

A Chemical Dynamics Study of the Reaction of the Methylidyne Radical (CH , $X^2\Pi$) with Dimethylacetylene (CH_3CCCH_3 , $X^1\text{A}_{1g}$)

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Supporting Information

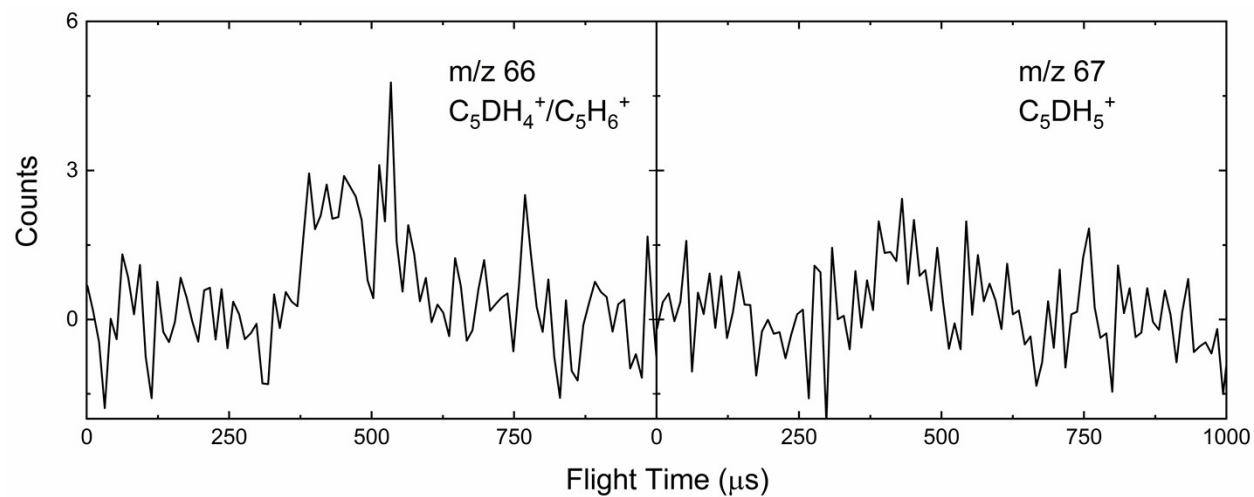


Figure S1. Time-of-flight (TOF) spectra for the reaction of D1-methylidyne radical (CD; $C_{\infty v}$; $X^2\Pi$) with dimethylacetylene (CH_3CCCH_3 ; D_{3d} ; X^1A_{1g}) recorded at mass-to-charge (m/z) ratios of 67 ($C_5DH_5^+$) and 66 ($C_5DH_4^+/C_5H_6^+$), respectively.

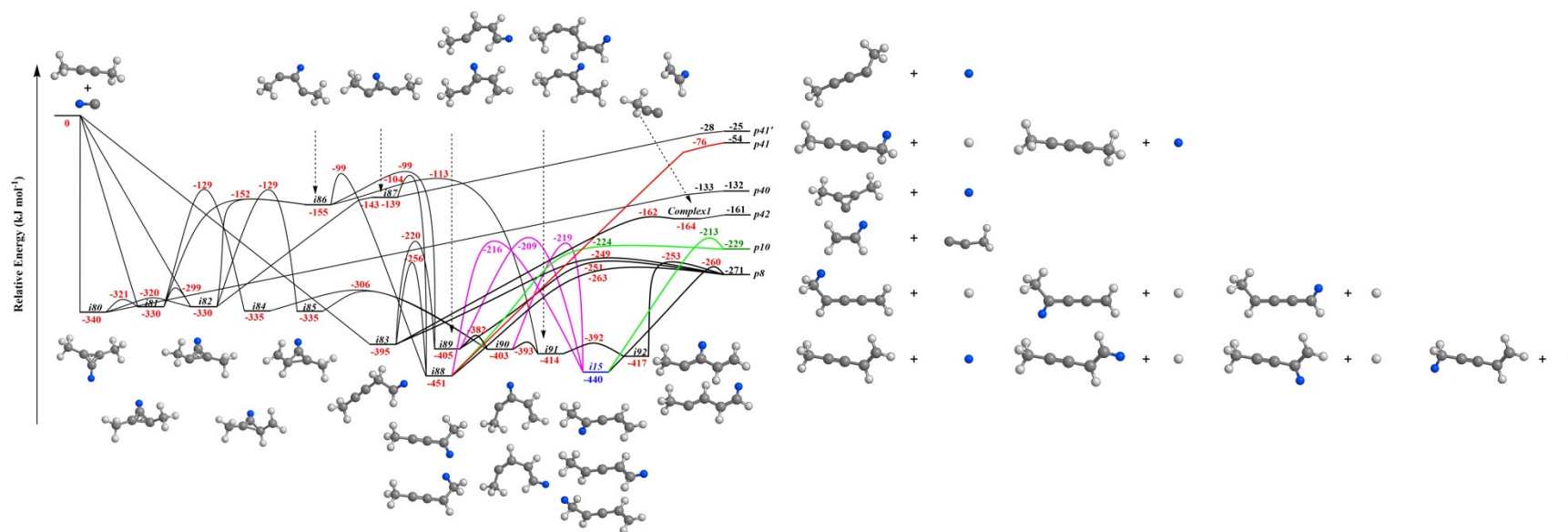


Figure S2. Portion of the C_5H_7 potential energy surface (PES) leading to **p8**, **p10**, **p40**, **p41**, **p41'**, and **p42**. H atoms from methylidyne radical and dimethylacetylene are colored in blue and grey, respectively.

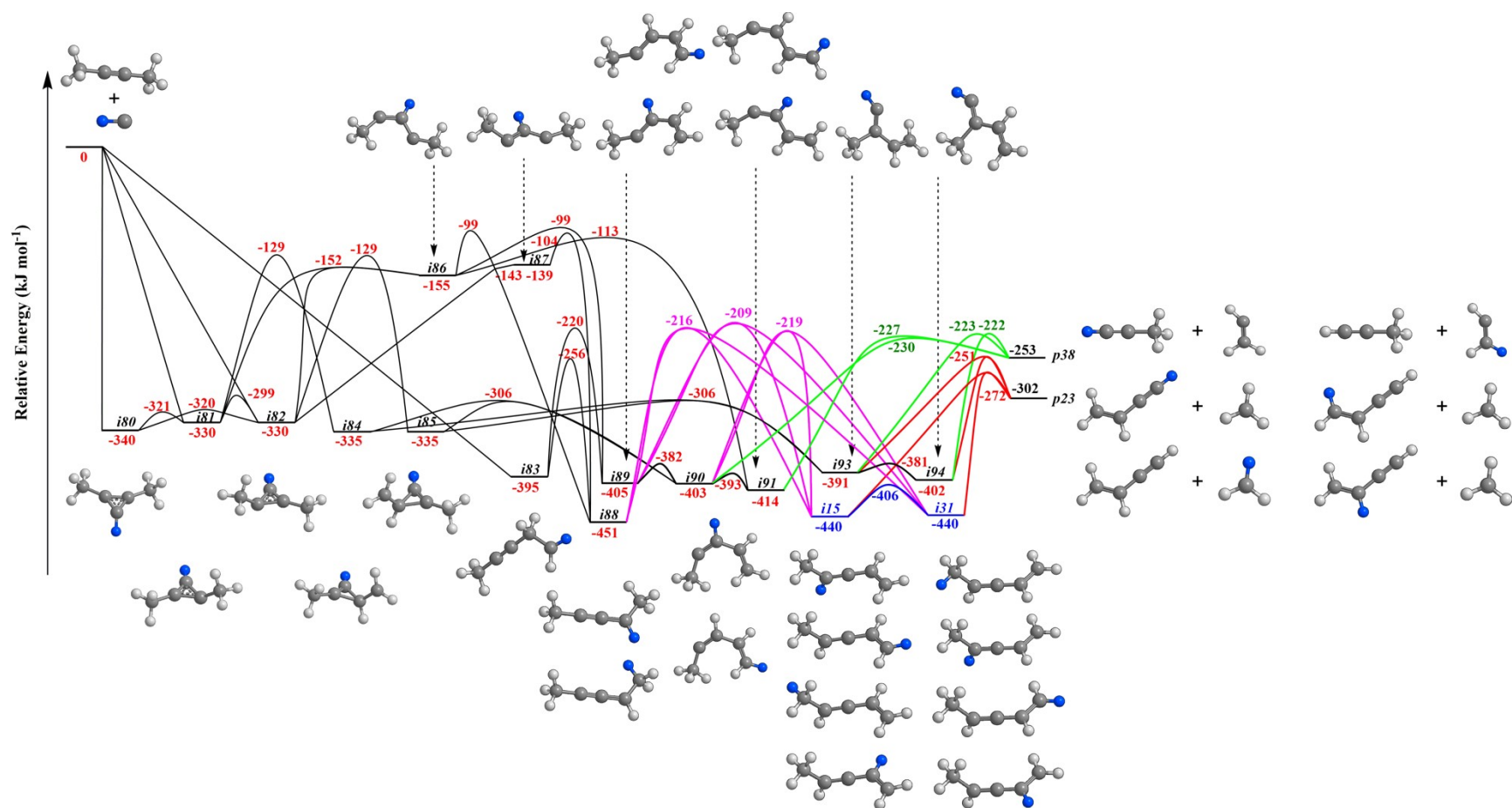


Figure S3. Portion of the C_5H_7 PES leading to **p23**, and **p38**. H atoms from methylidyne radical and dimethylacetylene are colored in blue and grey, respectively.

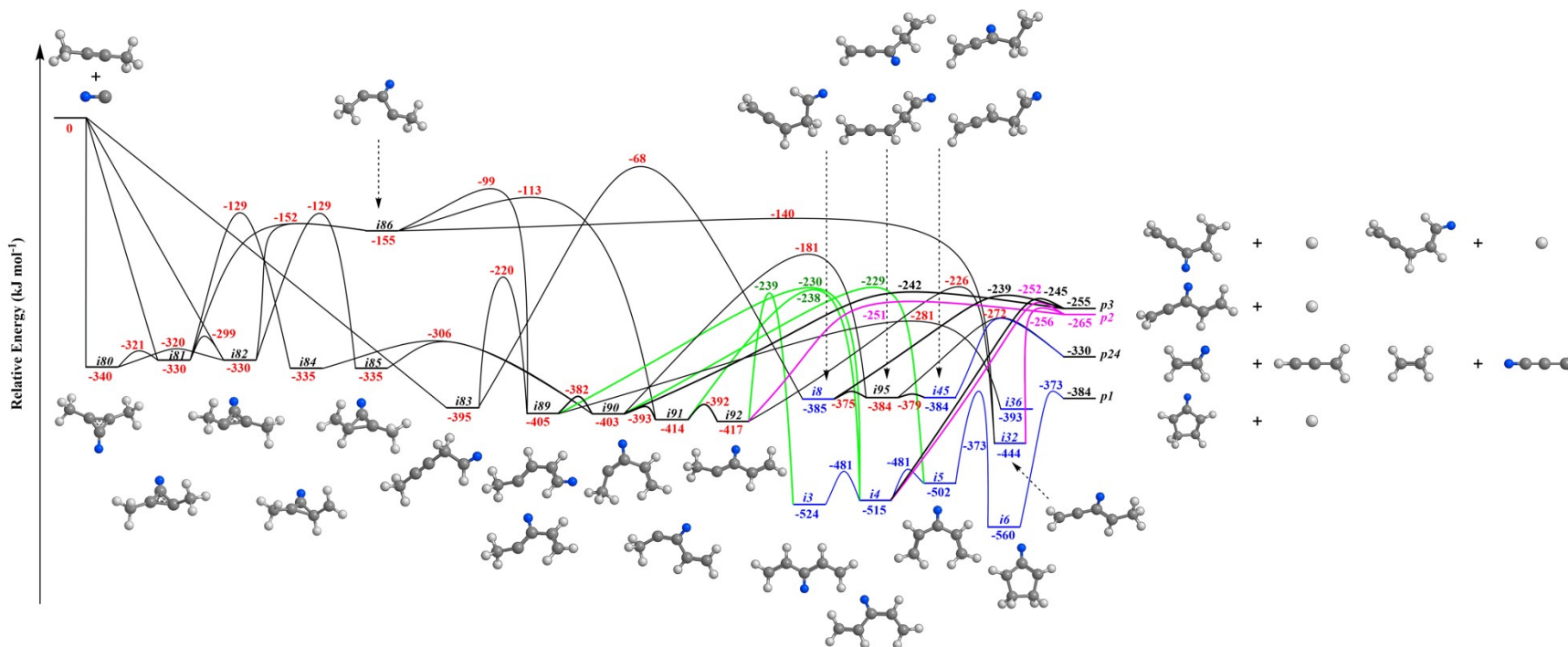


Figure S4. Portion of the C₅H₇ PES leading to **p1-p3** and **p24**. H atoms from methylidyne radical and dimethylacetylene are colored in blue and grey, respectively.

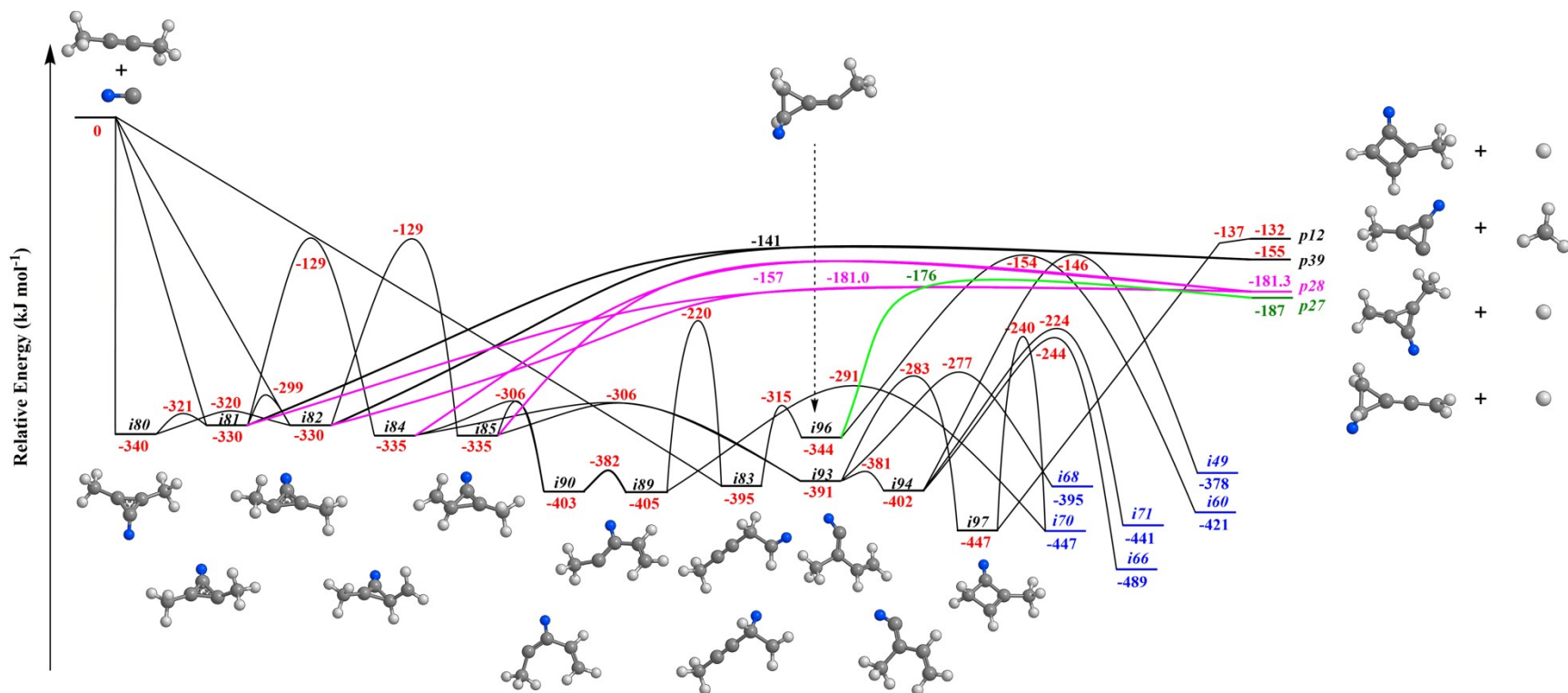


Figure S5. Portion of the C₅H₇ PES leading to **p12**, **p27**, **p28**, and **p39**. H atoms from methylidyne radical and dimethylacetylene are colored in blue and grey, respectively.

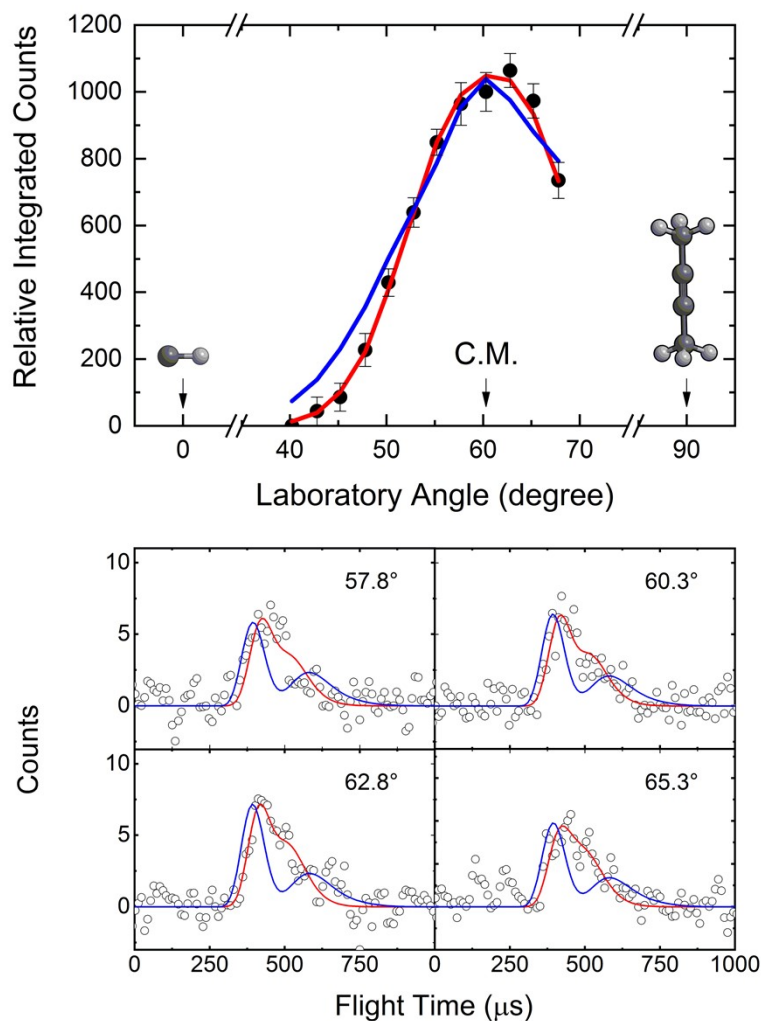


Figure S6. Laboratory angular distribution (top) and Time-of-flight (TOF) spectra (bottom) recorded at mass-to-charge (m/z) 65 ($C_5H_5^+$) from the reaction of the methylidyne radical (CH ; $C_{\infty v}$; $X^2\Pi$) with dimethylacetylene (CH_3CCCH_3 ; D_{3d} ; X^1A_{1g}). The directions of the methylidyne radical and dimethylacetylene beams are defined as 0° and 90° , respectively. The red solid lines represent the best-fits exploiting center-of-mass functions depicted in Figure S7 from the experimentally derived (red) with black circles defining the experimental data. Note that, the blue solid lines represent the best-fits exploiting center-of-mass functions depicted in Figure S7 from the dynamics simulations (blue) with **p8** as the sole product in the $CH-CH_3CCCH_3$ reaction.

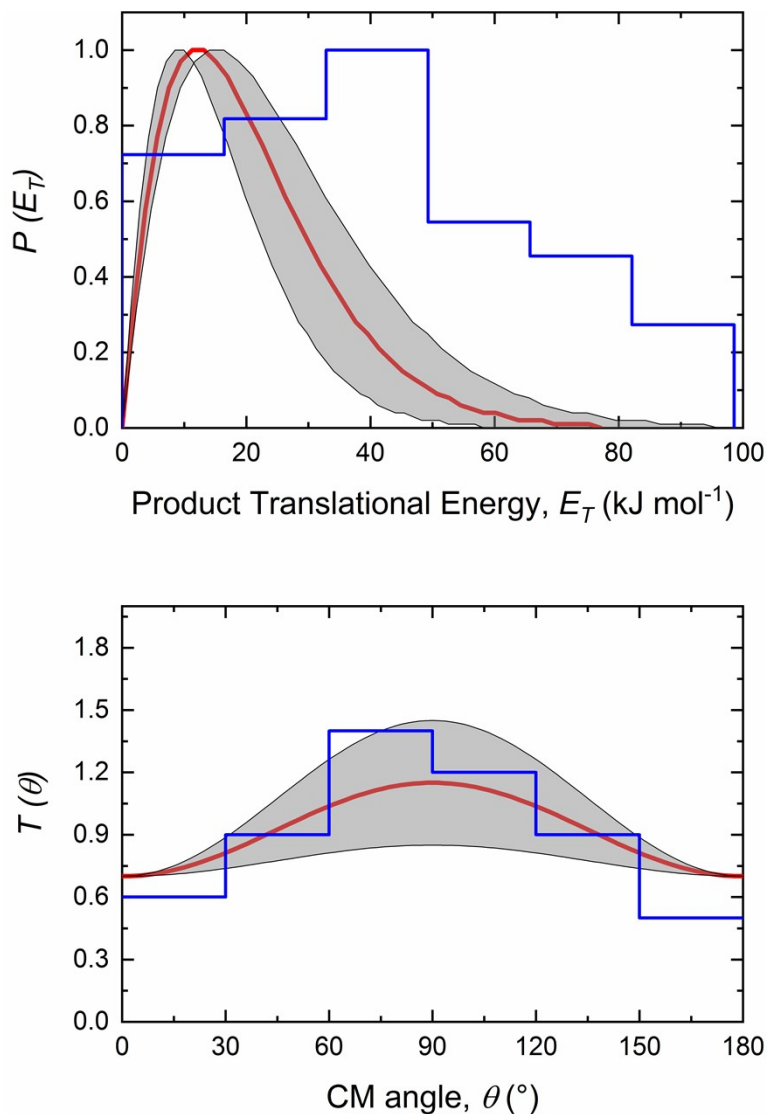


Figure S7. Center-of-mass (CM) translational energy $P(E_T)$ and angular $T(\theta)$ flux distributions for the reaction of the methylidyne radical (CH ; $C_{\infty v}$; $X^2\Pi$) with dimethylacetylene (CH_3CCCH_3 ; D_{3d} ; X^1A_{1g}). Shaded areas indicate the error limits of the best fits accounting for the uncertainties of the laboratory angular distribution and TOF spectra, with the red solid lines defining the best-fit functions. The center-of-mass function overlaid in blue are obtained from the dynamics simulations with **p8** as the sole product in the $\text{CH}-\text{CH}_3\text{CCCH}_3$ reaction.

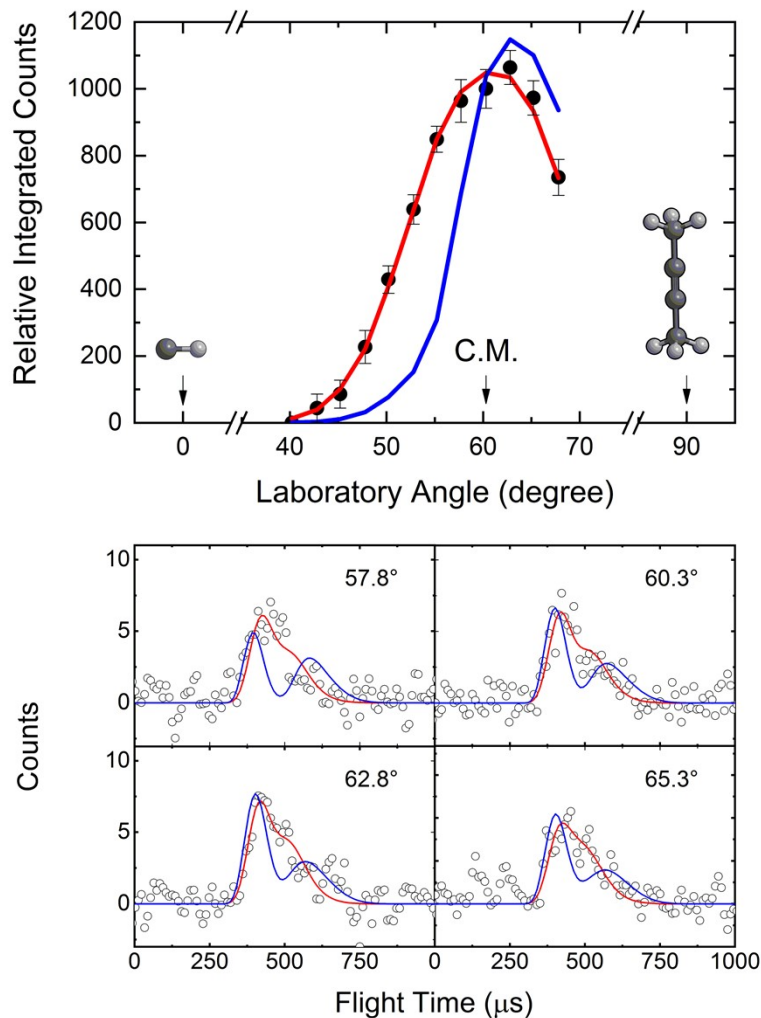


Figure S8. Laboratory angular distribution (top) and Time-of-flight (TOF) spectra (bottom) recorded at mass-to-charge (m/z) 65 ($C_5H_5^+$) from the reaction of the methylidyne radical (CH ; $C_{\infty v}$; $X^2\Pi$) with dimethylacetylene (CH_3CCCH_3 ; D_{3d} ; X^1A_{1g}). The directions of the methylidyne radical and dimethylacetylene beams are defined as 0° and 90° , respectively. The red solid lines represent the best-fits exploiting center-of-mass functions depicted in Figure S9 from the experimentally derived (red) with black circles defining the experimental data. Note that, the blue solid lines represent the best-fits exploiting center-of-mass functions depicted in Figure S9 from the dynamics simulations (blue) with **p28** as the sole product in the $CH-CH_3CCCH_3$ reaction.

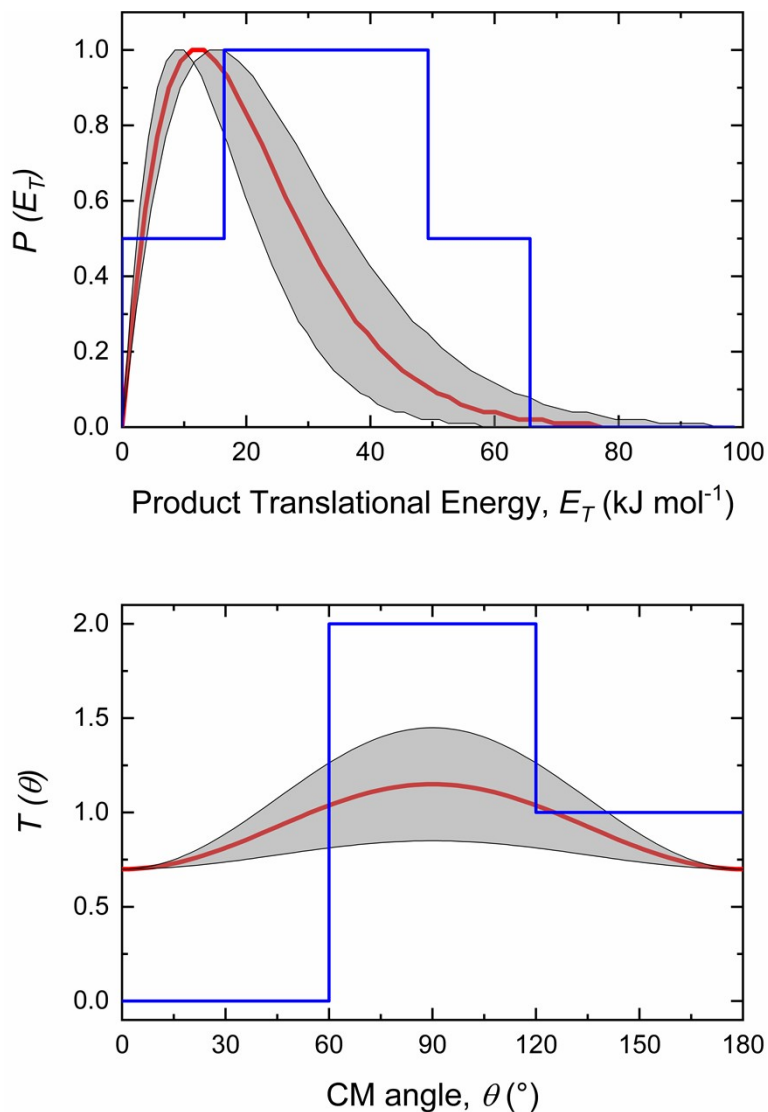


Figure S9. Center-of-mass (CM) translational energy $P(E_T)$ and angular $T(\theta)$ flux distributions for the reaction of the methylidyne radical ($\text{CH}; C_{\infty v}; X^2\Pi$) with dimethylacetylene ($\text{CH}_3\text{CCCH}_3; D_{3d}; X^1A_{1g}$). Shaded areas indicate the error limits of the best fits accounting for the uncertainties of the laboratory angular distribution and TOF spectra, with the red solid lines defining the best-fit functions. The center-of-mass function overlaid in blue are obtained from the dynamics simulations with **p28** as the sole product in the $\text{CH}-\text{CH}_3\text{CCCH}_3$ reaction.

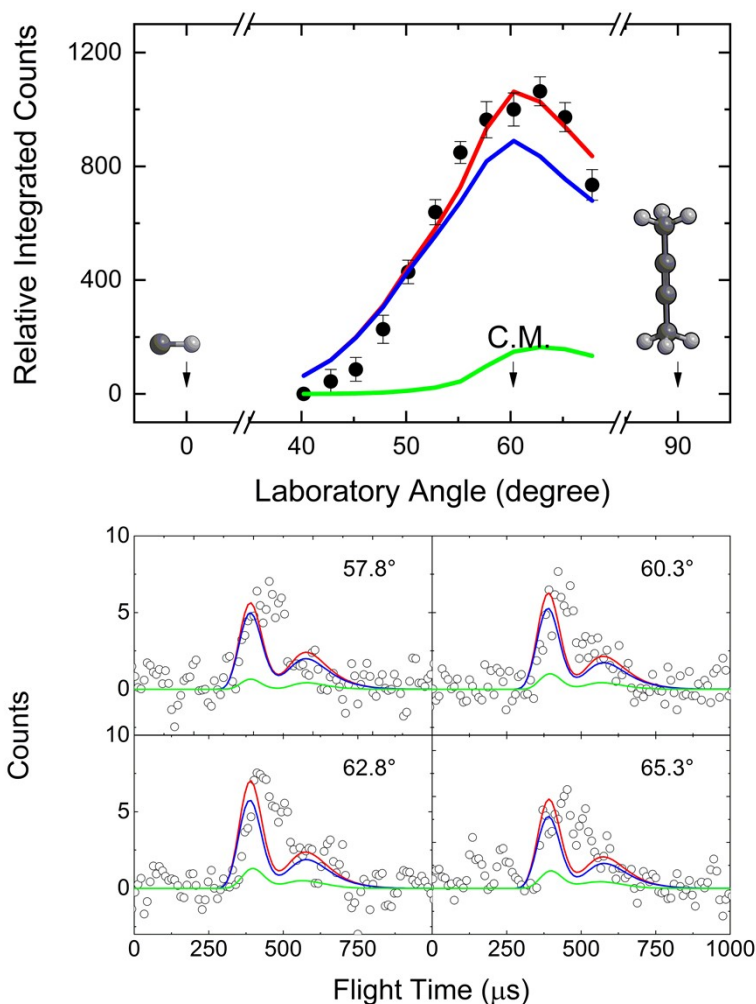


Figure S10. Laboratory angular distribution (top) and Time-of-flight (TOF) spectra (bottom) recorded at mass-to-charge (m/z) 65 ($C_5H_5^+$) from the reaction of the methylidyne radical (CH ; $C_{\infty v}$; $X^2\Pi$) with dimethylacetylene (CH_3CCCH_3 ; D_{3d} ; X^1A_{1g}) exploiting a two-channel fit: (i) **p8** (blue), (ii) **p28** (green). The ratio of these two channels is defined as 6 : 1. The directions of the methylidyne radical and dimethylacetylene beams are defined as 0° and 90° , respectively. The black circles defining the experimental data. Note that, the blue solid lines represent the best-fits exploiting center-of-mass functions depicted in Figure S7 from the dynamics simulations with **p8** as the sole product in the $CH-CH_3CCCH_3$ reaction, whereas the green solid lines represent the best-fits exploiting center-of-mass functions depicted in Figure S9 from the dynamics simulations with **p28** as the sole product in the $CH-CH_3CCCH_3$ reaction. The red solid lines correspond to the total fit.

Movies: Representative movies for reaction pathways:

SA1: **i80-82** → **p28**

SA2: **i80-82** → **p40**

SA3: **i80-82** → **i88** → **p10**

SA4: **i80-82** → **i88** → **p8**

SA5: **i83** → **p8**

SA6: **i83** → **i88** → **p8**

SA7: **i83** (\leftrightarrow **i96**) → **i88** → **p8**

SA8: **i83** (\leftrightarrow **i96**) → **p8**

Table S1. Relative energy (kJ mol⁻¹) of the potential energy profile computed from various candidate quantum chemistry methods.^a Critical points are named as in Figures 3-6 and transition states between two intermediates “iN” and “iM” are denoted as “iNTSiM”.

	Benchmark ^b	MP2	B3LYP	B97	B98	M05	M06	M06-2x	PBE0
i80TSi81	-321	-273	-316	-315	-313	-351	-336	-324	-343
i80TSi82	-320	N/A ^c	-316	-315	-313	-340	-336	-324	-328
i80TSp40	-133	-103	-115	-117	-113	-140	-133	N/A	-125
i80	-340	-290	-334	-334	-332	-355	-340	-347	-347
i81TSi82	-299	-219	-289	-291	-288	-315	-298	-296	-301
i81TSi84	-129	-273	-123	-126	-122	-148	-132	-135	-140
i81TSi86	-152	-273	-165	-164	-167	-153	-156	-149	-163
i81	-330	-273	-323	-323	-321	-343	-329	-336	-335
i82TSi85	-129	-289	-123	-126	-122	-148	-132	-135	-140
i82TSi86	-152	N/A	-165	-164	-167	-154	-156	-150	-158
i82TSi87	-143	N/A	-161	-158	-162	-149	-147	-142	-155
i82	-330	N/A	-323	-323	-321	-343	-329	-336	-335
i83	-395	-354	-389	-383	-387	-374	-379	-392	-382
i84TSi90	-306	-287	-304	-307	-308	-299	-371	-300	-304
i84	-335	-287	-326	-327	-326	-345	-332	-341	-337
i85TSi90	-306	N/A	-304	-307	-308	-299	-295	-300	-304
i85	-335	N/A	-326	-327	-326	-345	-332	-341	-337
i86TSi88	-99	-373	-114	-115	-116	-109	-110	-99	-107
i86TSi89	-99	N/A	-108	-109	-110	-102	-104	-107	-105
i86TSi91	-113	N/A	-113	-114	-116	-106	-110	-114	-111
i86	-155	N/A	-164	-165	-169	N/A	-157	-154	-153
i87TSi88	-104	-373	-119	-119	-120	-114	-116	-104	-111
i87	-139	-57	-154	-153	-163	-150	-149	-144	-142
i88TSp41-m3	-76	N/A	-83	-79	-45	-85	-79	N/A	N/A
i88	-451	-373	-460	-455	-458	-447	-449	-451	-451
i89TSi90	-382	-298	-386	-382	-384	-365	-371	-379	-377
i89	-405	-298	-404	-400	-403	-377	-386	-400	-395
i90TSi91	-393	-298	-387	-384	-387	-362	-370	-386	-380
i90	-403	N/A	-399	-396	-399	-374	-384	-398	-392
i91TSi92	-392	N/A	-396	-392	-395	-374	-379	-387	-387
i91	-414	N/A	-411	-407	-410	-384	-393	-407	-403
i92	-417	-299	-416	-411	-414	-388	-396	-410	-407
p40	-132	-103	-116	-121	-117	-145	-137	-141	-125
p41-m1	-25	N/A	-35	-36	-36	-17	-32	-21	-16
p41-m3	-54	N/A	-49	-83	-85	-89	-82	-67	-81
reactants	0	N/A	7	19	17	37	28	18	46
# of successful optimizations	36	20	36	36	36	35	36	34	35

a. The candidate potential energy profile seeks the maximum overlap with the benchmark, therefore, it has been shifted to minimize the RMSD.

b. The benchmark energy is computed at the CCSD(T)-F12/cc-pVTZ-f12//wB97X-D/6-311G(d,p) level of theory. The potential energy of the reactants is set to zero. Zero-point energy is included.

c. N/A denotes that the optimized structure is not found.

Table S2. The RMSD (in kJ mol^{-1} , defined in Equation (1)) associated with various quantum chemistry candidate methods in reproducing the CCSD(T)-F12/cc-pVTZ-f12// ω B97X-D/6-311G(d,p) potential energy profile of the reaction (see Figures 3-6). The basis set employed in these calculations is 6-311G(d,p). See Table S1 for the energies of each critical point from the candidate method.

Method	MP2	B3LYP	B97	B98	M05	M06	M06-2x	PBE0
RMSD	119.0	9.1	10.4	13.1	18.4	16.5	6.3	12.2

Table S3. Rate constant (k , in s^{-1}) for all unimolecular reactions in the CH + dimethylacetylene system calculated using RRKM theory at $E_C = 20.6 \text{ kJ mol}^{-1}$.

Reaction	k	Reaction	k	Reaction	k	Reaction	k	Reaction	k
i3 – i4	6.17E+12	i11 – p4	2.82E+10	i49 – i48 (rotation)	1.56E+12	i55 – i53	1.17E+08	i15 – i89	2.30E+08
i4 – i3	3.85E+12	i21 – p7	2.04E+10	i50 – i52	3.17E+08	i50 – p32	1.19E+10	i89 – i15	9.83E+08
i4 – i5	2.68E+12	i29 – p12	5.47E+06	i52 – i50	9.35E+07	i66 – i67	6.47E+08	i4 – i89	3.20E+07
i5 – i4	5.52E+12	i20 – p7	2.03E+10	i57 – p5	1.34E+09	i67 – i66	5.83E+11	i89 – i4	1.95E+09
i5 – i6	3.35E+10	i28 – i29	7.51E+08	i52 – p29	1.96E+08	i51 – p32	1.19E+10	i89 – i90	9.49E+12
i6 – i5	4.60E+10	i29 – i28	8.82E+08	i48 – i57	2.16E+08	i42 – i53	7.94E+10	i90 – i89	2.92E+13
i6 – p1	1.73E+11	i18 – i20	9.56E+12	i57 – i48	1.35E+09	i53 – i42	2.08E+08	i83 – p8	1.03E+10
i1 – i4	1.41E+13	i20 – i18	9.67E+12	i15 – i49	1.90E+03	i75 – p33	9.08E+10	i5 – i90	6.15E+07
i4 – i1	1.04E+06	i29 – i30	3.56E+09	i49 – i15	6.94E+04	i65 – p29	1.31E+09	i90 – i5	5.60E+09
i4 – p2	1.17E+09	i30 – i29	1.89E+09	i17 – i57	4.16E+07	i67 – p30	4.05E+10	i90 – p3	1.14E+11
i6 – i13	1.61E+10	i5 – i30	1.74E+10	i57 – i17	1.17E+08	i67 – p34	2.15E+11	i90 – p38	4.31E+11
i13 – i6	8.80E+10	i30 – i5	1.26E+12	i48 – i60	2.99E+06	i71 – p30	2.34E+09	i31 – i88	8.94E+08
i3 – i10	1.02E+04	i14 – i30	6.32E+07	i60 – i48	8.24E+05	i53 – i74	6.36E+11	i88 – i31	1.22E+08
i10 – i3	1.48E+06	i30 – i14	7.44E+08	i36 – i64	1.55E+04	i74 – i53	1.28E+11	i83 – i96	1.28E+11
i4 – p3	1.29E+09	i30 – p9	1.72E+11	i64 – i36	2.52E+12	i51 – i65	1.37E+08	i96 – i83	3.82E+13
i10 – i11	2.30E+12	i31 – i32	1.66E+08	i60 – p27	1.05E+08	i65 – i51	3.95E+07	i4 – i91	4.47E+07
i11 – i10	2.56E+12	i32 – i31	9.80E+07	i51 – i53	3.16E+08	i51 – p28	2.04E+08	i91 – i4	1.08E+09
i11 – i12	2.06E+12	i32 – p2	1.42E+10	i53 – i51	9.34E+07	i14 – i51	1.81E+10	i96 – p27	4.84E+09
i12 – i11	2.43E+12	i32 – p15	7.64E+10	i52 – i72	6.37E+11	i51 – i14	2.47E+12	i60 – i96	4.00E+06
i12 – i13	9.04E+10	i32 – i33	7.98E+08	i72 – i52	1.28E+11	i53 – p29	1.96E+08	i96 – i60	1.79E+08
i13 – i12	9.18E+09	i33 – i32	7.34E+09	i50 – p28	2.05E+08	i53 – i66	4.35E+12	i31 – i90	8.17E+08
i13 – p1	7.88E+11	i31 – i33	6.43E+07	i55 – i60	4.27E+07	i66 – i53	3.26E+09	i90 – i31	1.07E+10
i19 – i21	9.42E+12	i33 – i31	7.00E+08	i60 – i55	4.12E+06	i3 – i74	3.19E+07	i90 – i91	7.57E+12
i21 – i19	9.59E+12	i33 – i34	1.03E+13	i55 – p14	1.05E+11	i74 – i3	2.04E+09	i91 – i90	9.72E+11

i17 – i22	1.35E+10	i34 – i33	9.33E+12	i55 – i63	7.85E+08	i4 – i79	3.41E+07	i90 – i95	7.61E+07
i22 – i17	2.30E+10	i34 – p15	4.42E+10	i63 – i55	1.24E+09	i79 – i4	3.76E+09	i95 – i90	1.33E+07
i1 – i8	1.34E+10	i33 – i35	4.36E+12	i22 – i63	9.86E+12	i74 – i79	2.09E+12	i86 – i89	3.58E+10
i8 – i1	1.84E+04	i35 – i33	5.17E+12	i63 – i22	1.17E+13	i79 – i74	2.25E+12	i89 – i86	1.66E+04
i8 – p3	8.23E+09	i35 – i36	1.91E+14	i58 – i59	1.55E+12	i66 – i71	2.10E+07	i32 – i86	8.27E+04
i6 – i24	4.10E+05	i36 – i35	6.57E+13	i59 – i58	2.24E+12	i71 – i66	1.44E+08	i86 – i32	1.29E+12
i24 – i6	2.65E+08	i36 – p15	3.92E+10	i46 – i66	5.10E+11	i67 – i68	3.79E+12	i86 – i91	2.09E+11
i10 – i21	2.12E+12	i11 – i36	3.02E+03	i66 – i46	1.02E+04	i68 – i67	3.41E+12	i91 – i86	3.82E+04
i21 – i10	3.04E+12	i36 – i11	7.36E+02	i14 – i50	1.81E+10	i23 – i66	4.78E+10	i8 – i95	4.63E+11
i12 – i21	2.32E+12	i36 – i37	6.67E+10	i50 – i14	2.47E+12	i66 – i23	1.83E+08	i95 – i8	1.62E+12
i21 – i12	2.54E+12	i37 – i36	6.89E+11	i52 – i54	4.33E+07	i68 – i70	1.91E+10	i45 – i95	1.15E+12
i15 – p8	4.34E+10	i37 – p11	4.30E+08	i54 – i52	1.17E+08	i70 – i68	9.47E+09	i95 – i45	4.21E+12
i6 – i9	1.76E+07	i37 – p16	8.32E+06	i42 – i69	1.65E+08	i29 – i70	1.80E+09	i95 – p24	1.55E+11
i9 – i6	3.53E+09	i37 – i38	7.45E+11	i69 – i42	1.65E+08	i70 – i29	4.93E+08	i85 – i90	4.79E+12
i25 – i26	2.68E+12	i38 – i37	1.14E+12	i4 – i78	3.39E+07	i28 – i70	3.25E+09	i90 – i85	2.83E+11
i26 – i25	2.59E+12	i38 – p6	1.39E+09	i78 – i4	3.73E+09	i70 – i28	1.05E+09	i84 – p28	5.97E+08
i16 – i18	3.87E+06	i17 – i38	2.60E+07	i47 – i50	7.03E+12	i9 – i60	1.09E+08	i91 – p38	1.80E+10
i18 – i16	1.10E+06	i38 – i17	2.43E+07	i50 – i47	2.31E+09	i60 – i9	1.28E+07	i92 – p2	4.44E+10
i24 – i28	7.88E+07	i5 – i17	2.14E+09	i3 – i72	3.19E+07	i58 – i62	4.76E+10	i87 – i88	8.21E+11
i28 – i24	1.03E+07	i17 – i5	5.61E+11	i72 – i3	4.07E+09	i62 – i58	1.66E+12	i88 – i87	2.22E+03
i8 – i9	5.05E+09	i4 – i28	4.06E+09	i10 – i77	9.42E+12	i46 – i50	2.11E+12	i86 – i88	1.18E+11
i9 – i8	3.07E+11	i28 – i4	9.71E+11	i77 – i10	1.04E+13	i50 – i46	1.92E+08	i88 – i86	8.79E+02
i18 – i19	3.29E+12	i5 – i25	2.05E+08	i72 – i78	2.10E+12	i2 – i56	3.52E+08	i89 – p8	9.32E+10
i19 – i18	3.29E+12	i25 – i5	5.53E+10	i78 – i72	2.26E+12	i56 – i2	1.96E+08	i80 – i81	3.82E+12
i17 – i25	8.38E+08	i6 – i25	1.16E+05	i72 – i77	2.14E+09	i60 – i66	1.15E+11	i81 – i80	1.26E+13
i25 – i17	8.64E+08	i25 – i6	4.56E+07	i77 – i72	2.69E+09	i66 – i60	3.30E+08	i83 – i88	9.99E+09
i24 – i26	2.30E+10	i5 – i16	7.73E+05	i54 – i55	3.51E+12	i57 – i58	1.76E+12	i88 – i83	9.79E+08
i26 – i24	1.35E+10	i16 – i5	2.16E+08	i55 – i54	3.51E+12	i58 – i57	1.61E+12	i80 – i82	2.40E+12

i15 – i16	3.58E+05	i17 – i39	2.60E+12	i31 – i48	1.45E+09	i59 – i62	6.87E+10	i82 – i80	7.91E+12
i16 – i15	1.44E+07	i39 – i17	2.68E+12	i48 – i31	4.90E+10	i62 – i59	1.66E+12	i82 – i87	1.42E+08
i28 – p13	5.86E+09	i39 – i40	1.20E+11	i31 – i49	1.36E+09	i47 – i49	2.73E+12	i87 – i82	4.02E+12
i17 – p5	7.46E+08	i40 – i39	5.36E+11	i49 – i31	4.97E+10	i49 – i47	5.40E+08	i91 – i92	6.06E+12
i15 – i31	5.66E+11	i25 – i40	1.20E+11	i27 – i60	9.51E+08	i46 – i51	2.11E+12	i92 – i91	1.27E+13
i31 – i15	5.67E+11	i40 – i25	5.37E+11	i60 – i27	1.94E+08	i51 – i46	1.91E+08	i15 – i88	8.93E+08
i1 – i7	3.88E+09	i28 – i41	6.36E+08	i59 – p26	2.30E+09	i72 – i73	2.83E+12	i88 – i15	1.22E+08
i7 – i1	2.52E+05	i41 – i28	5.92E+08	i48 – p16	2.52E+08	i73 – i72	2.80E+12	i88 – p8	4.46E+09
i3 – i15	6.97E+07	i23 – i41	1.55E+09	i49 – p16	3.17E+08	i72 – p4	1.74E+11	i88 – p10	3.46E+08
i15 – i3	1.24E+09	i41 – i23	6.93E+09	i48 – p5	1.24E+09	i74 – i76	3.05E+12	i3 – i92	4.51E+07
i16 – p6	3.03E+09	i23 – i42	1.07E+08	i49 – p26	1.35E+09	i76 – i74	2.79E+12	i92 – i3	2.83E+09
i22 – i24	2.85E+12	i42 – i23	2.10E+11	i16 – i60	7.82E+08	i76 – p36	1.51E+11	i32 – i92	1.61E+08
i24 – i22	2.85E+12	i17 – p18	1.90E+09	i60 – i16	1.81E+08	i78 – p7	1.17E+11	i92 – i32	9.61E+08
i7 – i16	4.02E+12	i25 – p18	1.81E+09	i60 – p26	3.82E+08	i79 – p7	1.17E+11	i92 – p8	1.25E+11
i16 – i7	2.63E+12	i40 – p20	4.98E+07	i60 – p5	3.61E+08	i78 – i79	2.81E+12	i84 – i93	3.44E+12
i2 – i4	4.88E+11	i42 – p17	1.17E+01	i61 – i62	1.09E+13	i79 – i78	2.81E+12	i93 – i84	2.79E+11
i4 – i2	5.47E+08	i29 – p19	2.44E+10	i62 – i61	1.09E+13	i72 – i74	9.67E+08	i85 – p28	5.97E+08
i26 – p5	7.46E+08	i28 – i43	9.09E+10	i60 – i61	2.21E+08	i74 – i72	9.66E+08	i94 – p23	2.15E+11
i4 – i11	2.54E+02	i43 – i28	1.17E+12	i61 – i60	8.01E+10	i77 – p37	1.32E+12	i85 – i93	3.52E+12
i11 – i4	6.57E+04	i42 – i43	1.08E+07	i62 – p25	7.29E+07	i65 – p28	1.37E+09	i93 – i85	2.86E+11
i7 – p11	2.13E+09	i43 – i42	1.71E+05	i46 – i48	8.98E+13	i57 – p31	2.89E+09	i66 – i94	8.54E+06
i2 – i7	1.08E+13	i43 – p21	7.52E+08	i48 – i46	4.54E+09	i63 – p22	6.80E+10	i94 – i66	1.14E+10
i7 – i2	1.06E+13	i22 – p22	5.72E+10	i69 – p17	1.16E+01	i45 – i55	3.59E+10	i93 – i94	4.34E+12
i16 – i17	6.36E+12	i14 – p3	1.07E+10	i23 – i69	1.58E+08	i55 – i45	2.76E+12	i94 – i93	4.32E+12
i17 – i16	1.19E+13	i15 – p23	3.52E+11	i69 – i23	3.07E+11	i82 – i85	1.98E+08	i49 – i94	1.51E+07
i4 – i15	6.94E+07	i31 – p23	3.53E+11	i52 – i69	2.08E+08	i85 – i82	2.47E+07	i94 – i49	7.43E+06
i15 – i4	9.89E+08	i45 – p24	5.78E+10	i69 – i52	7.91E+10	i81 – i82	3.42E+12	i93 – i97	2.55E+10
i15 – p10	7.09E+08	i31 – i44	7.61E+07	i71 – p35	2.02E+09	i82 – i81	3.42E+12	i97 – i93	2.86E+09

i23 – p13	1.14E+10	i44 – i31	8.91E+08	i66 – p33	2.17E+08	i81 – p39	7.07E+09	i94 – p38	6.44E+10
i1 – i23	1.97E+10	i30 – i44	3.50E+12	i47 – i51	7.03E+12	i81 – p28	3.56E+11	i93 – p38	7.19E+10
i23 – i1	7.26E+04	i44 – i30	3.91E+12	i51 – i47	2.31E+09	i82 – p39	7.46E+09	i97 – p12	8.69E+06
i4 – i14	4.67E+09	i30 – i36	2.06E+09	i70 – p12	1.86E+07	i81 – i84	1.98E+08	i15 – i90	8.17E+08
i14 – i4	2.96E+10	i36 – i30	8.71E+08	i60 – i64	5.02E+00	i84 – i81	2.47E+07	i90 – i15	1.07E+10
i3 – i7	5.63E+08	i34 – i36	4.38E+12	i64 – i60	3.88E+08	i81 – i86	2.40E+08	i31 – i89	2.30E+08
i7 – i3	6.19E+11	i36 – i34	1.96E+12	i68 – p30	3.25E+10	i86 – i81	2.48E+12	i89 – i31	9.83E+08
i24 – p14	1.83E+10	i8 – i45	1.24E+12	i50 – i65	1.37E+08	i82 – i86	2.40E+08	i68 – i93	1.70E+10
i22 – p14	1.83E+10	i45 – i8	1.19E+12	i65 – i50	3.95E+07	i86 – i82	2.48E+12	i93 – i68	2.82E+10
i10 – p4	1.79E+10	i30 – i38	2.25E+11	i52 – i66	4.36E+12	i82 – p28	3.56E+11	i70 – i97	6.57E+08
i14 – i15	5.93E+07	i38 – i30	1.52E+12	i66 – i52	3.26E+09	i8 – i83	4.26E+03	i97 – i70	4.91E+08
i15 – i14	1.33E+08	i14 – i32	2.52E+12	i55 – i56	6.27E+12	i83 – i8	4.54E+03	i70 – i89	6.95E+09
i14 – p10	3.31E+08	i32 – i14	3.36E+12	i56 – i55	4.52E+12	i84 – i90	4.79E+12	i89 – i70	5.51E+09
i8 – i14	2.71E+09	i48 – i49 (H migration)	6.34E+07	i56 – p27	3.44E+08	i90 – i84	2.83E+11	i93 – p23	3.60E+11
i14 – i8	9.19E+08	i49 – i48 (H migration)	6.84E+07	i73 – p33	9.28E+10	i71 – i94	1.85E+07	i80 – p40	3.15E+09
i14 – p9	5.11E+10	i49 – i59	2.23E+08	i65 – i71	1.66E+12	i94 – i71	3.59E+09	i87 – p41-m1	1.85E+08
i25 – i27	1.18E+13	i59 – i49	1.71E+09	i71 – i65	8.80E+09	i83 – i89	5.12E+08	i88 – p41-m3	2.49E+05
i27 – i25	6.93E+12	i25 – i59	4.82E+07	i74 – i75	2.83E+12	i89 – i83	1.57E+09		
i27 – p6	3.60E+08	i59 – i25	1.74E+08	i75 – i74	2.75E+12	i36 – i89	8.79E+09		
i12 – p7	2.63E+10	i48 – i49 (rotation)	1.44E+12	i53 – i55	4.32E+07	i89 – i36	8.47E+09		

Table S4. Optimized Cartesian coordinates (in Å) and vibrational frequencies (in cm⁻¹) for all intermediates, transition states, reactants and products involved in the reactions of the methylidyne radical (CH) with dimethylacetylene (C₄H₆).

REACTANTS

Dimethylacetylene

C	-2.059168	-0.000411	0.000660
C	2.059183	-0.000403	0.000751
C	-0.600111	0.000929	-0.001496
C	0.600115	0.000883	-0.001473
H	-2.450766	1.017148	0.077127
H	-2.446784	-0.575349	0.845508
H	-2.451488	-0.444911	-0.917541
H	2.447402	-0.608870	0.821503
H	2.450351	1.013433	0.117545
H	2.451166	-0.407441	-0.934792

Frequencies

38.5950	199.0324	203.9345
400.8499	403.5262	732.0566
1047.9024	1053.1779	1065.2435
1070.8293	1181.4229	1419.9700
1421.0935	1484.5450	1485.1242
1489.7294	1490.2396	2401.6063
3049.6017	3050.7480	3119.0774
3121.5281	3122.7545	3123.7558

Methylidyne

C	0.000000	0.000000	0.160978
H	0.000000	0.000000	-0.965870

Frequencies

2831.0403

INTERMEDIATES

i80

C	1.938957	-0.612906	0.020057
C	-1.938954	-0.612910	0.020058
C	0.656313	0.113077	-0.021602
C	-0.656312	0.113074	-0.021619
C	-0.000001	1.413368	-0.123492
H	2.523444	-0.380566	-0.875569
H	1.793102	-1.693088	0.077877
H	2.530273	-0.287645	0.881047
H	-1.793099	-1.693091	0.077904
H	-2.523447	-0.380594	-0.875569
H	-2.530265	-0.287627	0.881044
H	-0.000030	2.240394	0.592853

Frequencies

96.4075	108.5116	204.4395
231.9117	401.0601	438.2794
681.7737	740.5535	950.6628
958.7421	1017.7644	1052.6412
1056.2825	1098.7978	1235.5556
1263.3868	1405.3690	1410.1711
1478.4611	1478.9120	1485.6533
1487.8892	1920.1049	3040.5230
3041.9158	3050.3284	3105.3928
3105.4656	3136.3741	3137.2389

i81

C	-1.923335	-0.602092	0.051633
C	1.900148	-0.599807	0.122872
C	-0.671204	0.168594	-0.057833
C	0.734009	0.154598	-0.441593
C	-0.017391	1.296930	0.089293
H	-1.794434	-1.428714	0.756273
H	-2.167938	-1.044099	-0.918764
H	-2.756256	0.020235	0.382839
H	1.967823	-1.600570	-0.311675
H	1.811743	-0.710846	1.215300
H	2.839691	-0.081337	-0.084202
H	-0.033988	2.335994	0.373997

Frequencies

136.4426	170.8719	178.9088
293.9342	388.0041	457.8550
660.9666	736.3642	806.7218
960.1977	989.0122	1035.0171
1062.2962	1082.3898	1134.4843
1363.7424	1399.7315	1402.9593
1479.3768	1481.8297	1484.5311
1496.4449	1821.1988	2974.2967
3048.9306	3085.2766	3115.8663
3122.3244	3141.7100	3275.8639

i82

C	-1.900134	-0.599815	0.122885
C	1.923331	-0.602087	0.051648
C	-0.734019	0.154603	-0.441609
C	0.671210	0.168604	-0.057875
C	0.017390	1.296936	0.089250
H	-1.811728	-0.710829	1.215316
H	-1.967792	-1.600588	-0.311639
H	-2.839689	-0.081368	-0.084197
H	2.167999	-1.044095	-0.918733
H	1.794382	-1.428712	0.756278
H	2.756236	0.020232	0.382911
H	0.033920	2.335916	0.374265

Frequencies

136.4177	170.8596	178.8979
293.9072	387.9908	457.8536
660.9975	736.3054	806.7261
960.2035	989.0103	1035.0146
1062.2951	1082.3887	1134.4779
1363.7475	1399.7313	1402.9612
1479.3733	1481.8278	1484.5303
1496.4423	1821.1988	2974.2885
3048.9302	3085.2758	3115.8623
3122.3243	3141.7092	3275.8663

C	2.588469	0.203053	-0.007504
C	-1.459275	-0.576104	0.011510
C	1.156601	-0.076450	0.000440
C	-0.021082	-0.308085	0.004496
C	-2.306234	0.653564	-0.014939
H	2.773665	1.276275	-0.097660
H	3.077730	-0.295207	-0.848207
H	3.059986	-0.145860	0.914527
H	-1.709995	-1.221823	-0.841878
H	-3.378669	0.560934	-0.133158
H	-1.702166	-1.181186	0.899783
H	-1.871421	1.630997	0.142573

Frequencies

41.3318	140.1861	161.9694
192.8957	321.7366	385.9520
454.7314	528.2636	709.0301
870.0121	986.1497	1062.3617
1064.7596	1098.3255	1178.0395
1208.2426	1364.4472	1427.7596
1450.5430	1461.0432	1485.7941
1490.1635	2399.7392	2978.0023
3018.1586	3050.8183	3121.4941
3125.1437	3164.4294	3282.3616

C	1.872436	-0.572995	-0.034298
C	-1.770965	-0.702559	-0.258221
C	0.630689	0.217418	0.048504
C	-0.832056	0.118396	0.489109
C	-0.079105	1.262090	-0.191586
H	1.679604	-1.516298	-0.552342
H	2.233415	-0.820314	0.968078
H	2.655671	-0.029529	-0.566884
H	-2.609729	-1.183358	0.230010
H	-1.642208	-0.840822	-1.326282
H	-0.198977	2.238980	-0.628513
H	-1.043769	0.217238	1.554877

Frequencies

156.8605	182.5775	268.9377
317.8650	400.5507	475.7529
540.7029	652.5528	754.0999
853.3243	957.7569	1002.2260
1031.6624	1071.5608	1086.5472
1133.2455	1160.9174	1380.2014
1405.6493	1475.7620	1480.7924
1488.0145	1892.5903	3049.0652
3095.6496	3120.1462	3134.1650
3152.0360	3260.3075	3279.8424

i85

C	-1.872348	-0.573034	-0.034294
C	1.770821	-0.702665	-0.258227
C	-0.630736	0.217569	0.048708
C	0.832077	0.118475	0.489110
C	0.079149	1.262104	-0.191708
H	-2.656105	-0.029069	-0.565598
H	-2.232552	-0.821940	0.967963
H	-1.679561	-1.515538	-0.553825
H	2.609504	-1.183613	0.229995
H	1.043917	0.217434	1.554839
H	1.641993	-0.840969	-1.326274
H	0.199027	2.238994	-0.628632

Frequencies

156.7434	182.5609	268.8837
317.8311	400.5631	475.7355
540.7094	652.5541	754.0927
853.3279	957.7528	1002.2307
1031.5566	1071.5493	1086.5218
1133.2474	1160.8991	1380.1823
1405.5774	1475.7648	1480.8273
1487.8963	1892.5987	3049.0686
3095.6704	3120.1673	3134.1433
3152.0288	3260.2951	3279.8482

C	2.210892	-0.486615	0.034935
C	-2.309830	-0.268452	0.086109
C	1.247383	0.613786	0.065763
C	-0.870611	-0.400674	-0.243617
C	-0.079059	0.768324	-0.069523
H	1.727200	-1.380573	-0.378450
H	2.565954	-0.714962	1.044415
H	3.083163	-0.221015	-0.569517
H	-2.416599	-0.669784	1.106038
H	-2.935672	-0.905412	-0.544752
H	-2.704468	0.759932	0.097221
H	-0.512232	1.773603	0.003048

Frequencies

74.5545	140.3806	176.0259
185.5889	303.8316	325.9720
491.0970	782.8779	822.8975
911.0031	968.4418	1023.5168
1042.9031	1056.2311	1194.2757
1332.8714	1365.4044	1376.8367
1432.8849	1448.4277	1457.7345
1494.9569	1603.1926	2969.3693
3017.9341	3039.9505	3043.4633
3097.0198	3101.6396	3112.9489

i87

C	-2.495315	0.141922	0.157204
C	-1.229478	-0.550039	-0.172221
C	-0.038138	0.198916	-0.241934
C	2.558672	0.088382	0.121452
C	1.166490	-0.349211	-0.006876
H	-3.363991	-0.330318	-0.308577
H	-2.491829	1.220381	-0.068082
H	-2.638448	0.043903	1.243771
H	-0.072579	1.276997	-0.481350
H	2.911664	-0.017791	1.152079
H	2.667179	1.142441	-0.170650
H	3.214618	-0.515437	-0.512941

Frequencies

112.9644	133.3743	151.4345
186.3531	224.2796	305.4179
395.3276	796.9283	813.0922
887.5557	961.0689	1024.1527
1033.2977	1059.0378	1178.1074
1340.5013	1374.2058	1397.4519
1445.0748	1453.6351	1472.1900
1489.7090	1596.8036	2949.9258
2969.2541	3004.6303	3043.0581
3085.6328	3103.4860	3106.4511

C	-2.387969	-0.493377	-0.000207
C	-1.343104	0.576414	-0.003867
C	0.006215	0.315154	-0.001392
C	2.629167	-0.211522	0.000877
C	1.202085	0.073782	0.000107
H	-2.959600	-0.481632	0.936234
H	-1.941996	-1.482516	-0.112706
H	-3.109287	-0.343549	-0.811299
H	-1.665561	1.613059	0.013194
H	2.888380	-0.914057	0.798341
H	3.208459	0.702787	0.151980
H	2.941245	-0.656801	-0.948852

Frequencies

33.3046	111.6247	132.9129
172.3840	310.0667	394.5465
542.4777	569.1424	739.7339
988.1689	1007.6678	1032.6123
1052.8042	1116.1741	1228.9922
1403.5137	1409.5816	1426.0763
1477.5230	1482.9778	1483.9793
1504.8737	2175.0640	3021.5632
3041.6640	3074.8810	3105.5478
3122.1624	3134.6954	3175.3814

C	0.916517	-0.183495	0.057585
C	2.380372	-0.266578	0.011432
C	-1.483730	0.475223	0.049463
C	-2.081273	-0.711746	-0.027492
C	-0.035696	0.715315	-0.061844
H	-1.513520	-1.620471	-0.201101
H	2.713428	-0.938210	-0.785228
H	2.785585	-0.645412	0.954404
H	2.820281	0.724384	-0.172776
H	-2.093256	1.362592	0.200245
H	-3.155186	-0.807319	0.080904
H	0.265524	1.752121	-0.251302

Frequencies

84.3654	163.8946	179.6634
217.6285	340.1785	583.8300
639.5775	832.3564	884.9073
955.6068	1008.2429	1033.7587
1039.8682	1052.0397	1128.3151
1298.5525	1335.4396	1405.9317
1445.9623	1461.6675	1479.6023
1707.6884	1762.5697	2996.3288
3052.5417	3082.0655	3108.8109
3155.5567	3177.1154	3248.7659

C	1.101041	0.630241	-0.126088
C	1.828972	-0.622035	0.113970
C	-1.341697	0.319815	0.178540
C	-1.530547	-0.962494	-0.127918
C	-0.125127	1.108027	-0.105818
H	2.049997	-1.136420	-0.826292
H	1.229444	-1.297008	0.741538
H	2.780105	-0.437229	0.621718
H	-2.142162	0.862706	0.677347
H	-0.788089	-1.536348	-0.672537
H	-2.450314	-1.471140	0.136861
H	-0.274833	2.174117	-0.274748

Frequencies

109.5132	167.2764	220.0797
336.2614	398.6552	575.8181
687.4241	841.5823	880.3386
945.6014	979.5278	1033.0066
1041.9776	1046.3214	1096.5216
1320.0481	1332.2190	1398.6587
1448.1438	1467.8236	1480.0307
1702.1051	1756.2152	3000.8710
3084.6298	3108.7178	3128.6246
3149.6076	3164.1864	3249.8909

i91

C	2.239654	-0.432334	0.001094
C	1.209191	0.613841	0.000122
C	-0.100494	0.746435	-0.001583
C	-2.377324	-0.214680	0.001624
C	-1.054774	-0.369906	-0.002158
H	2.910278	-0.324749	-0.856226
H	1.790271	-1.434470	-0.047859
H	2.848846	-0.381264	0.908153
H	-0.533811	1.747096	-0.001029
H	-3.047809	-1.066003	0.001961
H	-0.634789	-1.372834	-0.004612
H	-2.830511	0.772086	0.005011

Frequencies

42.7754	110.3823	176.5115
346.1783	376.2599	574.9042
625.5330	854.4251	884.6132
942.4073	984.2407	1021.4725
1040.2872	1044.5935	1170.3997
1291.0111	1335.1606	1399.6031
1451.4367	1457.2887	1471.4311
1702.5745	1758.3824	3003.5401
3085.7523	3113.4985	3129.3218
3155.0618	3175.2311	3247.2101

i92

C	2.549886	0.055386	0.000031
C	1.127292	-0.304901	-0.000083
C	-0.051746	0.278970	0.000067
C	-2.518179	0.188597	0.000010
C	-1.334989	-0.422747	-0.000011
H	3.058355	-0.344846	-0.881851
H	3.057035	-0.340714	0.884551
H	2.673850	1.147931	-0.002559
H	-0.094866	1.374986	-0.000216
H	-3.444920	-0.372712	0.000010
H	-2.596487	1.271853	0.000062
H	-1.286556	-1.508325	-0.000079

Frequencies

112.9170	149.7832	171.2156
263.4613	403.8317	473.7675
633.1945	841.0025	896.7048
937.1749	999.3129	1029.6943
1048.3692	1062.1246	1186.8993
1262.7367	1322.0902	1402.2040
1453.6118	1454.4376	1481.2040
1706.6022	1769.4017	3003.0111
3050.9842	3089.2933	3115.5826
3152.7104	3179.7095	3246.0295

C	1.645657	-0.750616	0.145542
C	-2.029215	-0.027533	0.169551
C	0.448431	0.156695	-0.065852
C	-0.858745	-0.520980	-0.222419
C	0.571341	1.464974	-0.116695
H	2.574817	-0.184434	0.220481
H	1.735732	-1.454987	-0.687631
H	1.518512	-1.335037	1.061796
H	-2.951330	-0.575233	0.012298
H	-2.096052	0.937708	0.660693
H	-0.821779	-1.507954	-0.680391
H	1.375285	2.184701	-0.048007

Frequencies

102.9476	171.3000	261.6658
362.4635	386.4312	540.4884
673.3776	721.2705	798.6869
867.8243	977.0530	1013.4844
1027.9982	1044.9835	1090.8615
1197.8916	1330.8930	1400.1791
1447.8758	1485.0847	1486.5042
1683.9837	1720.0312	3044.0666
3111.4776	3146.0426	3151.6889
3164.2685	3250.3988	3251.4852

i94

C	0.794003	1.299876	0.000134
C	-1.931302	0.100145	-0.000043
C	0.542052	-0.194153	-0.000009
C	-0.849644	-0.676805	-0.000179
C	1.542854	-1.052011	0.000050
H	0.344637	1.760719	0.884756
H	0.344434	1.760920	-0.884278
H	1.861735	1.519858	0.000030
H	-2.924954	-0.332338	-0.000177
H	-1.868159	1.183011	0.000213
H	-0.968796	-1.756231	-0.000429
H	2.623323	-0.998253	0.000165

Frequencies

135.1928	197.2613	280.8033
389.1809	391.3011	536.1238
666.7864	724.0003	778.1526
879.1659	938.7602	993.8843
1027.9638	1043.8026	1088.5990
1264.1358	1334.1066	1406.5647
1453.2889	1482.3150	1494.1751
1665.8430	1718.8947	3048.6703
3116.9225	3149.0471	3163.8913
3185.4207	3246.6659	3253.7063

i95

C	-2.439656	0.281487	-0.196990
C	-1.237366	-0.061811	0.166466
C	-0.032468	-0.405582	0.521922
C	2.235543	0.527999	0.037026
C	1.163345	-0.408710	-0.403360
H	-3.144220	-0.453346	-0.573057
H	0.821255	-0.154356	-1.418132
H	-2.773251	1.312054	-0.129131
H	0.143057	-0.693252	1.556321
H	3.273496	0.338343	-0.208031
H	1.976830	1.476667	0.492244
H	1.566439	-1.426408	-0.470591

Frequencies

74.1203	182.1761	206.0004
333.3492	342.9598	495.3017
561.7784	604.8186	782.7419
890.2142	905.6314	989.2762
1024.1559	1038.4601	1103.3377
1154.1011	1201.9159	1328.9280
1379.1120	1461.3347	1463.8863
1487.4654	2087.9895	2993.7538
3055.7199	3141.7405	3157.2439
3160.4227	3224.1807	3268.4395

C	2.284894	0.124550	-0.000092
C	-1.711186	-0.600572	-0.000184
C	0.952913	-0.498717	0.000147
C	-0.295872	-0.186584	0.000388
C	-1.345743	0.876463	-0.000029
H	2.201392	1.220077	-0.001809
H	2.859308	-0.173080	-0.881910
H	2.858455	-0.170434	0.883180
H	-2.116903	-1.021347	-0.914683
H	-2.117693	-1.021121	0.914074
H	-1.496852	1.437513	-0.916363
H	-1.497747	1.437549	0.916129

Frequencies

93.2360	155.2577	191.0862
347.7833	470.4091	675.2258
787.3538	841.8408	874.5650
970.5908	1043.4201	1047.5179
1052.6794	1077.8924	1080.2401
1180.2385	1197.3993	1400.8316
1453.1725	1463.1736	1476.1998
1486.7339	1894.7818	3005.8368
3084.9755	3108.5572	3125.0028
3133.7330	3208.3972	3227.1551

i97

C	1.948640	-0.000150	0.000652
C	-1.647498	0.002559	0.001561
C	0.456408	0.000734	-0.001820
C	-0.508371	-1.012973	-0.000799
C	-0.501715	1.011129	-0.000827
H	2.342396	1.012368	-0.106778
H	2.339068	-0.608759	-0.819189
H	2.335630	-0.419016	0.933820
H	-2.284265	0.004740	-0.889012
H	-2.280523	0.004784	0.894796
H	-0.475977	-2.094449	-0.003303
H	-0.461118	2.092543	-0.002936

Frequencies

38.1884	233.6603	332.2153
445.7019	527.0670	588.6913
686.1297	903.0309	935.8450
936.6754	972.5191	1034.5339
1056.1370	1092.2928	1186.8701
1199.2008	1246.6005	1279.7837
1409.1591	1473.9789	1488.7281
1495.3994	1605.6294	3045.6238
3051.6739	3090.1154	3118.1933
3138.1918	3229.2527	3236.5860

Complex 1

C	-1.581743	-1.105612	0.000221
C	-1.598323	0.344375	-0.000109
C	-1.263614	1.557588	-0.000098
H	-2.060317	-1.509236	-0.895077
H	-2.061583	-1.508860	0.895008
H	-0.533636	-1.429430	0.001005
C	1.957482	-0.021982	0.662875
C	1.957025	-0.022391	-0.663003
H	2.625759	-0.658580	1.234254
H	1.290383	0.627176	1.221614
H	2.624908	-0.659349	-1.234442
H	1.289524	0.626414	-1.221680

Frequencies

33.0399	78.2244	92.7184
98.7022	117.7460	170.4881
227.2217	350.2982	847.5458
876.4593	890.7781	950.4331
998.5441	1003.1656	1083.5226
1247.3201	1385.9001	1388.0736
1450.9153	1469.2861	1471.3605
1628.3415	1708.5207	3024.1223
3100.7184	3125.8270	3133.9813
3151.8671	3219.0317	3243.4602

TRANSITION STATES

i82 – i85

C	-1.925794	-0.600407	-0.044318
C	1.940346	-0.631564	-0.155049
C	-0.677774	0.178850	0.030639
C	0.763113	0.118905	0.304448
C	-0.024523	1.302668	-0.087407
H	-2.777570	0.027407	-0.310404
H	-2.120644	-1.078805	0.920240
H	-1.825257	-1.397460	-0.786304
H	1.834257	-1.684187	-0.397936
H	1.667584	-0.346308	1.135910
H	2.796249	-0.086798	-0.539216
H	-0.026834	2.355435	-0.312165

Frequencies

-2079.3846	147.8471	184.9303
230.8152	322.2704	407.9679
481.8187	682.2694	737.1394
746.8551	844.8580	959.5373
1005.4933	1020.6636	1054.2025
1132.2827	1174.6072	1369.7615
1405.7561	1411.0202	1483.3332
1490.9221	1841.6954	2128.0553
3045.6354	3112.5789	3122.7479
3140.1401	3245.3625	3290.5497

i81 – i82

C	1.960517	-0.585413	-0.104331
C	-1.960516	-0.585414	-0.104331
C	0.759279	0.178448	0.309741
C	-0.759278	0.178446	0.309742
C	-0.000001	1.237350	-0.092179
H	1.789021	-1.118652	-1.050648
H	2.238282	-1.334644	0.641758
H	2.811628	0.085252	-0.249417
H	-2.238254	-1.334676	0.641736
H	-1.789038	-1.118613	-1.050674
H	-2.811638	0.085247	-0.249370
H	-0.000003	2.195584	-0.595240

Frequencies

-787.2139	139.1552	147.8147
173.3081	257.2232	376.4617
595.2780	677.2884	907.5540
972.0971	997.5025	1016.4449
1054.9785	1089.2983	1186.1287
1297.6510	1398.6074	1407.0450
1472.3633	1475.1218	1498.0989
1499.0855	1718.3542	2991.3200
3000.8975	3079.4560	3080.9740
3121.1739	3121.6979	3231.4092

i81 – p39

C	-1.784003	-0.922607	0.066882
C	-0.807085	0.173452	-0.068270
C	0.374057	0.621680	-0.727221
C	-0.318165	1.354430	0.272254
H	-1.273967	-1.777880	0.518620
H	-2.118533	-1.237480	-0.923147
H	-2.640785	-0.651466	0.682625
H	-0.368737	2.252411	0.869168
C	2.368771	-0.641981	0.163503
H	2.581826	-1.159589	-0.757777
H	1.881803	-1.179769	0.965434
H	2.936938	0.243935	0.402190

Frequencies

-253.4621	65.3329	98.5887
144.5760	154.2524	327.6000
363.7157	370.0093	393.3509
639.2629	774.4011	888.9817
938.2535	1023.3485	1038.9539
1214.8994	1311.5893	1395.6710
1416.1241	1428.7971	1479.0272
1487.8426	1818.7587	3060.0701
3128.7567	3133.5124	3162.1701
3254.6344	3303.4536	3317.7897

i81 – p28

C	1.947945	-0.597032	-0.011167
C	-1.901649	-0.543712	0.261978
C	0.681268	0.155692	0.011728
C	-0.751806	0.108959	0.122006
C	0.030619	1.300119	-0.052091
H	1.918544	-1.344899	-0.807843
H	2.073022	-1.135307	0.932262
H	2.804449	0.060467	-0.165027
H	-1.916116	-1.620367	0.374424
H	-2.143365	-0.862777	-2.447468
H	-2.844484	-0.012426	0.283076
H	0.069688	2.371155	-0.164146

Frequencies

-195.9566	70.3114	86.3222
144.2539	206.6852	278.8007
440.5560	525.7798	720.8333
724.6121	779.6828	813.8848
849.9803	997.5379	1045.6420
1056.0241	1094.8771	1217.7084
1408.0015	1451.6213	1480.9402
1486.5331	1688.7281	1895.0474
3057.9540	3126.6094	3153.4991
3167.3402	3257.8608	3283.9445

i82 – p39

C	-2.362946	-0.643373	0.163500
C	1.779592	-0.924234	0.068752
C	-0.373265	0.623059	-0.728733
C	0.804519	0.173679	-0.064421
C	0.316667	1.356067	0.272273
H	-1.874307	-1.175776	0.968072
H	-2.577261	-1.167227	-0.753993
H	-2.933331	0.242156	0.398360
H	2.231230	-1.118925	-0.906412
H	1.241794	-1.831229	0.356154
H	2.558930	-0.714166	0.800189
H	0.365543	2.253976	0.869407

Frequencies

-255.7433	64.6050	92.7291
145.1204	154.0744	326.8084
366.0513	370.8822	391.6487
642.8975	774.7164	890.1775
938.7114	1019.1058	1038.5520
1215.2500	1310.6569	1394.9185
1416.5281	1428.6568	1479.3407
1484.8093	1819.1108	3058.8936
3130.4955	3133.6127	3153.2331
3255.3672	3303.7199	3317.3327

i81 – i84

C	-1.925752	-0.600440	0.044312
C	1.940318	-0.631594	0.155041
C	-0.677763	0.178870	-0.030630
C	0.763108	0.118953	-0.304444
C	-0.024539	1.302704	0.087428
H	-1.824985	-1.397875	0.785853
H	-2.120878	-1.078345	-0.920436
H	-2.777460	0.027231	0.310951
H	1.834098	-1.684173	0.398061
H	2.796312	-0.086865	0.539076
H	-0.026868	2.355479	0.312141
H	1.667553	-0.346409	-1.135886

Frequencies

-2079.3765	147.8382	184.7418
230.8325	322.2668	407.9838
481.8158	682.2775	737.1817
746.8411	844.8638	959.5495
1005.4819	1020.6790	1054.1846
1132.2898	1174.6310	1369.7439
1405.7444	1411.0024	1483.3257
1490.8792	1841.6973	2128.0876
3045.6439	3112.5975	3122.7186
3140.1425	3245.3397	3290.5655

i81 – i86

C	-2.135777	-0.515866	0.012867
C	-1.141793	0.543734	0.196630
C	0.113939	0.916012	-0.123731
H	-2.218307	-1.126318	0.916211
H	-1.856277	-1.169318	-0.819719
H	-3.119512	-0.070820	-0.171390
H	0.515794	1.919516	0.052442
C	2.204833	-0.372279	0.116552
C	0.789345	-0.282011	-0.334635
H	2.783784	-1.062245	-0.502680
H	2.182527	-0.821509	1.119164
H	2.728712	0.593157	0.199868

Frequencies

-318.5499	149.1400	155.3397
195.3914	210.5099	299.9865
462.7632	834.0493	875.7797
918.2889	972.5632	1026.1465
1034.6766	1053.4628	1196.3989
1358.3144	1365.3713	1390.0574
1446.7861	1451.4717	1463.8714
1494.6322	1608.4298	2971.2210
3025.8836	3054.9854	3061.0015
3100.8434	3106.8961	3116.4659

i82 – i86

C	-2.135776	-0.515860	-0.012868
C	2.204831	-0.372269	-0.116553
C	-1.141789	0.543737	-0.196631
C	0.789339	-0.282029	0.334627
C	0.113940	0.916006	0.123738
H	-1.856267	-1.169321	0.819709
H	-2.218319	-1.126302	-0.916217
H	-3.119507	-0.070811	0.171404
H	2.182539	-0.821578	-1.119129
H	2.783798	-1.062177	0.502730
H	2.728682	0.593177	-0.199938
H	0.515807	1.919505	-0.052437

Frequencies

-318.5405	149.2195	155.3381
195.3945	210.5099	299.9961
462.7729	834.0556	875.7886
918.2981	972.5665	1026.1464
1034.6793	1053.4703	1196.3946
1358.3070	1365.3723	1390.0567
1446.7958	1451.4708	1463.8704
1494.6396	1608.4372	2971.2160
3025.8855	3054.9816	3061.0014
3100.8457	3106.8894	3116.4707

i82 – p28

C	-1.901649	-0.543666	-0.262091
C	1.947939	-0.597044	0.011143
C	-0.751809	0.108978	-0.122031
C	0.681269	0.155694	-0.011723
C	0.030631	1.300121	0.052165
H	-2.143381	-0.863181	2.448171
H	-1.916128	-1.620314	-0.374600
H	-2.844481	-0.012371	-0.283154
H	2.073031	-1.135258	-0.932319
H	1.918519	-1.344964	0.807768
H	2.804446	0.060438	0.165064
H	0.069715	2.371149	0.164291

Frequencies

-194.2612	70.1932	86.2281
144.3041	206.6849	278.7984
440.5552	525.7820	720.8285
724.6039	779.6739	813.8916
849.9791	997.5361	1045.6430
1056.0277	1094.8740	1217.7010
1408.0037	1451.6205	1480.9418
1486.5411	1688.7580	1895.0603
3057.9505	3126.6053	3153.4928
3167.3353	3257.8511	3283.9417

i8 – i83

C	2.466791	0.296288	0.000026
C	-1.484635	-0.597755	0.000036
C	1.101884	0.048526	0.000007
C	0.004508	-0.563502	-0.000094
C	-2.037518	0.789446	0.000015
H	2.984689	0.442114	-0.935924
H	1.498425	-1.093092	-0.000235
H	2.984744	0.441557	0.936034
H	-1.815508	-1.160637	-0.876538
H	-1.815316	-1.160535	0.876749
H	-2.071710	1.346227	-0.926765
H	-2.071507	1.346342	0.926732

Frequencies

-1723.1898	108.0324	108.0883
182.8253	235.2459	347.2736
371.8228	378.3199	571.6392
590.3650	615.7496	771.5836
777.8275	1035.7937	1071.6256
1089.4776	1262.3789	1285.7583
1294.1694	1445.6224	1458.0815
1471.8362	2102.2961	2501.0426
3066.8342	3108.2788	3162.8527
3183.7064	3272.9078	3291.5776

i84 – i90

C	2.058381	-0.511070	-0.014359
C	-1.902115	-0.661744	-0.250537
C	0.767156	0.178118	0.062947
C	-1.066695	0.186248	0.451748
C	-0.084923	1.106225	-0.193941
H	1.934706	-1.490903	-0.483583
H	2.477571	-0.672155	0.982257
H	2.780009	0.064823	-0.606905
H	-2.602747	-1.305471	0.267705
H	-1.838076	-0.741436	-1.330155
H	-1.216213	0.289460	1.523123
H	-0.166079	2.069023	-0.687595

Frequencies

-604.4366	164.4482	176.3126
233.6358	316.8662	438.9144
524.2403	735.5890	777.2819
870.1500	912.5010	971.2717
1034.2333	1061.0378	1099.0210
1169.2586	1268.0764	1390.6828
1405.3620	1475.9867	1482.3900
1505.0358	1881.6683	3020.0798
3094.9198	3115.8800	3153.5609
3161.4707	3171.2704	3257.1198

i71 – i94

C	1.308079	-1.172477	0.000015
C	-2.031242	-0.318978	-0.000133
C	0.554335	0.112127	0.000070
C	-0.884864	0.337067	0.000322
C	0.914272	1.397829	-0.000164
H	1.046341	-1.765717	-0.881187
H	1.047078	-1.765339	0.881689
H	2.385986	-1.003123	-0.000475
H	-2.986282	0.191925	-0.000029
H	-2.043138	-1.408069	-0.000586
H	-0.460423	1.660470	0.000237
H	1.846959	1.956450	-0.000309

Frequencies

-2264.9419	95.2213	187.9549
209.6731	361.6812	432.8048
619.0166	647.2719	728.9903
776.3053	867.0785	961.9654
996.0440	1021.4205	1057.0635
1060.7516	1277.0651	1415.2315
1428.7371	1478.3752	1485.3994
1676.0634	1744.6266	1954.8668
3044.3782	3108.4375	3125.0355
3143.8132	3180.6991	3235.4852

i83 – i89

C	-1.162261	-0.022176	-0.168912
C	-2.590474	0.178367	0.038406
C	1.460250	-0.473490	-0.054249
C	2.411447	0.521704	-0.005070
C	0.034471	-0.266908	-0.021003
H	-2.866552	1.211166	-0.190531
H	-2.886081	-0.028500	1.073852
H	-3.174912	-0.471401	-0.618312
H	1.764365	-1.502164	-0.227265
H	2.131605	1.563194	0.086224
H	3.461754	0.263875	0.013662
H	0.649223	-0.661152	1.127336

Frequencies

-1821.0862	124.5911	135.1057
136.6962	317.2670	403.9089
536.6204	618.2042	669.0156
720.4182	741.8215	1017.9353
1034.4300	1045.8949	1064.2119
1176.6146	1258.3214	1406.2796
1422.1256	1453.4828	1482.3325
1485.9728	1572.7181	2181.3518
3023.5104	3092.7858	3117.3777
3171.8319	3178.4546	3277.2950

i36 – i89

C	-0.706900	-0.095016	-0.000011
C	-2.174466	-0.248559	0.000003
C	1.561985	0.422060	0.000000
C	1.620308	-0.899611	0.000003
C	0.154005	0.911995	-0.000002
H	0.234649	-1.105101	-0.000012
H	-2.513047	-0.801701	0.881594
H	-2.513084	-0.801578	-0.881650
H	-2.668497	0.730015	0.000084
H	2.418682	1.088987	-0.000002
H	2.425633	-1.620249	0.000011
H	-0.113927	1.964420	0.000018

Frequencies

-2060.9420	132.3661	217.4045
267.0726	392.4531	555.5581
629.4122	724.0909	823.4333
930.1316	937.6118	947.8797
1015.8617	1019.3698	1092.3509
1116.4643	1218.6673	1294.6029
1407.3332	1462.5541	1483.1962
1636.7561	1723.4016	1758.8280
3025.5030	3098.4875	3101.3438
3174.2439	3188.7912	3260.9412

i15 – i89

C	-1.033506	0.079658	0.428107
C	-2.419202	0.211477	-0.127161
C	1.451671	-0.498680	-0.032685
C	2.273133	0.567494	-0.003468
C	0.040017	-0.392522	-0.200479
H	-2.525742	1.259677	-0.424474
H	-3.178096	0.018969	0.632475
H	-2.602804	-0.409515	-1.010957
H	1.871408	-1.499728	-0.068630
H	1.882925	1.578868	0.002609
H	3.348328	0.440059	-0.014376
H	-0.668699	-1.192895	0.497465

Frequencies

-965.8275	51.6969	136.8599
165.6245	240.1292	410.1363
528.4591	637.4435	782.6766
862.8248	904.9471	976.4441
1026.9826	1069.7693	1121.1979
1194.0599	1311.7106	1394.0478
1428.9935	1464.5407	1488.9364
1595.2549	1700.1023	2268.3850
3028.7728	3110.4613	3134.7443
3164.7416	3184.0290	3262.7706

i4 – i89

C	0.962819	-0.151652	-0.283513
C	2.303076	-0.237245	0.126979
C	-1.417411	0.484993	0.074929
C	-1.984731	-0.728290	0.028943
C	-0.010399	0.775740	-0.118642
H	2.971095	-0.930144	-0.377514
H	1.371197	-1.106422	0.499450
H	2.759729	0.474530	0.820886
H	-2.049526	1.344381	0.285206
H	-1.403518	-1.612061	-0.214077
H	-3.045120	-0.858520	0.207980
H	0.276019	1.826951	-0.194108

Frequencies

-1757.2879	150.1007	184.0850
191.2384	331.3432	501.6636
633.3699	676.6425	825.1311
920.0648	929.9636	962.5691
1029.0351	1043.6460	1055.4201
1154.7638	1185.1644	1320.4222
1347.2377	1445.4600	1482.1984
1539.9076	1672.9561	2217.3213
3052.4049	3103.0769	3152.0274
3169.2527	3193.9654	3249.4836

i89 – i90

C	0.979153	0.301566	-0.024923
C	2.227064	-0.431279	0.033864
H	3.090634	0.219922	0.232462
H	2.413170	-0.943285	-0.915807
H	2.206353	-1.193812	0.822871
C	-1.502804	0.374437	0.058743
C	-1.796543	-0.920456	-0.030135
C	-0.146168	0.961161	-0.048954
H	-2.306235	1.089970	0.217847
H	-1.024962	-1.663690	-0.208448
H	-2.815464	-1.275072	0.070583
H	-0.127709	2.053392	-0.151085

Frequencies

-260.2377	53.0316	122.7424
229.1473	308.5608	552.4926
609.6095	819.7464	832.3586
945.1291	970.5220	992.6348
1033.6252	1040.3846	1098.1370
1310.9444	1337.6867	1406.1251
1438.9113	1462.8260	1474.6588
1706.5246	1835.4273	2986.0806
3025.4060	3041.5369	3092.6543
3147.7508	3166.8763	3244.6513

i83 – p8

C	-1.166823	-0.045653	-0.032870
C	-2.607332	0.161265	0.032861
C	1.436307	-0.421783	-0.166073
C	2.344302	0.559380	0.034526
C	0.022748	-0.211947	-0.079238
H	-2.863385	1.191189	-0.227487
H	-2.981082	-0.036625	1.040754
H	-3.127807	-0.505518	-0.658752
H	1.753756	-1.353788	-0.625208
H	1.598164	-1.452014	1.458612
H	2.045685	1.533542	0.402359
H	3.399451	0.375643	-0.125513

Frequencies

-900.2143	77.9422	140.5655
172.8082	329.2766	354.2457
420.1929	443.9335	545.3621
686.0673	726.2997	921.4417
1032.3941	1047.5068	1053.7101
1058.2374	1193.1330	1296.8652
1412.9187	1443.3106	1482.9089
1486.1254	1610.4334	2383.4463
3051.7859	3123.0161	3128.4377
3168.0357	3176.4895	3270.5475

i5 – i90

C	1.120784	0.505979	-0.236538
C	1.768960	-0.701495	0.085763
C	-1.350668	0.370086	0.054923
C	-1.557763	-0.948794	-0.061763
C	-0.075911	1.073633	0.027463
H	2.591086	-1.047415	-0.534017
H	1.385929	-1.393281	0.841375
H	2.245256	0.491267	0.412193
H	-2.222510	1.011293	0.166571
H	-0.749412	-1.657172	-0.204605
H	-2.561921	-1.354847	-0.033475
H	-0.120835	2.153694	0.132872

Frequencies

-1790.8494	94.8354	187.2376
309.7942	355.8123	432.1767
662.3699	679.9212	840.4800
906.1699	914.5817	943.0756
1023.8460	1030.6048	1055.7945
1129.3438	1167.1282	1326.8242
1380.5580	1437.9537	1471.2903
1542.7932	1679.1517	2235.1436
3055.4862	3155.9656	3166.5456
3177.1753	3198.9870	3253.3507

i90 – p3

C	1.011608	0.390185	0.000282
C	2.122559	-0.309462	-0.000207
C	-1.459518	0.368649	-0.000765
C	-1.683096	-0.942843	0.000542
C	-0.134786	1.016264	0.000529
H	2.643064	-0.522958	-0.928708
H	1.555920	-2.248027	-0.002486
H	2.642499	-0.525207	0.928091
H	-2.303758	1.052271	-0.002927
H	-0.868690	-1.661281	0.002869
H	-2.692877	-1.335418	-0.000777
H	-0.116758	2.103864	0.001649

Frequencies

-621.2520	57.4060	165.2486
254.3990	335.6166	343.7596
445.6299	574.9251	657.6542
744.8076	913.1107	919.5308
940.1578	963.7672	1024.4487
1039.7941	1051.7796	1144.9805
1341.6710	1365.5715	1451.8714
1475.5915	1713.7314	2017.5670
3141.0080	3156.7073	3159.9754
3183.8741	3225.9225	3252.3765

i90 – p38

C	1.211483	0.414484	-0.107601
C	2.065817	-0.734745	0.147679
C	-1.656142	0.294554	0.402871
C	-2.007998	-0.781652	-0.256641
C	0.336209	1.246933	-0.239145
H	2.516591	-1.100815	-0.777926
H	1.482525	-1.548933	0.590034
H	2.871138	-0.476520	0.839642
H	-2.110565	0.812671	1.239374
H	-1.403173	-1.166719	-1.074641
H	-2.920656	-1.331390	-0.021338
H	-0.132082	2.174258	-0.478115

Frequencies

-438.4840	32.5227	75.4463
87.0582	174.2539	268.8960
355.0724	373.4285	668.5606
736.7714	806.0882	905.9989
945.2148	948.0243	1035.6079
1063.6154	1098.0325	1394.9518
1410.9856	1479.7380	1480.7127
1661.7808	2128.4125	3042.8214
3090.9889	3112.4403	3128.4982
3181.0495	3216.1178	3433.9384

i31 – i88

C	2.374399	-0.464334	-0.033732
C	1.287050	0.571071	-0.010048
C	-0.011200	0.285773	0.003704
C	-2.635399	-0.193234	-0.130182
C	-1.231370	-0.015256	0.105233
H	2.974146	-0.381883	-0.946812
H	1.958228	-1.471912	0.010560
H	3.057407	-0.336741	0.812686
H	1.579836	1.617670	-0.024444
H	-3.059753	-1.184178	-0.044175
H	-3.230680	0.625566	-0.515320
H	-1.980066	0.027361	1.097653

Frequencies

-2025.9399	85.7446	102.8762
159.6939	242.5026	301.5711
490.2423	548.7880	652.6388
668.6609	782.2811	950.9479
1002.6993	1027.7037	1034.4691
1109.6333	1265.8816	1405.8407
1420.3537	1473.2207	1481.7643
1530.5684	2084.1538	2259.6275
3034.2461	3090.2182	3138.9200
3156.6987	3162.1531	3276.9487

i83 – i96

C	-2.363506	0.162142	0.000020
C	1.665485	-0.607339	0.000022
C	-0.997247	-0.350062	-0.000040
C	0.239247	-0.357724	-0.000007
C	1.584715	0.885485	-0.000011
H	-2.378759	1.259157	0.002815
H	-2.910534	-0.185466	0.880571
H	-2.908847	-0.180996	-0.883322
H	2.061720	-1.070983	0.902284
H	2.061780	-1.071058	-0.902175
H	1.651287	1.427207	0.932630
H	1.651190	1.427126	-0.932707

Frequencies

-710.3413	43.9616	123.7328
191.5602	363.7314	366.6851
592.6172	681.9856	724.9092
819.7721	1024.5855	1043.4000
1058.1364	1064.2696	1193.1190
1213.8466	1224.2111	1407.1617
1447.1904	1474.0406	1477.2437
1485.8643	2093.7761	3021.0592
3091.8810	3095.5130	3115.8547
3163.7520	3177.4356	3297.4674

i4 – i91

C	2.170372	-0.513665	0.074639
C	1.246161	0.516412	-0.203894
C	-0.067773	0.711216	0.030151
C	-2.367790	-0.184093	0.036751
C	-1.045678	-0.355206	-0.075629
H	3.062665	-0.605313	-0.537458
H	1.953742	-1.327577	0.771297
H	2.321094	0.739474	0.487452
H	-0.441986	1.716715	0.206883
H	-3.056579	-1.015854	-0.050611
H	-2.796233	0.796264	0.222074
H	-0.654453	-1.351689	-0.271742

Frequencies

-1815.4563	130.7478	169.9555
292.0044	369.5628	425.0854
613.3790	682.6903	855.8881
897.5743	926.9123	934.1158
1034.2419	1043.0260	1070.5133
1159.5880	1187.0851	1309.6219
1336.1755	1451.3395	1471.3232
1573.7801	1670.0624	2235.2727
3064.8217	3149.5325	3158.8544
3165.7862	3203.7246	3246.7188

i96 – p27

C	2.285515	0.177755	0.000038
C	-1.510267	-0.810180	0.000064
C	0.970022	0.140587	-0.000037
C	-0.307370	0.047016	-0.000060
C	-1.628168	0.706079	-0.000028
H	2.838040	0.274810	0.928363
H	2.838117	0.274576	-0.928244
H	2.864169	-1.821195	-0.000151
H	-1.750424	-1.339664	-0.915721
H	-1.750257	-1.339531	0.915936
H	-1.949122	1.191657	-0.915484
H	-1.948920	1.191809	0.915435

Frequencies

-531.6535	156.6894	177.8428
227.3101	308.4671	371.7206
568.3802	658.9693	663.5771
787.1873	902.2681	923.3867
951.3269	1014.9082	1031.6602
1056.4949	1078.7210	1083.8426
1181.4920	1361.5176	1456.8284
1473.5761	1537.7226	2108.7001
3135.0320	3137.6460	3151.5956
3219.3544	3232.2649	3238.0561

i60 – i96

C	2.279690	0.187684	0.065617
C	-1.651873	-0.637264	0.090527
C	0.996331	-0.374348	-0.188064
C	-0.281275	-0.132803	-0.038863
C	-1.376337	0.861294	-0.049495
H	2.430580	0.983202	0.795710
H	3.085063	-0.027216	-0.628282
H	1.911924	-1.056283	0.417671
H	-2.095565	-1.147596	-0.759809
H	-1.982445	-1.003543	1.058138
H	-1.632739	1.337945	-0.990222
H	-1.516035	1.486117	0.828455

Frequencies

-1951.3892	159.7631	187.1866
319.8272	380.4219	523.9753
687.9228	772.0085	840.8783
871.2013	954.7712	993.5064
1033.6213	1045.7112	1072.7955
1077.8992	1122.6860	1167.8431
1279.3863	1449.1880	1452.0185
1485.7171	1831.0397	2216.9513
3086.0330	3116.1037	3123.7176
3196.0626	3213.2454	3222.1526

i31 – i90

C	2.346531	-0.428240	0.193629
C	1.176175	0.327683	-0.334362
C	-0.085719	0.531177	-0.164266
C	-2.268984	-0.582209	-0.111578
C	-1.417619	0.367239	0.313962
H	2.884530	-0.927400	-0.614771
H	2.015774	-1.178396	0.922148
H	3.043836	0.252186	0.687743
H	0.564838	1.392211	-0.826220
H	-3.285897	-0.619879	0.259499
H	-1.965118	-1.332023	-0.832747
H	-1.760262	1.119405	1.020036

Frequencies

-2101.4804	94.4428	114.8034
178.1984	226.5378	285.4629
402.1568	571.0742	657.3219
740.9244	890.7742	989.1405
1002.4962	1035.4812	1044.3587
1125.3786	1310.3444	1390.9545
1428.1266	1471.3128	1484.7815
1610.1728	1999.5276	2388.6101
3021.9409	3110.1510	3132.2672
3161.3756	3171.0988	3261.6915

i90 – i91

C	2.009688	-0.633666	-0.005024
C	1.187322	0.573031	-0.177957
C	-0.057968	0.954244	-0.025597
H	2.506506	-0.907649	-0.939878
H	1.387442	-1.483528	0.308798
H	2.784879	-0.477535	0.750508
H	-0.342446	1.979114	-0.264885
C	-2.050814	-0.520111	-0.296263
C	-1.138011	0.050897	0.479045
H	-2.819025	-1.164202	0.118192
H	-2.060153	-0.362125	-1.370343
H	-1.158509	-0.130445	1.552387

Frequencies

-129.4330	152.7649	161.7488
306.3387	446.4926	453.7094
686.3716	780.9487	884.4538
969.5622	970.9567	1030.3248
1049.2836	1050.8925	1113.5060
1271.9819	1318.5021	1391.0701
1440.1679	1463.4053	1481.3337
1712.8069	1771.7220	3004.7114
3088.4962	3115.2290	3121.1139
3144.6881	3158.2927	3241.6040

i90 – i95

C	1.691784	-0.749050	0.069607
C	1.332550	0.587214	0.160410
C	0.110448	1.034258	-0.010328
C	-1.987360	-0.367868	0.285484
C	-0.848732	-0.077667	-0.458528
H	2.342282	-1.086071	-0.736395
H	0.171081	-0.974329	-0.300151
H	1.770155	-1.335617	0.985041
H	-0.250534	2.048647	0.111716
H	-2.804143	-0.943436	-0.135262
H	-2.045412	-0.111849	1.338231
H	-0.975572	-0.158656	-1.543046

Frequencies

-2307.3209	167.7843	299.1555
363.0359	412.4060	536.6999
618.0213	727.3410	796.6461
833.6718	878.7096	934.7468
1003.7918	1024.0245	1069.6129
1098.4873	1245.3227	1258.7558
1282.1325	1383.2512	1441.1829
1477.3676	1538.2910	1762.2926
3075.5136	3108.1403	3152.3558
3186.0968	3216.1515	3251.1819

i86 – i89

C	2.014749	-0.656930	0.045318
C	-2.349583	-0.276691	-0.022918
C	1.441453	0.562535	-0.316149
C	-0.882877	-0.176778	-0.065962
C	0.053044	0.735753	0.131524
H	1.471364	-1.447617	0.579872
H	2.325040	0.405019	0.663548
H	3.009939	-0.912007	-0.315119
H	-2.667545	-1.116010	0.599905
H	-2.764123	-0.428903	-1.022967
H	-2.784340	0.642966	0.389162
H	-0.251044	1.729221	0.474716

Frequencies

-1049.2627	148.8917	161.2642
207.9630	291.5004	351.5682
536.6385	675.3568	851.9713
910.5626	1008.5404	1050.2069
1057.2270	1068.8565	1123.3871
1272.8233	1323.2603	1400.1913
1410.1334	1464.9752	1481.5485
1521.7010	1703.5163	2250.0258
3020.5411	3029.1823	3065.9368
3098.4248	3120.7141	3157.2385

i32 – i86

C	1.872993	-0.651763	0.047572
C	-2.166546	-0.295997	0.059279
C	1.398004	0.681466	-0.016859
C	-0.715661	-0.259795	-0.246026
C	0.050612	0.896679	0.015024
H	0.724275	-1.076991	-0.308544
H	1.934618	-1.070380	1.053955
H	2.739788	-0.918630	-0.556675
H	-2.282393	-0.899333	0.970777
H	-2.727611	-0.818829	-0.720682
H	-2.623942	0.683145	0.252233
H	-0.401144	1.877475	0.154994

Frequencies

-1525.5102	107.2227	150.0574
318.8639	435.6112	521.9260
556.1217	667.6197	847.8006
888.4590	965.0177	996.4894
1036.9240	1064.4960	1115.9070
1237.2409	1319.6790	1347.9337
1381.7021	1442.3547	1463.7309
1493.1767	1506.3325	1707.6957
3001.2360	3068.7417	3093.1823
3098.9658	3144.8114	3158.3463

i86 – i91

C	2.209646	-0.459537	-0.006815
C	-2.304985	-0.207871	0.003635
C	1.220861	0.621607	-0.037519
C	-0.943966	-0.449881	0.170652
C	-0.092996	0.744390	0.022529
H	1.695301	-1.413259	0.170668
H	2.944888	-0.295021	0.785925
H	2.750619	-0.519638	-0.955471
H	-3.020988	-1.018135	0.138290
H	-1.615016	-0.784838	-0.917690
H	-2.747218	0.792235	-0.127233
H	-0.538950	1.746408	-0.009383

Frequencies

-1196.7439	87.7418	172.2171
188.6762	349.5009	381.1302
564.5641	631.3708	859.3162
905.1129	995.9467	1046.5280
1049.8690	1060.6138	1160.6036
1281.5216	1327.1940	1385.3551
1405.5960	1462.4321	1469.7547
1532.4500	1720.6760	2224.8911
2984.9885	3014.6198	3041.3155
3098.8810	3116.7627	3153.3333

i8 – i95

C	-1.352243	-0.429919	0.320201
C	-1.721362	0.950127	-0.105054
H	-2.111704	-1.142559	-0.011742
H	-1.312320	-0.494676	1.412655
H	-2.206174	1.113388	-1.060284
H	-1.289452	1.806983	0.398202
C	-0.002820	-0.884699	-0.244143
C	2.216344	0.439977	0.078378
C	1.112018	-0.229911	-0.085810
H	0.020334	-1.810015	-0.814217
H	2.864569	0.255349	0.929175
H	2.523123	1.198074	-0.635220

Frequencies

-100.5678	163.2613	190.0743
300.0476	333.4342	553.4462
558.9940	683.3247	778.0797
883.1888	893.0486	897.1521
1021.1254	1070.2816	1099.0134
1155.4442	1279.1205	1303.0299
1361.5948	1466.4098	1481.4795
1494.8681	2078.9665	3050.8034
3101.6462	3145.8756	3154.9329
3164.1320	3227.7313	3264.3948

i45 – i95

C	2.557845	-0.142778	0.008890
C	1.295813	0.177014	-0.010449
C	0.031504	0.488519	-0.031894
H	3.102567	-0.331911	-0.910805
H	3.101777	-0.226810	0.944465
H	-0.232210	1.542221	-0.097836
C	-2.453542	0.110475	-0.010962
C	-1.105155	-0.514337	0.022620
H	-3.335580	-0.503615	-0.142409
H	-2.590468	1.162798	0.207972
H	-0.998721	-1.125694	0.933481
H	-1.006156	-1.230344	-0.804107

Frequencies

-101.2374	103.1116	164.8619
317.2077	375.5082	439.1433
534.3862	568.1716	841.7999
884.9277	891.4301	918.3691
1027.5497	1078.4351	1108.7960
1162.3146	1189.5665	1300.0701
1391.8061	1452.9077	1467.8598
1488.0171	2087.7594	2972.1743
3029.3099	3143.5730	3153.4595
3163.5916	3225.4998	3271.7440

i95 – p24

C	-2.435573	-0.480310	-0.047657
C	-1.354557	0.291103	-0.101966
C	-0.264769	0.921695	-0.106523
C	2.301658	-0.341165	-0.401454
C	1.420094	-0.226005	0.628583
H	-3.055463	-0.508945	0.841257
H	-2.739847	-1.072808	-0.902966
H	0.145549	1.878627	-0.362541
H	3.046214	0.422718	-0.596714
H	2.233496	-1.157360	-1.111357
H	0.778485	-1.057990	0.893254
H	1.590446	0.503854	1.413172

Frequencies

-640.7503	60.6280	134.5540
222.5286	315.5800	382.4729
426.5488	488.7873	719.6685
741.9297	795.6011	827.4355
876.3140	982.6242	1027.0484
1029.9261	1162.6553	1240.2407
1292.6748	1464.0203	1467.4581
1576.2274	1934.2087	3147.3684
3149.0683	3158.6096	3232.9267
3238.9872	3257.8136	3350.8620

i85 – i90

C	-2.058387	-0.511072	-0.014354
C	1.902135	-0.661734	-0.250533
C	-0.767156	0.178104	0.062928
C	1.066693	0.186248	0.451739
C	0.084915	1.106224	-0.193939
H	-2.780155	0.065049	-0.606510
H	-2.477361	-0.672561	0.982287
H	-1.934798	-1.490713	-0.484002
H	2.602741	-1.305469	0.267733
H	1.838120	-0.741432	-1.330152
H	1.216202	0.289447	1.523117
H	0.166049	2.069062	-0.687520

Frequencies

-604.4425	164.3851	176.2542
233.6283	316.8589	438.9114
524.2424	735.5888	777.2871
870.1497	912.5013	971.2664
1034.2156	1061.0195	1099.0198
1169.2622	1268.0816	1390.6848
1405.3408	1475.9601	1482.3942
1505.0341	1881.6692	3020.0860
3094.9350	3115.9068	3153.5609
3161.4688	3171.2643	3257.1221

i84 – p28

C	1.930472	-0.565776	-0.033698
C	-1.924025	-0.627947	-0.166475
C	0.654057	0.170276	-0.033461
C	-0.781123	0.062668	0.078110
C	-0.035289	1.287979	-0.057763
H	1.928357	-1.317614	-0.825525
H	2.029517	-1.093561	0.918881
H	2.780109	0.102660	-0.166326
H	-1.921529	-1.709215	-0.146217
H	-2.874068	-0.112903	-0.208983
H	-0.956646	-0.195721	1.823352
H	-0.050287	2.363160	-0.115462

Frequencies

-1035.9967	85.8686	185.9488
224.4998	312.7220	458.6653
577.6375	620.1583	666.5657
738.4760	789.1509	807.2029
866.2479	1003.3074	1043.8910
1045.5034	1093.7246	1224.1734
1398.8532	1453.0208	1476.0718
1481.7188	1626.9705	1882.1080
3048.5000	3116.9789	3148.1778
3162.8896	3261.2945	3281.6204

i91 – p38

C	2.533676	-0.431376	0.058287
C	1.334639	0.389946	-0.011579
C	0.250134	0.932264	-0.070815
C	-2.696710	-0.067191	0.090415
C	-1.502983	-0.571431	-0.099651
H	3.247364	-0.145946	-0.718533
H	2.290387	-1.489790	-0.078141
H	3.023967	-0.318149	1.028201
H	-0.472631	1.715120	-0.120807
H	-3.592008	-0.690551	0.106537
H	-2.855557	0.999011	0.243311
H	-1.154061	-1.582967	-0.260514

Frequencies

-406.9659	44.8827	97.5235
118.7188	191.5368	267.5974
350.7858	358.3106	669.0498
766.9550	791.5774	913.4770
945.5804	954.5574	1046.6878
1067.0857	1093.2906	1404.5854
1421.1839	1484.1027	1487.3411
1662.1807	2137.0902	3044.7846
3085.3903	3112.9583	3126.4708
3164.2415	3238.6485	3424.2335

i92 – p2

C	2.411856	-0.305797	0.000052
C	1.146783	0.045666	-0.000031
C	-0.088926	0.469799	-0.000074
C	-2.515525	0.046549	0.000066
C	-1.263244	-0.404601	-0.000054
H	2.921457	-0.544088	-0.928205
H	2.921347	-0.544013	0.928389
H	3.436669	1.429850	0.000043
H	-0.262606	1.545622	-0.000104
H	-3.358749	-0.633530	0.000100
H	-2.734484	1.109945	0.000151
H	-1.069298	-1.473482	-0.000128

Frequencies

-659.7105	108.4980	142.2853
228.4709	312.8772	371.8166
411.1828	576.5041	580.4447
762.3440	908.9094	920.5284
935.9031	948.3379	1023.9332
1034.5636	1103.1128	1194.2682
1312.0150	1345.0673	1446.2999
1485.4869	1719.2070	2023.4061
3140.3190	3144.9217	3155.5661
3183.6085	3229.4953	3250.9561

i87 – i88

C	-2.388847	-0.409967	0.039736
C	-1.368134	0.673040	-0.083418
C	-0.044347	0.285889	0.011539
C	2.557839	-0.183832	0.079981
C	1.164841	-0.008529	-0.331307
H	-3.298883	-0.073463	0.539804
H	-2.048443	-1.368009	0.450934
H	-2.669084	-0.585203	-1.011032
H	-0.311480	0.566128	1.119098
H	2.928037	-1.186558	-0.150859
H	2.657746	-0.033543	1.164201
H	3.213992	0.541043	-0.411335

Frequencies

-596.4376	111.6492	125.8668
152.1042	189.5740	206.5556
461.4290	574.4080	705.7244
798.5483	910.6855	1016.9506
1042.5190	1062.8845	1076.9147
1319.1733	1370.2266	1408.3859
1438.4901	1461.6066	1485.6774
1496.6694	1896.3951	2469.4204
2998.4573	3004.9158	3064.0344
3081.6561	3109.0408	3125.8306

i86 – i88

C	2.465269	-0.342740	0.096036
C	1.208606	0.288750	-0.312186
C	-0.046391	0.460788	-0.069743
C	-2.321368	-0.451115	-0.121732
C	-1.303166	0.442506	0.512951
H	2.938499	-0.880768	-0.729753
H	2.281830	-1.062144	0.905891
H	3.178250	0.398265	0.470334
H	-0.637097	1.305206	-0.633738
H	-2.396595	-1.279040	0.598873
H	-2.070404	-0.878435	-1.099869
H	-3.312177	0.007782	-0.143701

Frequencies

-432.1733	129.6448	134.6183
153.2472	206.7841	230.7841
455.5281	579.1600	737.1713
777.0063	925.3256	1011.0063
1032.3029	1059.5142	1076.4016
1305.0187	1375.3756	1405.6682
1443.4245	1464.6260	1486.7437
1492.5740	1875.0888	2485.2511
3006.0911	3007.7085	3074.4379
3080.5156	3105.2079	3122.7222

i89 – p8

C	1.077436	-0.015104	0.023232
C	2.506731	-0.275289	0.005933
C	-1.507165	0.450419	0.060319
C	-2.295128	-0.619105	-0.036218
C	-0.073180	0.376069	0.002677
H	2.765675	-0.990566	-0.778373
H	2.843238	-0.680889	0.963399
H	3.053711	0.653903	-0.182763
H	-1.939526	1.436561	0.190157
H	-1.886617	-1.613618	-0.174079
H	-3.372334	-0.517302	0.021624
H	0.283687	2.209972	-0.375625

Frequencies

-772.6917	57.9947	105.4255
145.6407	198.8867	333.5441
408.4184	525.0715	605.7484
704.0511	724.5980	971.2721
1034.9914	1043.6238	1049.8376
1054.7942	1205.7754	1334.9091
1413.7824	1448.3588	1475.8143
1483.6947	1700.3444	2277.9364
3044.3272	3114.8343	3127.1674
3162.1734	3189.9017	3259.0849

i80 – i81

C	-1.910447	-0.635605	0.026189
C	1.937627	-0.582900	0.070593
C	-0.657355	0.146047	-0.040458
C	0.688548	0.128543	-0.295641
C	-0.053559	1.350259	0.139347
H	-1.962711	-1.145005	0.992988
H	-1.916976	-1.402374	-0.750496
H	-2.790414	0.000751	-0.076059
H	1.857072	-1.655836	-0.121004
H	2.154005	-0.435453	1.139972
H	2.794922	-0.198759	-0.487605
H	-0.164779	2.398612	-0.097978

Frequencies

-620.4370	91.2039	179.4744
183.0982	337.1645	407.0907
493.2063	741.4424	781.7621
905.4296	960.5502	1038.3583
1047.6009	1096.1811	1182.3459
1283.1950	1400.1398	1404.7436
1479.1712	1481.4301	1489.0869
1491.8715	1787.3642	2985.9296
3059.8110	3086.5971	3126.0344
3132.4262	3156.3649	3224.5366

i83 – i88

C	2.621799	0.195303	-0.002035
C	-1.388276	-0.547171	-0.001498
C	1.188377	-0.068014	-0.008836
C	0.002814	-0.294179	-0.021061
C	-2.396882	0.549919	-0.041790
H	2.896120	0.914301	-0.778630
H	3.180923	-0.726332	-0.182781
H	2.944146	0.599681	0.961694
H	-1.736073	-1.543028	-0.252520
H	-1.977645	-0.145712	1.037427
H	-3.417393	0.310276	-0.303929
H	-2.057072	1.575668	-0.029938

Frequencies

-1916.8474	62.0129	129.8245
174.9856	315.2220	340.4965
478.2193	529.9281	652.4983
717.6612	776.5360	1007.1182
1049.8413	1055.9757	1115.0804
1217.9033	1251.3069	1390.6243
1418.3357	1428.1876	1481.6508
1489.6889	2233.5909	2332.0067
3045.7839	3112.4520	3122.2507
3173.6244	3192.6460	3301.7222

i80 – i82

C	-1.939457	-0.579745	0.075613
C	1.909939	-0.638260	0.029419
C	-0.693546	0.129340	-0.311438
C	0.652825	0.137727	-0.037515
C	0.055852	1.342406	0.134733
H	-2.140644	-0.429892	1.147648
H	-1.862527	-1.653318	-0.114547
H	-2.803994	-0.196875	-0.472050
H	1.737264	-1.703240	-0.128044
H	2.373464	-0.488685	1.007446
H	2.614931	-0.274757	-0.722725
H	0.167834	2.397961	-0.062602

Frequencies

-613.2366	121.8198	181.6487
188.9386	351.0872	411.0461
490.6435	739.0008	781.8826
924.0220	969.2205	1039.8109
1049.9074	1095.6001	1160.7208
1295.2080	1405.0458	1410.3415
1479.5056	1488.9773	1492.8582
1495.6543	1784.0127	2985.3367
3056.6443	3086.9074	3125.6848
3127.4949	3152.3512	3236.3039

i82 – i87

C	-2.424757	-0.014273	0.251266
C	-1.137489	-0.438408	-0.352269
C	-0.052189	0.455338	-0.279975
C	2.489300	-0.055627	0.213318
C	1.094346	-0.232390	-0.197115
H	-3.285943	-0.470054	-0.243765
H	-2.560766	1.077463	0.320302
H	-2.427194	-0.405121	1.279332
H	-0.116263	1.547861	-0.147736
H	2.679930	-0.580120	1.154665
H	2.721965	1.008235	0.360897
H	3.173000	-0.466102	-0.535039

Frequencies

-150.4413	135.3659	144.5781
162.2482	286.7858	326.1552
347.7940	802.5765	865.3782
914.9552	961.6768	1030.1273
1033.9758	1060.7521	1166.6233
1352.0194	1369.2263	1397.0858
1439.1511	1460.1126	1468.3797
1495.1227	1643.1712	2963.7016
2975.3922	3006.0657	3052.5581
3090.7051	3106.0984	3113.9411

i91 – i92

C	-2.541785	-0.189357	-0.004527
C	-1.143496	0.193173	0.007170
H	-3.150810	0.504650	-0.598828
H	-2.944100	-0.193552	1.013326
H	-2.695076	-1.193510	-0.424335
C	0.117822	0.528581	0.001549
C	2.526416	-0.034639	-0.003596
C	1.249871	-0.413204	0.002475
H	0.403859	1.589232	-0.003367
H	3.332043	-0.759181	-0.004677
H	2.802927	1.015774	-0.008082
H	0.998194	-1.470739	0.007538

Frequencies

-267.2738	28.5504	104.3884
258.9197	315.0124	462.6419
608.4139	843.2543	852.2936
939.7893	986.3713	993.6320
1028.0073	1041.8162	1146.3509
1284.7545	1323.1886	1411.5672
1450.3231	1455.9705	1477.2843
1703.3280	1839.0410	2988.6888
3008.3733	3036.0966	3098.4259
3148.3463	3168.2253	3246.9713

i15 – i88

C	2.374418	-0.464295	0.033788
C	1.287027	0.571066	0.010000
C	-0.011208	0.285721	-0.003761
C	-2.635384	-0.193162	0.130236
C	-1.231361	-0.015418	-0.105297
H	3.057290	-0.336926	-0.812796
H	1.958260	-1.471906	-0.010129
H	2.974318	-0.381546	0.946755
H	1.579787	1.617676	0.024320
H	-3.059993	-1.183957	0.043731
H	-1.980184	0.027637	-1.097617
H	-3.230427	0.625550	0.515942

Frequencies

-2025.8934	85.9546	103.1665
159.7558	242.6959	301.6855
490.2913	548.7964	652.7298
668.8079	782.3044	951.1024
1002.7195	1027.7430	1034.4883
1109.6441	1265.8995	1405.8493
1420.4212	1473.2205	1481.7550
1530.5737	2084.0742	2259.5842
3034.1375	3090.0880	3138.8415
3156.6393	3162.1165	3276.8753

i88 – p8

C	-2.325486	-0.361186	-0.250372
C	-1.383792	0.547807	0.048156
C	0.013732	0.275320	0.023787
C	2.635202	-0.194117	-0.008780
C	1.200006	0.066869	0.010520
H	-2.773134	-1.325280	1.598309
H	-2.056493	-1.354385	-0.588382
H	-3.374047	-0.091736	-0.256809
H	-1.677218	1.549833	0.345703
H	3.022674	-0.289214	1.007592
H	3.167840	0.621845	-0.500986
H	2.852406	-1.119226	-0.545294

Frequencies

-536.8555	82.0990	131.9059
161.5158	244.4756	298.5726
333.9013	417.7333	546.4190
725.4806	741.6603	974.5095
1011.4869	1047.4264	1055.3577
1058.5475	1202.2421	1314.7241
1416.8785	1442.7053	1484.8760
1488.1738	1655.0190	2372.0947
3060.9788	3129.5323	3140.0964
3163.8583	3174.4056	3262.6722

i88 – p10

C	-2.371782	0.487354	0.007284
C	-1.300965	-0.558973	-0.079797
C	-0.012478	-0.318186	0.020601
C	2.514886	0.171926	0.201538
C	1.224012	-0.077062	0.118787
H	-2.960441	0.508343	-0.915510
H	-1.946010	1.477227	0.172571
H	-3.063381	0.259864	0.824615
H	-1.621654	-1.587149	-0.236629
H	3.144782	0.565480	-2.005296
H	3.243927	-0.630325	0.163102
H	2.880739	1.176207	0.386672

Frequencies

-391.1542	130.9927	140.9869
166.2624	184.2466	265.9241
315.7058	530.8598	539.0945
586.3706	808.1651	860.2634
896.3550	1032.0038	1042.8967
1057.5805	1122.6439	1313.9622
1409.9703	1447.9135	1487.9909
1492.1864	1709.5241	2187.2631
3041.7762	3102.8506	3143.9840
3152.0337	3160.7254	3238.3283

i3 – i92

C	2.493623	0.107052	0.144579
C	1.183303	-0.236021	-0.247191
C	-0.035882	0.328616	-0.170549
C	-2.478802	0.156883	0.101809
C	-1.270839	-0.407519	-0.002247
H	3.335658	-0.343949	-0.372244
H	1.873367	-0.999347	0.545882
H	2.709540	0.932851	0.826713
H	-0.111558	1.411547	-0.303018
H	-3.372083	-0.439604	0.242432
H	-2.606203	1.233800	0.045637
H	-1.177140	-1.489366	0.056191

Frequencies

-1828.4700	121.7094	188.9604
255.0401	369.0235	458.6860
542.4097	673.2458	855.4316
899.5955	920.1123	936.1503
1030.1100	1033.6681	1126.4094
1153.9955	1209.2621	1277.2992
1322.3865	1451.2858	1475.9259
1611.1181	1678.9777	2223.3133
3067.6353	3087.4662	3154.5156
3167.8098	3200.5200	3251.3648

i32 – i92

C	-2.415002	-0.189987	0.000104
C	-0.935556	-0.152494	-0.000157
C	0.045439	0.752246	-0.000098
C	2.492759	-0.201113	0.000113
C	1.172803	-0.161542	-0.000111
H	-2.788453	-0.718080	0.881716
H	-2.788884	-0.717707	-0.881542
H	-2.829933	0.824281	0.000465
H	0.017351	1.837193	0.000109
H	3.035532	-1.138598	0.000123
H	3.075424	0.718725	0.000266
H	0.116304	-1.088471	-0.000242

Frequencies

-2281.9290	105.9362	136.6497
223.6709	328.0318	379.7600
551.0437	598.2925	860.7606
872.5728	921.4102	952.0014
1032.8698	1036.8438	1086.3549
1129.0925	1223.4517	1393.8760
1427.8237	1461.0511	1479.6835
1713.5022	1746.0088	1915.5180
3033.5089	3110.9085	3120.0555
3120.4857	3199.0086	3230.0997

i92 – p8

C	-2.607959	0.070770	-0.000156
C	-1.164207	-0.112983	0.000057
C	0.051105	-0.077238	0.000207
C	2.495977	0.301495	-0.000235
C	1.428277	-0.492828	0.000129
H	-3.058326	-0.383266	0.884515
H	-3.057790	-0.381837	-0.885833
H	-2.848806	1.137596	0.000613
H	0.287216	1.804673	0.001190
H	3.491974	-0.122426	-0.000361
H	2.402531	1.380513	-0.000449
H	1.564038	-1.570553	0.000319

Frequencies

-742.7514	36.0923	96.8534
144.8624	201.6257	404.5182
406.1578	503.3069	599.3661
715.3105	752.6626	975.4214
1019.4454	1044.7262	1053.0765
1055.1603	1179.6279	1323.7421
1411.7495	1445.4195	1477.4683
1480.3363	1714.6840	2273.3056
3047.4526	3119.0378	3125.7864
3156.9310	3170.8138	3253.7261

i84 – i93

C	-1.741596	-0.711566	0.048632
C	1.816758	-0.567173	0.296112
C	-0.573361	0.202206	-0.060076
C	0.833847	-0.025458	-0.507739
C	-0.182041	1.409757	0.151086
H	-1.495109	-1.554079	0.701162
H	-1.993024	-1.122994	-0.933262
H	-2.613059	-0.192686	0.450809
H	2.818931	-0.727277	-0.082736
H	1.625508	-0.786425	1.340886
H	1.048758	0.123846	-1.562560
H	-0.313650	2.413022	0.517611

Frequencies

-666.5029	125.7426	157.6916
308.9365	331.6043	512.8926
540.0214	645.0092	688.8021
765.1781	781.5106	957.5138
973.1386	1035.6149	1074.0782
1192.3832	1287.8311	1393.7353
1404.3393	1479.1871	1483.5468
1511.3380	1836.7705	3049.5748
3116.5080	3149.0287	3152.5126
3163.3872	3255.0425	3303.4701

i85 – p28

C	-1.930472	-0.565776	-0.033698
C	1.924025	-0.627947	-0.166475
C	-0.654057	0.170275	-0.033460
C	0.781123	0.062668	0.078111
C	0.035289	1.287979	-0.057763
H	-2.780111	0.102664	-0.166296
H	-2.029505	-1.093587	0.918868
H	-1.928369	-1.317592	-0.825546
H	1.921530	-1.709215	-0.146217
H	2.874068	-0.112903	-0.208984
H	0.956647	-0.195721	1.823352
H	0.050287	2.363160	-0.115463

Frequencies

-1035.9972	85.8622	185.9490
224.4989	312.7221	458.6653
577.6377	620.1584	666.5659
738.4759	789.1511	807.2030
866.2479	1003.3072	1043.8910
1045.5037	1093.7245	1224.1736
1398.8531	1453.0208	1476.0715
1481.7194	1626.9704	1882.1080
3048.4998	3116.9787	3148.1781
3162.8893	3261.2943	3281.6200

i94 – p23

C	-0.859220	1.659938	0.028924
C	1.888506	0.194543	-0.044615
C	-0.479793	-0.601072	-0.000378
C	0.956094	-0.749174	0.047790
C	-1.593395	-1.112549	-0.035842
H	-0.424491	1.953113	-0.919948
H	-0.323262	1.929936	0.931792
H	-1.939918	1.678907	0.087696
H	2.937092	-0.074867	-0.001634
H	1.651089	1.242744	-0.167322
H	1.268244	-1.783805	0.165555
H	-2.641910	-1.296147	-0.071417

Frequencies

-536.9359	57.2967	173.5668
226.2978	296.5552	312.3768
453.0098	478.1647	541.4020
575.2347	684.2186	718.6971
830.3740	893.1495	970.4579
1028.2072	1096.9140	1325.1568
1419.1658	1431.5183	1445.0167
1711.5843	2024.3536	3100.0903
3169.8847	3185.5268	3266.0985
3270.0879	3274.8758	3451.0215

i85 – i93

C	-1.741607	-0.711536	-0.048676
C	1.816761	-0.567141	-0.296138
C	-0.573351	0.202197	0.060051
C	0.833831	-0.025521	0.507758
C	-0.182010	1.409761	-0.151008
H	-2.612677	-0.192976	-0.452116
H	-1.993927	-1.121875	0.933451
H	-1.494669	-1.554814	-0.700046
H	2.818908	-0.727355	0.082724
H	1.625535	-0.786132	-1.340972
H	1.048710	0.123593	1.562614
H	-0.313622	2.413008	-0.517579

Frequencies

-666.5345	125.8025	157.7040
308.9188	331.6306	512.8974
540.0599	645.0091	688.8301
765.2034	781.5445	957.5477
973.1201	1035.5407	1074.1106
1192.3920	1287.8185	1393.7291
1404.3196	1479.2522	1483.4912
1511.3355	1836.7724	3049.5225
3116.4371	3149.0000	3152.5115
3163.3839	3255.0544	3303.4602

i66 – i94

C	-0.986106	1.197872	0.000072
C	1.993794	0.221936	-0.000110
C	-0.421509	-0.197304	0.000054
C	0.967464	-0.626928	0.000141
C	-1.574828	-0.854618	-0.000117
H	-0.911627	1.775320	-0.921338
H	-0.911845	1.775188	0.921577
H	-2.144455	0.425617	-0.000113
H	3.019612	-0.127667	-0.000055
H	1.834315	1.296068	-0.000408
H	1.145824	-1.699092	0.000407
H	-1.904715	-1.891178	-0.000308

Frequencies

-2212.6910	135.5802	222.8439
330.5473	474.4314	515.9516
612.3048	639.2689	751.8463
863.4569	951.3035	952.5982
971.5968	1020.4068	1046.6216
1054.1326	1109.8206	1314.9781
1327.6632	1421.8215	1444.5941
1664.7433	1738.7113	1906.6860
3086.4277	3154.3269	3164.5658
3178.5032	3187.6209	3248.3177

i94 – i93

C	-1.172404	-1.155058	0.001704
C	-0.505430	0.205222	0.081801
C	-1.142171	1.323107	-0.165974
H	-1.093985	-1.668543	0.965003
H	-0.662404	-1.775140	-0.741481
H	-2.226587	-1.071906	-0.267669
H	-2.141175	1.615541	-0.460008
C	1.929632	-0.099260	-0.339258
C	0.935387	0.207496	0.482866
H	2.960145	-0.101520	-0.001906
H	1.747468	-0.346241	-1.380826
H	1.146449	0.458770	1.520059

Frequencies

-119.1643	189.3209	259.1895
302.7229	371.1878	571.0753
679.3130	689.4630	779.9009
863.7598	966.7711	1000.3881
1019.7057	1033.9068	1086.6976
1207.8088	1324.5833	1400.7671
1445.2218	1478.2500	1485.8840
1694.5187	1733.0643	3043.6843
3112.9956	3143.7321	3146.3432
3160.2777	3239.9652	3244.7077

i49 – i94

C	0.390731	1.288642	-0.052744
C	-1.782168	0.015218	0.023169
C	0.582796	-0.201155	-0.002167
C	-0.644047	-0.884918	-0.022933
C	1.846299	-0.667639	0.072227
H	0.520577	1.832468	0.880883
H	0.788440	1.811461	-0.920907
H	-1.058286	1.075886	-0.285605
H	-2.060142	0.414746	1.001526
H	-2.663053	-0.255491	-0.557953
H	-0.715889	-1.951687	-0.187434
H	2.826692	-0.228276	-0.035820

Frequencies

-1971.3994	210.3241	293.0094
350.9883	458.9297	514.4605
632.6055	669.0419	678.0760
736.7445	830.2833	899.6665
948.6448	994.6560	1016.7479
1035.2106	1173.7279	1258.3343
1377.1721	1386.1920	1410.5157
1456.0258	1501.3500	1663.7300
3062.2589	3099.1497	3157.3029
3188.4635	3215.1829	3284.3046

i93 – i97

C	1.898863	-0.259196	0.131076
C	-1.790718	-0.108684	0.203920
C	0.446612	0.053056	-0.062672
C	-0.662949	-0.852429	-0.151113
C	-0.174987	1.240508	-0.219287
H	2.512019	0.639211	0.041695
H	2.237486	-0.979166	-0.620318
H	2.076609	-0.704816	1.113904
H	-2.771294	-0.310732	-0.227175
H	-1.808549	0.434563	1.139481
H	-0.679899	-1.802354	-0.676285
H	0.132701	2.283767	-0.182841

Frequencies

-773.2380	160.0508	245.9770
334.3503	500.7794	608.4916
678.0938	739.3897	781.6425
886.8944	918.0001	955.9230
1006.7985	1025.2005	1070.0192
1200.7363	1301.2376	1408.8388
1420.1877	1489.1254	1495.5438
1528.1245	1602.0115	3044.6199
3108.4112	3122.1863	3138.9562
3160.0210	3190.5904	3233.0534

i94 – p38

C	0.791526	1.403254	0.012092
C	-2.125202	0.073358	-0.020195
C	1.045214	-0.044532	-0.000966
C	-1.115440	-0.761593	0.026118
C	1.724150	-1.057154	-0.018196
H	0.217801	1.688216	0.896379
H	0.225944	1.704024	-0.872441
H	1.741137	1.941434	0.019949
H	-3.156791	-0.282220	-0.010445
H	-1.991272	1.151309	-0.071133
H	-1.089074	-1.842141	0.077107
H	2.130771	-2.040617	-0.032537

Frequencies

-485.2558	27.6326	197.4123
219.6849	228.2954	281.8478
325.4807	376.3974	554.3385
682.0258	832.7464	901.9161
935.0024	938.9079	1038.8533
1065.1816	1111.1842	1404.0944
1417.9429	1485.7027	1495.5852
1659.0770	2071.5352	3058.0980
3093.1756	3132.8837	3142.9983
3182.3587	3236.2084	3461.5541

i93 – p38

C	1.561831	-0.997620	0.185755
C	0.932030	0.314591	-0.026442
C	0.859211	1.528487	-0.098349
H	2.622910	-0.867043	0.409215
H	1.467387	-1.622083	-0.705215
H	1.085127	-1.522931	1.015463
H	0.590912	2.551445	-0.216889
C	-2.118864	-0.022008	0.317233
C	-1.156785	-0.445359	-0.464607
H	-3.145593	-0.374248	0.210729
H	-1.927989	0.702029	1.105955
H	-1.157289	-1.135714	-1.300798

Frequencies

-495.5192	48.0600	153.1182
161.5853	189.9887	311.1281
346.0781	384.6827	555.1919
703.8826	811.6451	900.5320
931.2889	953.5939	1038.2553
1066.2731	1103.0715	1392.2846
1414.6788	1485.0234	1487.3821
1663.4921	2086.4918	3058.5988
3096.5789	3135.0747	3139.6679
3182.2590	3213.3468	3464.1147

i97 – p12

C	-1.962100	-0.108816	0.110288
C	1.547504	0.036872	-0.211486
C	-0.498380	0.048870	-0.027740
C	0.684471	-0.978511	-0.140640
C	0.372215	1.057419	-0.100082
H	-2.456736	0.863223	0.164864
H	-2.207704	-0.676773	1.014697
H	-2.376343	-0.664508	-0.738314
H	2.501885	-0.057568	2.361971
H	2.617658	0.121558	-0.339395
H	0.765356	-2.056481	-0.165137
H	0.293625	2.135538	-0.080724

Frequencies

-308.4076	65.8603	107.4393
178.6699	251.8727	313.3856
552.6499	596.8841	645.9826
733.3590	773.5512	852.5743
900.6515	1004.1403	1048.4945
1068.3160	1161.2715	1171.6242
1258.8181	1410.9351	1470.8655
1485.0248	1515.9003	1715.3929
3030.4651	3086.6701	3132.4886
3225.3660	3243.9101	3261.6915

i15 – i90

C	2.346589	0.428160	0.193685
C	1.176151	-0.327579	-0.334379
C	-0.085734	-0.531114	-0.164393
H	3.043892	-0.252413	0.687606
H	2.015897	1.178271	0.922274
H	2.884612	0.927408	-0.614653
C	-2.269108	0.582010	-0.111650
C	-1.417548	-0.367121	0.314157
H	-3.285871	0.619870	0.259823
H	-1.965547	1.331322	-0.833469
H	-1.759878	-1.118858	1.020845
H	0.564795	-1.391741	-0.826938

Frequencies

-2101.7855	94.3779	114.8581
178.2637	226.3553	285.4591
402.1159	571.0291	657.4120
740.9251	890.8834	989.2389
1002.5190	1035.5088	1044.3538
1125.3288	1310.3627	1390.9549
1428.1318	1471.2906	1484.8094
1610.2322	1999.5992	2388.6302
3021.9505	3110.1387	3132.2059
3161.3625	3171.0911	3261.7125

i31 – i89

C	1.033504	0.079661	0.428105
C	2.419201	0.211477	-0.127160
C	-1.451671	-0.498680	-0.032684
C	-2.273131	0.567495	-0.003468
C	-0.040016	-0.392525	-0.200480
H	3.178094	0.018991	0.632483
H	2.525735	1.259671	-0.424497
H	2.602810	-0.409534	-1.010941
H	-1.871410	-1.499728	-0.068628
H	-1.882920	1.578868	0.002608
H	-3.348327	0.440062	-0.014375
H	0.668698	-1.192893	0.497471

Frequencies

-965.8309	51.6848	136.8576
165.6248	240.1295	410.1365
528.4587	637.4446	782.6775
862.8261	904.9458	976.4443
1026.9823	1069.7690	1121.1978
1194.0605	1311.7112	1394.0464
1428.9937	1464.5392	1488.9367
1595.2559	1700.1015	2268.3837
3028.7722	3110.4607	3134.7424
3164.7415	3184.0292	3262.7705

i68 – i93

C	1.829120	-0.428308	0.000005
C	-1.894330	-0.128085	0.000009
C	0.428830	0.098977	-0.000030
C	-0.763167	-0.811135	-0.000026
C	0.035719	1.364949	-0.000002
H	2.562447	0.379285	-0.000558
H	2.003537	-1.054496	-0.881132
H	2.003829	-1.053423	0.881848
H	-2.940827	-0.398654	0.000079
H	-1.327042	1.129564	0.000008
H	-0.674312	-1.893878	0.000018
H	0.555337	2.313213	0.000002

Frequencies

-2080.6669	136.3609	216.1649
327.1942	479.3113	610.1010
610.9460	659.5348	673.0174
845.0552	902.7905	968.3858
981.6087	1025.7003	1044.4977
1057.2873	1184.4147	1312.0971
1412.9517	1481.6644	1484.4164
1638.7941	1702.4621	1761.4761
3041.9894	3102.5559	3145.1600
3179.4084	3249.9972	3250.9440

i70 – i97

C	1.928696	-0.061927	0.030334
C	-1.600406	0.104152	0.020194
C	0.449968	0.033365	-0.089191
C	-0.459985	1.047568	-0.051805
C	-0.623321	-0.998972	-0.027652
H	2.217280	-0.511091	0.987238
H	2.384263	0.928545	-0.033151
H	2.356690	-0.683969	-0.761872
H	-1.365946	-0.697636	1.060738
H	-2.639507	0.123358	-0.279898
H	-0.382407	2.114987	0.104344
H	-0.740086	-2.019314	-0.368682

Frequencies

-2053.6503	119.6190	259.3803
328.3041	591.5248	662.3279
679.1713	787.2779	814.6429
903.7957	971.8871	989.7292
1038.5049	1063.9206	1170.2087
1227.1636	1271.3453	1279.1044
1327.4165	1411.3589	1477.5301
1491.8027	1639.1082	1974.6931
3036.6655	3096.0533	3131.0098
3219.1872	3232.9670	3243.3797

i70 – i89

C	0.613792	0.007460	0.140338
C	2.068025	-0.232881	0.041983
C	-1.520310	0.386284	0.079477
C	-1.284010	-0.984862	-0.082270
C	-0.253558	1.010460	-0.118242
H	2.283008	-0.996347	-0.712126
H	2.483060	-0.585412	0.991056
H	2.595004	0.685940	-0.246759
H	-2.401194	0.824477	0.536310
H	-0.822345	-1.344247	-0.993410
H	-1.852217	-1.736865	0.465478
H	-0.028952	2.033684	-0.408263

Frequencies

-740.5863	143.5128	235.4413
260.3122	464.1586	634.0906
687.4908	773.2835	874.6444
932.2229	941.3369	1005.9509
1037.5001	1049.3798	1071.8933
1199.1017	1304.6277	1394.3444
1420.0374	1461.7265	1479.7727
1521.4187	1617.6207	3013.4565
3088.4773	3101.6791	3121.6181
3165.4476	3198.6809	3223.1888

i93 – p23

C	1.730160	-1.128832	0.177155
C	-2.066574	-0.180970	0.258867
C	0.241474	0.514906	-0.143921
C	-0.907017	-0.330832	-0.375739
C	0.802689	1.598040	-0.029319
H	2.635775	-0.595047	0.437090
H	1.714725	-1.598708	-0.800353
H	1.233513	-1.658536	0.982185
H	-2.901641	-0.838655	0.047739
H	-2.207383	0.595967	1.001420
H	-0.782217	-1.126458	-1.103615
H	1.502835	2.387561	0.113280

Frequencies

-573.9845	72.5002	77.3489
217.2424	244.4774	321.1374
494.5212	527.7310	557.8237
570.0735	693.8442	698.0450
870.5543	918.0819	969.9273
1030.8242	1109.6239	1330.3936
1418.4544	1425.6705	1437.2253
1696.5547	2029.3504	3095.5706
3160.5186	3183.7128	3257.6286
3257.9176	3265.3639	3452.2658

i80 – p40

C	1.967340	-0.595826	0.112538
C	-1.967357	-0.595794	0.112547
C	0.664486	0.063920	-0.096093
C	-0.664493	0.063933	-0.096089
C	0.000007	1.258370	-0.457458
H	2.628732	-0.377560	-0.728955
H	1.877654	-1.675067	0.243830
H	2.433321	-0.168448	1.004862
H	-1.877688	-1.675043	0.243787
H	-2.628771	-0.377473	-0.728915
H	-2.433302	-0.168451	1.004906
H	0.000157	3.274420	1.507816

Frequencies

-189.1591	53.8332	66.6810
78.7372	87.8041	206.5467
294.3763	424.5198	492.9112
734.9173	801.5108	1012.6277
1030.6875	1048.9134	1086.4668
1330.6204	1332.1386	1402.0102
1408.0135	1479.6807	1485.1535
1488.1354	1488.9262	1896.9902
3056.9372	3057.7704	3132.3381
3132.3532	3147.3602	3147.7490

i87 – p41-m1

C	2.615385	0.134792	0.100184
C	-2.541577	0.204124	0.144889
C	1.223588	-0.250991	-0.028469
C	-1.307886	-0.526144	-0.178239
C	-0.025039	-0.171348	-0.120286
H	3.292239	-0.597139	-0.348099
H	2.878681	0.236510	1.158141
H	2.783779	1.108829	-0.374880
H	-2.592891	0.362035	1.231027
H	-3.440655	-0.334257	-0.159926
H	-2.541609	1.199007	-0.319184
H	-0.166372	1.682420	-0.695553

Frequencies

-624.4541	83.7581	94.2938
117.9572	129.4778	182.0626
264.6664	418.3681	475.4761
521.8387	727.5422	859.1734
994.3144	1008.4969	1046.9151
1072.8988	1375.3345	1398.5481
1448.5639	1461.9941	1465.8385
1476.4124	1481.3078	1914.6238
3006.395	3021.8003	3067.0013
3091.7095	3109.8765	3119.8252

i88 – p41-m3

C	2.654190	-0.267466	-0.008688
C	1.231970	0.037261	0.010741
C	-0.043159	-0.032649	0.009618
C	-2.758248	-0.044560	-0.010334
C	-1.307046	-0.033084	0.016811
H	3.149760	0.200032	-0.866309
H	2.824491	-1.348534	-0.073277
H	3.152015	0.096343	0.896536
H	1.673281	3.237289	-0.008751
H	-3.135979	-0.858231	-0.639290
H	-3.153830	0.895188	-0.411288
H	-3.175976	-0.179102	0.993488

Frequencies

-168.8653	48.1757	53.3944
65.1297	72.2710	88.7521
91.9673	125.4975	365.2925
371.7060	640.7936	995.9713
1021.4280	1024.3655	1027.6008
1032.0868	1411.8946	1416.3907
1467.5138	1470.7943	1476.6234
1477.3215	1667.6116	1808.7506
3016.2195	3017.6181	3081.0784
3082.8344	3085.5263	3087.5103

i83 - Complex 1

C	-2.009219	-0.932570	0.003065
C	-1.591377	0.451814	-0.124983
C	-1.120839	1.598974	0.080345
H	-1.512544	-1.563430	-0.738290
H	-3.093071	-1.029707	-0.092926
H	-1.727407	-1.297799	0.997127
C	2.355812	0.458156	-0.023223
C	1.978785	-0.810030	0.032946
H	3.398531	0.734626	-0.143509
H	1.631585	1.262977	0.051174
H	2.689925	-1.626823	-0.037716
H	0.934012	-1.077910	0.155240

Frequencies

-52.6614	37.3608	61.5792
83.9812	96.9508	115.5551
183.6796	348.5325	836.6125
841.3309	870.9311	956.5369
973.5887	1004.4614	1074.7312
1241.9577	1385.1510	1392.3734
1451.5615	1463.0209	1470.6158
1559.1193	1713.0977	3036.2370
3107.9834	3126.0466	3137.3117
3155.5934	3220.8473	3245.2168

PRODUCTS

p38 including r1

C	-0.219309	-0.000049	-0.000487
C	1.238422	0.000063	0.000065
C	-1.418043	0.000183	0.000101
H	1.625265	1.019893	-0.061176
H	1.625734	-0.563676	-0.851769
H	1.623707	-0.456790	0.914489
H	-2.481130	-0.000610	0.000383

Frequencies

345.6904	348.5038	682.8639
682.9795	951.9958	1056.5401
1060.9036	1416.6621	1481.6220
1487.1634	2257.1935	3057.6595
3132.0095	3132.4546	3484.7942

p39 including r2

C	-1.524574	0.054857	-0.001553
C	-0.052656	-0.011958	-0.002572
C	1.089015	-0.857835	0.000157
C	1.145322	0.553943	0.000514
H	-1.891262	-0.375250	0.934442
H	-1.912526	-0.569459	-0.809944
H	-1.903718	1.072145	-0.104077
H	1.764866	1.438516	0.000298

Frequencies

51.0268	333.3637	383.8329
766.7491	905.8706	921.4238
1015.6511	1043.7603	1214.5759
1328.5760	1398.4025	1478.0412
1483.3541	1803.5350	3058.6354
3132.6782	3153.6193	3249.3435

p40 including H

C	1.964741	-0.530458	-0.002155
C	-1.964741	-0.530458	-0.002155
C	0.664150	0.166375	-0.003548
C	-0.664150	0.166375	-0.003548
C	0.000000	1.416092	0.000948
H	2.616807	-0.092356	-0.761318
H	1.868477	-1.603668	-0.173041
H	2.447011	-0.367756	0.965736
H	-1.868477	-1.603668	-0.173037
H	-2.616805	-0.092359	-0.761321
H	-2.447013	-0.367753	0.965734

Frequencies

106.6634	115.7906	201.6987
287.9918	421.9525	492.7620
735.1999	798.1811	1017.0935
1031.5793	1052.5613	1085.5674
1327.9242	1334.1151	1404.5069
1409.7260	1482.5953	1487.6508
1490.1742	1490.5355	1897.3263
3055.1780	3056.0051	3129.3246
3129.3515	3146.9792	3147.3925

p41-m1 including H

C	2.568524	0.181310	-0.000516
C	-2.404517	0.382523	-0.014580
C	1.136923	-0.040133	-0.009252
C	-1.365954	-0.671951	-0.012662
C	-0.065326	-0.280229	-0.005003
H	3.065853	-0.490774	-0.706142
H	2.951484	-0.069448	0.994354
H	2.846068	1.214143	-0.225251
H	-2.630560	0.506905	1.058128
H	-3.337962	0.042472	-0.468181
H	-2.112786	1.367579	-0.400829

Frequencies

37.1099	111.7589	136.7999
209.1378	217.5150	443.6031
547.4488	726.2439	789.2720
1020.9404	1036.2214	1063.8710
1079.0862	1329.5504	1356.9005
1398.7426	1424.5305	1464.3290
1486.3563	1500.2205	2152.6232
2989.3460	3039.4253	3052.4857
3112.4611	3114.8121	3117.1015

p41-m3 including H

C	-2.720198	0.009252	0.001384
C	2.720201	0.008960	-0.001614
C	-1.269092	-0.012993	-0.006700
C	1.269076	-0.012128	0.007032
C	-0.000039	-0.008479	0.000116
H	-3.117311	0.422198	-0.932720
H	-3.103694	0.623062	0.824359
H	-3.133572	-0.998626	0.119714
H	3.107486	0.318892	-0.978830
H	3.134798	-0.980764	0.220197
H	3.112603	0.707563	0.745972

Frequencies

16.3272	47.7974	60.7661
66.1999	68.6091	371.2411
371.9596	634.1908	1004.5881
1017.6306	1018.9933	1024.5301
1027.6799	1409.5038	1414.1084
1468.9423	1470.2872	1473.8465
1475.6521	1689.1690	1808.5110
3013.6116	3014.9108	3078.5841
3078.9516	3081.1769	3081.6558

p42 including r8

C	0.662180	-0.000023	-0.000018
C	-0.662353	-0.000121	-0.000218
H	1.232150	-0.923294	0.000530
H	1.230524	0.924249	-0.000145
H	-1.230724	-0.924023	0.000178
H	-1.230909	0.923936	0.000852

Frequencies

839.2527	982.4793	991.2431
1072.0636	1241.4943	1387.9480
1470.8495	1715.0755	3142.8807
3162.9756	3224.7554	3251.2187

RADICALS

r1

C	0.586124	0.030174	0.000070
C	-0.705694	-0.145146	-0.000004
H	1.281449	-0.806476	-0.000191
H	1.031818	1.027773	-0.000133
H	-1.595847	0.468530	-0.000073

Frequencies

713.5131	840.0178	933.4653
1052.5848	1393.7358	1668.6491
3080.9921	3175.0374	3245.4203

r2

C	-0.000134	-0.000001	0.000023
H	-1.080503	0.038158	-0.000046
H	0.507588	-0.954443	-0.000046
H	0.573721	0.916289	-0.000046

Frequencies

470.9451	1399.8856	1409.5749
3117.6199	3301.0861	3304.8947

r8

C	1.123284	0.027275	0.000131
C	-0.320711	-0.140148	-0.000084
C	-1.552808	0.068747	0.000067
H	1.570476	-0.421470	-0.889846
H	1.569551	-0.409861	0.896285
H	1.361383	1.096088	-0.007126

Frequencies

122.1309	356.0273	826.0899
862.9238	976.1288	1393.8684
1404.9662	1457.5578	1492.4161
3044.7347	3116.6419	3133.0016