

Looking at the big picture in ASM/EDA analysis: the case of the *ortho-para* regioselectivity rule in Diels-Alder reactions

Nicolás Grimblat* and Ariel M. Sarotti*

grimblat@iquir-conicet.gov.ar

sarotti@iquir-conicet.gov.ar

Instituto de Química Rosario (IQUIR, CONICET-UNR) and Facultad de Ciencias Bioquímicas y Farmacéuticas, Universidad Nacional de Rosario, Suipacha 531, S2002LRK Rosario, Argentina.

Supporting Information

Table of contents

- **Table S1** D/I-ASM energies. Page S2

- **Table S2** EDA energies. Page S3

- Cartesian coordinates, energies, and number of imaginary vibrational frequencies of stationary points at M06-2X/def2-TZVPP. Page S4-S9

Table S1

Energies from the distortion/interaction-Activation Strain Model of the reaction of methyl acrylate with all dienes under study

1 + 2 ortho			
$r(\text{C}\cdots\text{C}) / \text{\AA}$	ΔE_{dist}	ΔE	ΔE_{int}
2.19	51.75	11.84	-39.91
2.29	28.41	14.96	-13.45
2.33	20.54	14.39	-6.15
2.40	15.40	13.03	-2.37
2.47	12.05	11.32	-0.73
2.53	9.94	9.52	-0.43
2.60	8.68	7.79	-0.90
2.73	7.43	4.99	-2.44
2.95	6.57	1.99	-4.58

1 + 2 meta			
$r(\text{C}\cdots\text{C}) / \text{\AA}$	ΔE_{dist}	ΔE	ΔE_{int}
2.08	56.36	13.77	-42.59
2.18	30.94	17.53	-13.41
2.22	22.16	16.92	-5.24
2.29	16.10	15.43	-0.66
2.35	11.92	13.47	1.55
2.42	9.19	11.32	2.13
2.55	6.58	7.28	0.70
2.67	5.60	4.23	-1.36
2.93	4.12	0.23	-3.89

1 + 3 meta			
$r(\text{C}\cdots\text{C}) / \text{\AA}$	ΔE_{dist}	ΔE	ΔE_{int}
2.21	49.80	13.20	-36.61
2.32	29.93	15.86	-14.07
2.35	22.93	15.36	-7.57
2.42	18.18	14.19	-4.00
2.48	14.94	12.70	-2.24
2.55	12.76	11.11	-1.65
2.62	11.34	9.55	-1.79
2.74	9.93	6.92	-3.01
2.80	9.63	5.93	-3.70
2.97	9.10	4.01	-5.09

1 + 3 para			
$r(\text{C}\cdots\text{C}) / \text{\AA}$	ΔE_{dist}	ΔE	ΔE_{int}
2.11	53.78	14.91	-38.87
2.21	29.81	18.46	-11.35
2.28	21.49	17.83	-3.65
2.35	15.63	16.28	0.65
2.42	11.49	14.23	2.74
2.48	8.69	11.95	3.27
2.55	6.88	9.68	2.80
2.74	4.62	4.34	-0.28
2.85	4.13	2.19	-1.94
3.02	3.74	0.45	-3.28

1 + 4 ortho/para			
$r(\text{C}\cdots\text{C}) / \text{\AA}$	ΔE_{dist}	ΔE	ΔE_{int}
2.18	59.09	6.13	-52.96
2.22	53.13	8.71	-44.42
2.39	27.08	11.56	-15.52
2.46	20.42	11.10	-9.33
2.53	16.15	10.03	-6.13
2.59	13.41	8.71	-4.70
2.66	11.68	7.33	-4.35
2.72	10.65	6.02	-4.63
2.78	10.01	4.86	-5.16
2.90	9.29	3.11	-6.19

1 + 4 meta/meta			
$r(\text{C}\cdots\text{C}) / \text{\AA}$	ΔE_{dist}	ΔE	ΔE_{int}
2.06	57.95	13.45	-44.50
2.20	32.89	17.25	-15.64
2.27	24.40	16.62	-7.78
2.34	18.54	15.12	-3.43
2.41	14.54	13.14	-1.40
2.47	11.97	11.00	-0.98
2.54	10.47	8.92	-1.55
2.61	9.63	7.06	-2.57
2.73	8.82	4.15	-4.66
2.89	8.07	1.51	-6.55

1 + 5 ortho/meta			
$r(\text{C}\cdots\text{C}) / \text{\AA}$	ΔE_{dist}	ΔE	ΔE_{int}
2.21	40.70	7.02	-33.68
2.25	34.55	7.03	-27.52
2.32	24.57	7.77	-16.80
2.35	17.15	7.24	-9.91
2.42	12.31	5.97	-6.34
2.49	9.15	4.33	-4.82
2.56	7.20	2.61	-4.59
2.63	6.06	1.01	-5.05
2.69	5.38	-0.37	-5.76
2.93	4.30	-3.68	-7.98

1 + 5 meta/para			
$r(\text{C}\cdots\text{C}) / \text{\AA}$	ΔE_{dist}	ΔE	ΔE_{int}
2.23	35.09	9.22	-25.87
2.26	25.57	9.87	-15.71
2.30	18.30	9.40	-8.90
2.37	13.25	8.27	-4.98
2.43	9.85	6.81	-3.04
2.50	7.68	5.25	-2.43
2.57	6.37	3.77	-2.60
2.69	5.12	1.36	-3.76
2.80	4.51	-0.34	-4.85
2.94	3.66	-1.95	-5.61

Table S2

Energies from the Energy Decomposition Analysis of the reaction of methyl acrylate with all dienes under study

1 + 2 <i>ortho</i>				
$r(\text{C}\cdots\text{C}) / \text{\AA}$	ΔE_{int}	ΔE_{Pauli}	ΔE_{elstat}	ΔE_{oi}
2.19	-39.87	153.4	-79.46	-113.81
2.29	-13.13	98.7	-52	-59.83
2.33	-5.81	79.62	-42.48	-42.95
2.40	-2.12	64.11	-35.07	-31.16
2.47	-0.44	51.86	-29.16	-23.14
2.53	-0.24	41.93	-24.58	-17.59
2.60	-0.66	34.19	-20.86	-13.99
2.73	-2.3	22.87	-15.61	-9.56
2.95	-4.43	11.19	-9.87	-5.75

1 + 2 <i>meta</i>				
$r(\text{C}\cdots\text{C}) / \text{\AA}$	ΔE_{int}	ΔE_{Pauli}	ΔE_{elstat}	ΔE_{oi}
2.08	-45.68	145.19	-75.9	-114.97
2.18	-13.12	103.26	-54.11	-62.27
2.22	-4.94	86.62	-45.71	-45.85
2.29	-0.36	72.17	-38.66	-33.87
2.35	1.8	60.34	-32.97	-25.57
2.42	2.34	50.01	-28.11	-19.56
2.55	0.85	34.46	-20.84	-12.77
2.67	-1.21	23.66	-15.8	-9.07
2.93	-3.75	10.09	-8.89	-4.95

1 + 3 <i>meta</i>				
$r(\text{C}\cdots\text{C}) / \text{\AA}$	ΔE_{int}	ΔE_{Pauli}	ΔE_{elstat}	ΔE_{oi}
2.21	-40.91	149.92	-77.57	-113.26
2.31	-11.08	104.9	-54.21	-61.77
2.35	-3.39	87.62	-45.57	-45.44
2.42	0.86	73.11	-38.85	-33.4
2.48	2.95	60.98	-32.65	-25.38
2.55	3.4	50.73	-28.13	-19.2
2.61	2.94	42.26	-23.83	-15.49
2.74	-0.14	24.11	-15.51	-8.74
2.80	-1.76	16.63	-11.55	-6.84
2.97	-3.11	9.51	-7.97	-4.65

1 + 3 <i>para</i>				
$r(\text{C}\cdots\text{C}) / \text{\AA}$	ΔE_{int}	ΔE_{Pauli}	ΔE_{elstat}	ΔE_{oi}
2.11	-36.97	150.73	-80.64	-107.06
2.21	-13.75	100.45	-55.13	-59.07
2.28	-7.3	82.18	-45.72	-43.76
2.35	-3.74	67.18	-38.46	-32.46
2.42	-1.98	55.19	-32.42	-24.75
2.48	-1.46	45.26	-27.83	-18.89
2.55	-1.56	37.36	-23.79	-15.13
2.74	-2.81	25.46	-18.17	-10.1
2.85	-3.46	21.28	-15.9	-8.84
3.02	-4.91	12.57	-11.53	-5.95

1 + 4 <i>ortho/para</i>				
$r(\text{C}\cdots\text{C}) / \text{\AA}$	ΔE_{int}	ΔE_{Pauli}	ΔE_{elstat}	ΔE_{oi}
2.18	-52.52	210.21	-111.32	-151.41
2.22	-44.96	186.08	-99.31	-131.73
2.39	-15.19	99.88	-56.05	-59.02
2.46	-8.98	78.27	-45	-42.25
2.53	-5.82	61.74	-36.8	-30.76
2.59	-4.44	49.06	-30.58	-22.92
2.66	-4.21	39.22	-25.9	-17.53
2.72	-4.42	31.76	-22.13	-14.05
2.78	-5.02	25.85	-19.33	-11.54
2.90	-6.02	17.94	-15.33	-8.63

1 + 4 <i>meta/meta</i>				
$r(\text{C}\cdots\text{C}) / \text{\AA}$	ΔE_{int}	ΔE_{Pauli}	ΔE_{elstat}	ΔE_{oi}
2.06	-44.47	145.83	-79.46	-110.84
2.20	-15.29	103.59	-57.21	-61.67
2.27	-7.44	86.64	-48.76	-45.32
2.34	-3.08	72.65	-41.68	-34.05
2.41	-1.11	60.61	-35.84	-25.88
2.47	-0.76	50.23	-31.04	-19.95
2.54	-1.35	41.91	-26.97	-16.29
2.61	-2.38	34.61	-23.65	-13.34
2.73	-4.44	24.14	-18.53	-10.05
2.89	-6.35	14.57	-13.87	-7.05

1 + 5 <i>ortho/meta</i>				
$r(\text{C}\cdots\text{C}) / \text{\AA}$	ΔE_{int}	ΔE_{Pauli}	ΔE_{elstat}	ΔE_{oi}
2.21	-34.08	128.48	-70.3	-92.26
2.25	-26.94	115	-63.42	-78.52
2.32	-16.21	92.48	-52.06	-56.63
2.35	-9.38	74.67	-43.22	-40.83
2.42	-5.82	60.57	-36.36	-30.03
2.49	-4.32	49.31	-30.98	-22.65
2.56	-4.1	40.36	-26.73	-17.73
2.63	-4.6	33.24	-23.38	-14.46
2.69	-5.33	27.55	-20.69	-12.19
2.93	-7.58	14.04	-14.11	-7.51

1 + 5 <i>meta/para</i>				
$r(\text{C}\cdots\text{C}) / \text{\AA}$	ΔE_{int}	ΔE_{Pauli}	ΔE_{elstat}	ΔE_{oi}
2.23	-25.48	115.24	-63.21	-77.51
2.26	-15.31	95.59	-52.93	-57.97
2.30	-8.51	79.33	-44.56	-43.28
2.37	-4.62	66	-37.83	-32.79
2.43	-2.72	54.9	-32.33	-25.29
2.50	-2.13	45.61	-27.78	-19.96
2.57	-2.33	37.86	-24.02	-16.17
2.69	-3.54	26.26	-18.36	-11.44
2.80	-4.65	18.91	-14.65	-8.91
2.94	-5.39	12.58	-11.2	-6.77

Table S3

Cartesian coordinates (Å), energies (Hartree), and imaginary vibrational frequencies of the optimized structures.

1

M062X/def2TZVPP geometry

C	1.317365	-0.647473	-0.000001
C	0.039941	0.110015	0.000000
C	2.472189	-0.001035	-0.000001
O	-0.061812	1.306908	0.000001
O	-1.012436	-0.720373	0.000000
C	-2.286515	-0.081954	0.000001
H	1.247306	-1.726352	-0.000001
H	3.415898	-0.528214	-0.000002
H	2.485943	1.081482	0.000000
H	-3.021300	-0.880388	0.000001
H	-2.395867	0.541933	0.885418
H	-2.395868	0.541934	-0.885415

Number of imaginary frequencies = 0

ZPE Energy (M062X/def2TZVPP) = -306.367305

Free Energy (M062X/def2TZVPP) = -306.398155

2

M062X/def2TZVPP geometry

C	0.436647	0.091518	-0.000005
C	1.824804	-0.339049	-0.000003
C	2.872048	0.481899	0.000004
C	-0.563134	-0.796114	0.000000
H	1.994061	-1.411960	-0.000006
H	3.884419	0.104696	0.000006
H	2.742802	1.557277	0.000008
O	-1.884815	-0.552904	0.000004
C	-2.277994	0.802199	-0.000001
H	0.243515	1.156484	-0.000007
H	-0.368592	-1.861990	0.000002
H	-3.363667	0.809871	0.000009
H	-1.904116	1.313073	0.890732
H	-1.904134	1.313063	-0.890746

Number of imaginary frequencies = 0

ZPE Energy (M062X/def2TZVPP) = -270.380553

Free Energy (M062X/def2TZVPP) = -270.410859

3

M062X/def2TZVPP geometry

C	-2.166565	-0.768170	0.000224
C	-1.485347	0.370292	-0.000256
C	-0.020695	0.455844	-0.000056
C	0.618848	1.629826	0.000186
O	0.572865	-0.759578	-0.000148
C	1.981025	-0.786511	-0.000006
H	-3.247297	-0.768988	0.000082
H	-1.658427	-1.722345	0.000648
H	-2.000013	1.323044	-0.000744
H	1.692707	1.723299	0.000298
H	0.035476	2.537174	0.000274
H	2.269752	-1.833600	0.000134
H	2.380728	-0.294931	-0.890494
H	2.380555	-0.294713	0.890438

Number of imaginary frequencies = 0

ZPE Energy (M062X/def2TZVPP) = -270.382389

Free Energy (M062X/def2TZVPP) = -270.412513

4

M062X/def2TZVPP geometry

C	1.473231	1.476088	0.306370
C	1.013107	0.235613	0.118907
C	-0.401713	-0.153250	0.154489
C	-1.364655	0.641569	-0.312711
O	1.788643	-0.854720	-0.119022
C	3.182601	-0.657836	-0.140232
O	-2.687416	0.406232	-0.319265
C	-3.115711	-0.814578	0.244449
H	2.516426	1.734266	0.223897
H	0.779534	2.260944	0.561284
H	-0.610419	-1.141383	0.540334
H	-1.139200	1.601221	-0.760692
H	3.630669	-1.635011	-0.296867
H	3.470761	0.011843	-0.954370
H	3.531245	-0.238231	0.806969
H	-4.198731	-0.827870	0.168753
H	-2.814840	-0.881612	1.292880
H	-2.696422	-1.661895	-0.303523

Number of imaginary frequencies = 0

ZPE Energy (M062X/def2TZVPP) = -384.874500

Free Energy (M062X/def2TZVPP) = -384.908337

5

M062X/def2TZVPP geometry

C	-1.829080	2.018189	-0.319027
C	-1.594596	0.928603	0.404609
C	-0.441309	0.036382	0.250123
C	0.786569	0.490368	-0.013552
O	1.837156	-0.331960	-0.223976
C	3.096249	0.252915	0.033910
H	-2.669316	2.663759	-0.103985
H	-1.187042	2.292037	-1.146736
H	-2.287411	0.642675	1.191502
H	0.975763	1.557823	-0.060871
H	3.849698	-0.478096	-0.246312
H	3.203836	0.497887	1.093161
H	3.234420	1.160674	-0.560843
O	-0.644186	-1.298089	0.480747
C	-1.563047	-1.905170	-0.409176
H	-2.544947	-1.427214	-0.356711
H	-1.195953	-1.851101	-1.437099
H	-1.651523	-2.945767	-0.107604

Number of imaginary frequencies = 0

ZPE Energy (M062X/def2TZVPP) = -384.859446

Free Energy (M062X/def2TZVPP) = -384.895521

TS-1+2-MN

M062X/def2TZVPP geometry

C	-1.404657	0.769814	-0.947683
C	-0.212905	1.489411	-1.001277
C	0.403344	1.975037	0.128434
C	-2.046713	0.538377	0.260458

O	-3.154161	-0.231014	0.406680
C	-3.398990	-1.190925	-0.599292
H	-1.708950	0.220713	-1.827519
H	0.346091	1.462612	-1.928009
H	-0.169709	2.272163	0.994637
H	1.389630	2.414646	0.060589
H	-2.012995	1.286964	1.039105
H	-2.497928	-1.772707	-0.812573
H	-3.742545	-0.715829	-1.521133
H	-4.178160	-1.845456	-0.219391
C	0.683530	0.046068	1.234005
C	-0.565955	-0.541758	1.335083
C	1.604640	-0.496294	0.224835
O	2.872268	-0.081627	0.408225
O	1.277603	-1.218347	-0.684536
C	3.806828	-0.553561	-0.555008
H	1.127461	0.588143	2.055437
H	-0.750420	-1.434054	0.753887
H	-1.123559	-0.447862	2.256021
H	4.770551	-0.149941	-0.260284
H	3.834321	-1.641955	-0.559792
H	3.535785	-0.206544	-1.551252

Number of imaginary frequencies = 1 (-536.9257)
 ZPE Energy (M062X/def2TZVPP) = -576.716673
 Free Energy (M062X/def2TZVPP) = -576.756074

TS-1+2-ON

M062X/def2TZVPP geometry

C	-2.298583	0.211059	-1.058113
C	-1.074626	0.854602	-1.246695
C	-0.383308	1.416030	-0.208635
C	-2.911883	0.091467	0.175713
O	0.857330	1.880315	-0.410637
C	1.517962	2.368451	0.742449
H	-2.677464	-0.380559	-1.882272
H	-0.557535	0.753935	-2.191838
H	-0.854275	1.710289	0.721047
H	-3.852681	-0.438841	0.238905
H	-2.795408	0.875702	0.911451
H	1.699098	1.554124	1.445441
H	0.928505	3.154920	1.219923
H	2.466641	2.779640	0.410112
C	-0.362097	-0.703753	1.194675
C	-1.666648	-1.167063	1.193747
C	0.565024	-1.220882	0.201892
O	1.836122	-0.814421	0.431389
O	0.267447	-1.920548	-0.739229
C	2.776881	-1.194221	-0.563433
H	0.044416	-0.140469	2.021861
H	-1.879426	-2.030819	0.579773
H	-2.243639	-1.087987	2.105564
H	3.738005	-0.814081	-0.229416
H	2.811698	-2.277294	-0.668259
H	2.508542	-0.755477	-1.524084

Number of imaginary frequencies = 1 (-479.7328)
 ZPE Energy (M062X/def2TZVPP) = -576.721151
 Free Energy (M062X/def2TZVPP) = -576.760211

TS-1+3-MN

M062X/def2TZVPP geometry

C	2.218372	-0.365448	-0.536779
C	1.231446	-1.047512	0.189690
C	0.745496	-0.524195	1.364455
C	2.726312	0.841201	-0.105854
H	3.429889	1.363344	-0.740678
H	2.374756	-0.689106	-1.557948
O	0.668797	-2.093350	-0.471379
H	1.391856	0.091057	1.965833
H	-0.105618	-0.947814	1.875715
H	2.857723	1.027319	0.950577
C	-0.473609	-2.679862	0.100008
H	-1.283222	-1.950388	0.191754
H	-0.255423	-3.099338	1.086409
H	-0.780767	-3.475212	-0.573105
C	0.046932	1.581647	0.580216
C	1.104600	2.127074	-0.128180
C	-1.027686	0.932447	-0.174884
O	-2.143015	0.750533	0.566085
O	-0.950840	0.588756	-1.329123
C	-3.256629	0.217102	-0.139537
H	-0.176170	1.878426	1.593881
H	1.020297	2.144170	-1.205095
H	1.661531	2.938142	0.320569
H	-3.573433	0.903349	-0.924022
H	-3.006724	-0.738081	-0.598983
H	-4.045636	0.091893	0.595631

Number of imaginary frequencies = 1 (-538.5433)
 ZPE Energy (M062X/def2TZVPP) = -576.716979
 Free Energy (M062X/def2TZVPP) = -576.755566

TS-1+3-PN

M062X/def2TZVPP geometry

C	1.836227	0.095528	0.335586
C	0.893263	-0.180249	1.359490
C	0.105445	0.793450	1.876099
C	2.030847	1.383905	-0.128209
H	2.760569	1.519733	-0.914526
O	2.427782	-0.879299	-0.379773
H	0.655941	-1.210321	1.583450
H	0.338586	1.841605	1.787809
H	-0.701690	0.541730	2.550652
H	1.920198	2.205466	0.560497
C	-0.852641	1.519919	-0.410789
C	0.296015	1.742162	-1.151929
C	-1.444250	0.200084	-0.459411
O	-2.666499	0.139892	0.113244
O	-0.910526	-0.779087	-0.944589
C	-3.265379	-1.147125	0.124639
H	-1.403753	2.315200	0.066905
H	0.536851	1.012530	-1.914307
H	0.572254	2.764170	-1.376440
H	-3.360846	-1.538927	-0.886738
H	-2.666561	-1.843357	0.712230
H	-4.244591	-1.019456	0.576515
C	1.945335	-2.207765	-0.263293
H	0.872624	-2.238379	-0.461641
H	2.163728	-2.619182	0.724488
H	2.481455	-2.782306	-1.013058

Number of imaginary frequencies = 1 (-464.1776)
ZPE Energy (M062X/def2TZVPP) = -576.721224
Free Energy (M062X/def2TZVPP) = -576.759828

TS-1+4-MMN

M062X/def2TZVPP geometry

C	-1.106479	1.185860	0.070100
C	0.069506	1.168031	0.826096
C	0.285227	0.207788	1.790750
C	-2.094490	0.240230	0.261490
O	-3.163942	0.277998	-0.571791
H	-1.184558	1.789917	-0.821986
O	1.153620	1.928720	0.507645
H	-0.544832	-0.204724	2.339646
H	1.256642	0.153146	2.261526
H	-2.288749	-0.187060	1.238744
C	1.125974	2.662112	-0.699470
H	0.352939	3.434371	-0.673172
H	0.967464	1.999793	-1.552144
H	2.099211	3.138699	-0.783037
C	0.186133	-1.612882	0.443870
C	-1.045358	-1.629050	-0.179336
C	1.338582	-1.112896	-0.322681
O	2.513149	-1.376747	0.273502
O	1.253486	-0.504137	-1.362008
C	3.651841	-0.809948	-0.365303
H	0.405028	-2.231953	1.300931
H	-1.099802	-1.388411	-1.231426
H	-1.815952	-2.276072	0.216807
H	4.507732	-1.097896	0.237120
H	3.752388	-1.193120	-1.379381
H	3.557855	0.274798	-0.402400
C	-4.183959	-0.656417	-0.296542
H	-4.469693	-0.624789	0.758448
H	-3.868359	-1.669055	-0.555656
H	-5.039681	-0.381280	-0.906644

Number of imaginary frequencies = 1 (-505.5637)
ZPE Energy (M062X/def2TZVPP) = -691.210466
Free Energy (M062X/def2TZVPP) = -691.252402

TS-1+4-OPN

M062X/def2TZVPP geometry

C	-1.914004	0.690459	-0.149600
C	-0.744442	0.889813	-0.920118
C	0.350677	1.501333	-0.406959
C	-2.052805	1.165968	1.143468
H	-3.001956	0.987607	1.629087
O	-2.886545	-0.141629	-0.562889
H	-0.624329	0.390913	-1.869969
H	0.339411	2.076287	0.509425
O	1.490436	1.531375	-1.104914
H	-1.545382	2.075343	1.423839
C	0.447148	-0.185755	1.734311
C	-0.862723	-0.143378	2.179219
C	0.801480	-1.124915	0.702146
O	2.126719	-1.099897	0.404158
O	0.031064	-1.864326	0.117435
C	2.519778	-1.945369	-0.665938
H	1.232394	0.400249	2.188855
H	-1.491349	-0.992593	1.942562

H	-1.071135	0.340407	3.124625
H	2.021573	-1.648184	-1.588781
H	3.595299	-1.826756	-0.764866
H	2.271272	-2.983520	-0.450832
C	-2.627077	-1.025067	-1.643040
H	-1.717325	-1.596516	-1.450958
H	-2.546081	-0.478379	-2.584702
H	-3.485124	-1.689078	-1.691393
C	2.616312	2.026194	-0.397994
H	2.849856	1.365138	0.437795
H	2.428285	3.040431	-0.038594
H	3.445143	2.038770	-1.099391

Number of imaginary frequencies = 1 (-419.6554)
ZPE Energy (M062X/def2TZVPP) = -691.220931
Free Energy (M062X/def2TZVPP) = -691.263099

TS-1+5-MPN

M062X/def2TZVPP geometry

C	-1.130800	0.822638	0.563144
C	0.002258	0.826387	1.398073
C	0.484733	-0.309364	1.979504
C	-1.852289	-0.351064	0.367883
O	-1.469703	1.850183	-0.237564
H	0.632997	1.703523	1.393599
H	-0.132301	-1.171546	2.176349
H	1.427914	-0.284508	2.508192
H	-1.906697	-1.066329	1.178289
C	0.829407	-1.550900	-0.061829
C	-0.403255	-1.468771	-0.682689
C	1.853407	-0.588253	-0.441386
O	3.078855	-0.917164	0.018791
O	1.653531	0.418538	-1.086624
C	4.112405	0.002078	-0.304738
H	1.143236	-2.424341	0.489282
H	-0.510050	-0.803497	-1.529486
H	-1.035826	-2.346696	-0.688707
H	4.200034	0.119037	-1.383883
H	3.910087	0.978124	0.135863
H	5.026160	-0.415643	0.107009
C	-0.531355	2.895212	-0.418342
H	0.426978	2.491835	-0.751043
H	-0.400743	3.469112	0.502172
H	-0.952083	3.542054	-1.182746
O	-2.916804	-0.322733	-0.472436
C	-3.786168	-1.426956	-0.354532
H	-4.224862	-1.472424	0.645963
H	-4.575365	-1.288784	-1.087934
H	-3.266583	-2.366559	-0.560795

Number of imaginary frequencies = 1 (-458.1449)
ZPE Energy (M062X/def2TZVPP) = -691.206716
Free Energy (M062X/def2TZVPP) = -691.248774

TS-1+5-OMN

M062X/def2TZVPP geometry

C	2.207119	0.107588	-0.359433
C	0.982904	0.506893	-0.912823
C	0.083082	-0.432850	-1.363149
C	2.575742	-1.215298	-0.208396
H	3.530296	-1.428612	0.253175

H	2.788391	0.854011	0.163030
O	0.519784	1.784506	-0.879607
H	0.401908	-1.429447	-1.630462
H	2.251040	-1.962718	-0.917848
C	1.224556	2.724639	-0.094723
H	2.220376	2.913688	-0.504610
H	1.298907	2.387315	0.940301
H	0.644879	3.642796	-0.139213
C	-0.034349	-1.633279	0.883952
C	1.264718	-1.936499	1.238759
C	-0.609072	-0.378466	1.342661
O	-1.918406	-0.266280	1.037032
O	0.004172	0.500207	1.910804
C	-2.482009	1.018377	1.275258
H	-0.691600	-2.354415	0.421253
H	1.713560	-1.349036	2.026584
H	1.606332	-2.959430	1.155477
H	-2.417169	1.277000	2.330788
H	-1.954717	1.768667	0.686569
H	-3.520303	0.952868	0.963390
O	-1.127515	-0.046543	-1.781184
C	-2.028150	-1.098339	-2.069028
H	-2.900590	-0.646672	-2.532346
H	-1.579322	-1.814040	-2.762849
H	-2.323517	-1.603695	-1.148061

Number of imaginary frequencies = 1 (-459.1422)
 ZPE Energy (M062X/def2TZVPP) = -691.210282
 Free Energy (M062X/def2TZVPP) = -691.252122

P-1+2-MN

M062X/def2TZVPP geometry

C	1.733973	0.516770	1.074206
C	0.968174	1.596487	1.149979
C	0.173990	2.123338	-0.009689
C	1.955290	-0.278040	-0.182594
O	1.871953	-1.672027	0.065061
C	0.611127	-2.149071	0.471961
H	2.279453	0.167119	1.944067
H	0.903689	2.139956	2.085578
H	0.745108	2.907434	-0.516770
H	-0.740995	2.592704	0.349728
H	3.003613	-0.153250	-0.464618
H	-0.100789	-2.169063	-0.357891
H	0.196883	-1.547043	1.288451
H	0.758680	-3.167081	0.826730
C	-0.150835	1.028193	-1.021048
C	1.104694	0.208518	-1.373121
C	-1.306343	0.129338	-0.628412
O	-1.758979	0.329999	0.614209
O	-1.787511	-0.682293	-1.373412
C	-2.830090	-0.521771	1.013503
H	-0.496515	1.483447	-1.951746
H	0.831415	-0.648112	-1.989626
H	1.734211	0.853339	-1.988296
H	-3.065758	-0.247028	2.036490
H	-3.692289	-0.375873	0.365347
H	-2.520289	-1.564563	0.956987

Number of imaginary frequencies = 0
 ZPE Energy (M062X/def2TZVPP) = -576.795747

Free Energy (M062X/def2TZVPP) = -576.834088

P-1+2-ON

M062X/def2TZVPP geometry

C	2.643107	-0.100891	0.841872
C	1.618780	0.703963	1.086002
C	0.685971	1.034873	-0.036292
C	2.769328	-0.688579	-0.533368
O	-0.401587	1.768330	0.470594
C	-1.106795	2.500801	-0.504127
H	3.356896	-0.357214	1.613565
H	1.423921	1.157065	2.048643
H	1.224874	1.652709	-0.771420
H	3.514505	-1.481987	-0.562191
H	3.104331	0.081743	-1.236997
H	-1.589187	1.847822	-1.235241
H	-0.438371	3.195445	-1.024790
H	-1.873717	3.069658	0.016538
C	0.240276	-0.254522	-0.796608
C	1.407857	-1.244692	-0.985828
C	-0.884445	-0.881403	0.000677
O	-2.088397	-0.516468	-0.465367
O	-0.741570	-1.604090	0.946755
C	-3.196917	-0.978049	0.302694
H	-0.168625	0.049343	-1.759036
H	1.199194	-2.130266	-0.387266
H	1.461879	-1.555955	-2.028565
H	-4.085260	-0.612543	-0.202685
H	-3.200796	-2.065457	0.348411
H	-3.140177	-0.581537	1.315046

Number of imaginary frequencies = 0

ZPE Energy (M062X/def2TZVPP) = -576.793111
 Free Energy (M062X/def2TZVPP) = -576.831889

P-1+3-MN

M062X/def2TZVPP geometry

C	-2.251847	0.264481	-0.520574
C	-1.360760	0.901320	0.227095
C	-0.631591	0.123800	1.288272
C	-2.463574	-1.196752	-0.243665
H	-3.078041	-1.656424	-1.015884
H	-2.795166	0.782630	-1.299099
O	-1.101745	2.239050	0.088637
H	-1.337611	-0.150870	2.076572
H	0.157347	0.709751	1.754003
H	-3.007569	-1.319281	0.699397
C	0.205614	2.516067	-0.380271
H	0.365806	2.055462	-1.359027
H	0.968890	2.150519	0.314145
H	0.291408	3.596700	-0.461552
C	-0.062614	-1.182329	0.681659
C	-1.115844	-1.937936	-0.150492
C	1.155398	-0.818190	-0.147061
O	2.153035	-0.374127	0.637780
O	1.252285	-0.877063	-1.341373
C	3.329561	0.042672	-0.049698
H	0.304461	-1.797861	1.503870
H	-0.723554	-2.067091	-1.157696
H	-1.274244	-2.931093	0.269640
H	3.754363	-0.786281	-0.613097

H	3.098151	0.853466	-0.739530
H	4.021095	0.378705	0.716310

Number of imaginary frequencies = 0
ZPE Energy (M062X/def2TZVPP) = -576.797264
Free Energy (M062X/def2TZVPP) = -576.836300

P-1+3-PN

M062X/def2TZVPP geometry

C	-1.645420	-0.117918	-0.085090
C	-1.159098	0.358116	1.063105
C	0.056130	-0.229150	1.729105
C	-1.058143	-1.277805	-0.831163
H	-0.631253	-0.904868	-1.764044
O	-2.722382	0.376048	-0.748271
H	-1.637561	1.189060	1.561876
H	-0.241591	-0.872195	2.562972
H	0.666736	0.565498	2.155589
H	-1.873046	-1.949282	-1.106966
C	0.893456	-1.058761	0.754315
C	-0.000672	-2.022746	-0.020490
C	1.701153	-0.197955	-0.200037
O	2.307893	0.820965	0.425196
O	1.836936	-0.409271	-1.374811
C	3.115186	1.650979	-0.405674
H	1.636992	-1.622978	1.325482
H	0.597010	-2.647467	-0.682171
H	-0.488045	-2.677509	0.704927
H	3.904724	1.066353	-0.874561
H	2.508013	2.110051	-1.183848
H	3.535892	2.408234	0.248016
C	-3.360958	1.503152	-0.198170
H	-2.668823	2.345785	-0.120627
H	-3.764695	1.281755	0.793375
H	-4.173717	1.758156	-0.872351

Number of imaginary frequencies = 0
ZPE Energy (M062X/def2TZVPP) = -576.811900
Free Energy (M062X/def2TZVPP) = -576.850089

P-1+4-OPN

M062X/def2TZVPP geometry

C	2.147277	-0.019721	0.197330
C	1.222196	-0.773603	-0.393880
C	-0.009874	-1.094108	0.395750
C	1.882718	0.499265	1.575954
H	2.627646	1.250721	1.831866
O	3.331426	0.374924	-0.319102
H	1.296441	-1.181707	-1.389743
H	0.243671	-1.766911	1.229810
O	-0.919006	-1.753603	-0.452906
H	1.977650	-0.315944	2.299383
C	-0.621226	0.188558	1.045677
C	0.471003	1.102963	1.637774
C	-1.412768	0.908196	-0.025561
O	-2.712298	0.575677	0.008885
O	-0.956063	1.672763	-0.829180
C	-3.504047	1.125962	-1.040424
H	-1.322747	-0.126740	1.816890
H	0.484999	2.028973	1.064984
H	0.225223	1.355043	2.668575

H	-3.133735	0.785032	-2.005774
H	-4.515410	0.769963	-0.871147
H	-3.469722	2.213489	-1.011866
C	3.601201	-0.043097	-1.639038
H	2.840139	0.335780	-2.325348
H	3.629020	-1.133925	-1.702154
H	4.572674	0.365080	-1.902203
C	-1.918351	-2.477731	0.224859
H	-2.587475	-1.822635	0.788052
H	-1.471927	-3.210048	0.906597
H	-2.497700	-3.004369	-0.530140

Number of imaginary frequencies = 0
ZPE Energy (M062X/def2TZVPP) = -691.291760
Free Energy (M062X/def2TZVPP) = -691.333609

P-1+5-MPN

M062X/def2TZVPP geometry

C	-1.054739	0.905907	0.320059
C	0.014918	1.233782	1.050063
C	0.715559	0.134826	1.800320
C	-1.570443	-0.513495	0.384549
O	-1.799704	1.722883	-0.442289
H	0.397738	2.241737	1.095957
H	0.127418	-0.204941	2.659684
H	1.673653	0.475413	2.183387
H	-2.059810	-0.619689	1.366583
C	0.912842	-1.059984	0.851012
C	-0.429137	-1.555395	0.302791
C	1.854678	-0.671808	-0.277660
O	2.980114	-0.114043	0.196158
O	1.667134	-0.853665	-1.448132
C	3.933941	0.261926	-0.792865
H	1.419391	-1.866034	1.387760
H	-0.313697	-1.824210	-0.747093
H	-0.735825	-2.448827	0.846371
H	4.252456	-0.608775	-1.363461
H	3.502158	0.990579	-1.476745
H	4.771300	0.693160	-0.253399
C	-1.372944	3.062090	-0.524407
H	-0.355697	3.121278	-0.920595
H	-1.402947	3.542757	0.457356
H	-2.060276	3.563510	-1.199399
O	-2.530429	-0.712607	-0.617210
C	-3.241512	-1.915187	-0.478889
H	-3.671623	-2.006417	0.525992
H	-4.047581	-1.896487	-1.208673
H	-2.612561	-2.789573	-0.671783

Number of imaginary frequencies = 0
ZPE Energy (M062X/def2TZVPP) = -691.285835
Free Energy (M062X/def2TZVPP) = -691.328271

P-1+5-OMN

M062X/def2TZVPP geometry

C	-2.290488	-0.791012	-0.056664
C	-1.549325	0.310769	0.068326
C	-0.359377	0.255312	0.997315
C	-1.825314	-2.018517	0.674460
H	-2.387427	-2.893664	0.351910
H	-3.163977	-0.833327	-0.688999

O	-1.732586	1.502699	-0.524245
H	-0.740184	0.104345	2.018144
H	-1.998023	-1.922765	1.752640
C	-2.793341	1.573587	-1.448099
H	-3.753065	1.393478	-0.955873
H	-2.656350	0.840069	-2.246546
H	-2.776544	2.577914	-1.861093
C	0.522007	-0.988440	0.664826
C	-0.328119	-2.249042	0.412698
C	1.350885	-0.618583	-0.547007
O	2.581386	-0.211956	-0.203293
O	0.964072	-0.652447	-1.681835
C	3.380263	0.271366	-1.280320
H	1.204042	-1.140795	1.499747
H	-0.214979	-2.534717	-0.632227
H	0.040400	-3.071930	1.025038
H	3.531137	-0.510238	-2.022632
H	2.891954	1.120867	-1.754746
H	4.326973	0.569396	-0.840954
O	0.362177	1.451405	0.939937
C	1.219021	1.654796	2.037826
H	1.634570	2.654394	1.934259
H	0.664123	1.594818	2.980677
H	2.039691	0.933117	2.055975

Number of imaginary frequencies = 0

ZPE Energy (M062X/def2TZVPP) = -691.285274

Free Energy (M062X/def2TZVPP) = -691.327317