253

v74	3083.6	64.7872	3153.3	32.0551
v75	3093.65	39.555	3157.65	3.3491
v76	3095.58	15.3675	3158.46	8.5779
v77	3097	55.4044	3162.79	30.7729
v78	3109.25	17.2621	3177.11	20.9041

Normal modes	tsR5-O ₂ H		tsR6-O ₂ H	
	Frequency(cm ⁻¹)	IR Inten	Frequency(cm ⁻¹)	IR Inten
v1	-716.37	174.5419	-419.76	30.6858
v2	11.53	1.1077	26.74	1.4338
v3	54.52	1.0525	50.59	0.4635
v4	70.97	0.4327	63.98	1.0036
v5	132.2	0.168	134.53	0.9436
v6	159.78	1.2114	136.92	0.0253
v7	175.38	0.0948	238.93	1.6433
v8	269.25	0.3882	264.39	0.0773
v9	291.78	1.3957	288.89	0.3795
v10	319.78	0.5222	331.14	0.1138
v11	395.77	0.1272	397.07	0.8335
v12	495.8	0.648	492.42	0.7711
v13	532.64	1.0127	534.6	0.1062
v14	600.15	1.3879	568.23	3.059
v15	644.25	11.0005	685.44	0.3926
v16	735.78	0.9598	702.02	5.8043
v17	745.99	0.1226	733.22	0.3734
v18	770.6	10.2864	781.08	0.276
v19	793.19	6.3382	795.96	6.1231
v20	827.96	1.8492	827.94	2.6429
v21	847.04	7.4273	848.93	0.2959
v22	860.38	4.4339	886.86	1.8852
v23	887.38	0.811	887.61	1.1277
v24	889.28	11.8902	894.37	26.7081
v25	908.74	18.3546	910.9	8.6293
v26	912.38	5.1111	922.67	3.4347
v27	923.88	0.8485	924.52	3.2344
v28	951.15	5.6343	929.28	19.7909
v29	961.14	0.6407	962.17	0.0795
v30	983.75	12.2083	963.48	9.9241
v31	987.64	2.0908	1003.02	2.832
v32	1011.17	6.8354	1016.13	9.9875
v33	1035.33	10.7554	1046.22	0.6794
v34	1049.25	3.0756	1051.99	0.6426
v35	1050.28	0.1808	1057.75	3.2557

v36	1058.69	2.0102	1075.56	0.0114
v37	1095.98	13.981	1108.46	37.4992
v38	1140.41	2.2916	1132.2	0.8842
v39	1157.86	6.6953	1146.84	0.05
v40	1163.42	0.7126	1167.1	10.3544
v41	1197.51	4.4788	1199.3	0.024
v42	1203.94	4.7689	1209.76	3.9474
v43	1219.07	0.2409	1214.41	1.9075
v44	1225.14	0.8788	1236.6	2.7532
v45	1249.51	0.5167	1247.17	0.69
v46	1276.46	1.5214	1259.83	0.5131
v47	1289.32	1.0117	1293.14	1.1107
v48	1294.97	1.6672	1307.63	0.0561
v49	1302.33	1.0462	1310.32	1.8178
v50	1315.76	0.4763	1311.29	0.3221
v51	1318.19	1.6682	1321.3	1.7202
v52	1324.53	0.5539	1326.16	1.3754
v53	1335.71	1.5413	1344.4	0.5109
v54	1348.22	3.2167	1354.18	4.9442
v55	1359.04	0.3854	1365.48	0.29
v56	1367.98	0.6056	1369.65	0.7588
v57	1422.88	1.6119	1458.37	17.9869
v58	1471.12	4.5909	1469.87	4.773
v59	1496.04	1.2596	1492.36	1.3606
v60	1498.76	2.0571	1496	1.2026
v61	1508.58	12.2207	1504.88	10.6079
v62	1523.48	4.0006	1523.67	4.1736
v63	1589.71	13.4338	1716.93	10.1756
v64	2951.66	21.4571	2949.84	11.4299
v65	2982.48	20.1287	2953.21	21.9928
v66	3037.35	7.6821	3032.47	14.3828
v67	3038.76	31.3387	3035.93	5.4257
v68	3045.07	13.6183	3038.34	18.5954
v69	3048.98	73.904	3045.66	38.5631
v70	3052.95	28.8134	3048.57	47.5375
v71	3054.13	15.7368	3054.61	14.4922
v72	3067.21	2.9892	3067.65	15.3314
v73	3079.93	48.0367	3068.67	25.0619

v74	3084.78	44.781	3074.77	75.8192
v75	3088.51	51.2097	3082.04	4.4966
v76	3092.82	36.9823	3085.5	32.7305
v77	3098.74	29.4799	3090.07	79.3461
v78	3105.54	15.2297	3123.43	30.057
