Electronics Supplementary Information (ESI)

Molecular Tailoring Approach – New Guide to Quantify the Energy of Push-Pull Effect: Case Study on the *(E)* 3-(1H-pyrrol-2-yl)prop-2-enones

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1. Table S1. The R_1 and R_2 substituents and their Hammett constants for the studied *(E)* 3-(1H-pyrrol-2-yl)prop-2-enones **1**–**35**

N Comp	R_1 (R_2=H)	N Comp	R_2 (R_1=H)	σ_p[a]
1	H			0.00
2	$N(CH_3)_2$	**19**	$N(CH_3)_2$	–0.83
3	NH_2	**20**	NH_2	–0.66
4	$NHNH_2$	**21**	$NHNH_2$	–0.55
5	OH	**22**	OH	–0.37
6	OCH_3	**23**	OCH_3	–0.27
7	CH_3	**24**	CH_3	–0.17
8	$CH_2C_6H_5$	**25**	$CH_2C_6H_5$	–0.09
9	F	**26**	F	0.06
10	SH	**27**	SH	0.15
11	Cl	**28**	Cl	0.23
12	$CONH_2$	**29**	$CONH_2$	0.36
13	CHO	**30**	CHO	0.42
14	CCl_3	**31**	CCl_3	0.46
15	CF_3	**32**	CF_3	0.54
16	CN	**33**	CN	0.66
17	NO_2	**34**	NO_2	0.78
18	NO	**35**	NO	0.91

[a]Taken from ref. 10

2. Table S2. The calculated E_π(MTA) energy (kcal mol^{-1}), bond length (l, Å), vibration frequency (ν, cm^{-1}) and chemical shifts (δ, ppm) for the enones **1**–**35**

N	Energy	Bond lengths				Frequency	Chemical shifts		
Comp	$-E_\pi$(MTA)	l(C_2–C_6)	l(C_6=C_7)	l(C_7–C_8)	l(C_8=O_9)	$\nu_{C=O}$	δC_6	δC_7	$\Delta\delta_{C=C}$[e]
1	3.66	1.4281	1.3551	1.4646	1.2177	1749	136.90	118.90	18.00
2	5.88	1.4153	1.3631	1.4559	1.2216	1733	134.34	113.87	20.47
3	5.15	1.4184	1.3605	1.4583	1.2207	1737	135.28	115.09	20.19
4[a]	5.31	1.4191	1.3615	1.4575	1.2208	1737	135.22	114.83	20.39
5[b]	4.68	1.4208	1.3584	1.4606	1.2197	1742	135.91	116.41	19.50
6[a]	4.92	1.4206	1.3598	1.4593	1.2201	1740	135.85	115.88	19.97
7	4.24	1.4251	1.3569	1.4624	1.2188	1745	136.49	117.67	18.82
8[a]	4.21	1.4255	1.3568	1.4624	1.2188	1745	136.43	118.12	18.31
9	3.67	1.4250	1.3553	1.4645	1.2178	1748	136.61	118.16	18.45
10[c]	3.26	1.4303	1.3537	1.4666	1.2171	1751	136.62	120.34	16.28
11	3.43	1.4274	1.3546	1.4655	1.2174	1750	136.06	119.13	16.93
12[d]	2.87	1.4313	1.3530	1.4683	1.2162	1754	137.30	121.26	16.04
13[a]	2.28	1.4342	1.3513	1.4712	1.2152	1754	136.74	123.91	12.83
14	2.60	1.4329	1.3516	1.4699	1.2158	1756	136.83	122.13	14.70
15	2.44	1.4337	1.3511	1.4704	1.2155	1757	136.84	122.19	14.65
16	2.33	1.4341	1.3509	1.4715	1.2151	1758	135.73	123.12	12.61
17	1.94	1.4357	1.3495	1.4742	1.2141	1760	136.15	125.42	10.73
18[a]	1.74	1.4355	1.3501	1.4742	1.2141	1760	138.03	126.58	11.45
19	2.54	1.4351	1.3488	1.4855	1.2300	1704	140.53	109.92	30.61
20	2.19	1.4343	1.3475	1.4821	1.2232	1741	139.55	112.30	27.25
21[a]	2.7	1.4345	1.3482	1.4766	1.2254	1730	139.10	110.68	28.42
22[a]	3.13	1.4309	1.3503	1.4709	1.2085	1790	143.55	108.91	34.64
23[a]	3.12	1.4319	1.3505	1.4723	1.2108	1764	143.08	107.77	35.31
24	3.23	1.4311	1.3518	1.4781	1.2211	1742	137.59	117.95	19.64
25[b]	4.07	1.4307	1.3522	1.4738	1.2213	1734	138.16	118.13	20.03
26	4.13	1.4270	1.3540	1.4535	1.1907	1850	146.34	105.42	40.92
27[a]	3.98	1.4290	1.3531	1.4677	1.2092	1744	136.77	118.24	18.53
28	5.15	1.4255	1.3564	1.4540	1.1900	1831	141.64	116.98	24.66
29[d]	5.59	1.4255	1.3568	1.4528	1.2254	1760	141.72	113.21	28.51
30[a]	5.15	1.4287	1.3577	1.4584	1.2209	1728	142.87	113.96	28.91
31	5.5	1.4259	1.3555	1.4601	1.2090	1760	143.81	112.93	30.88
32	5.39	1.4236	1.3574	1.4562	1.2131	1762	142.79	112.46	30.33
33	5.8	1.4218	1.3591	1.4560	1.2187	1717	140.68	119.90	20.78
34	6.92	1.4202	1.3614	1.4383	1.1901	1858	149.32	101.25	48.07
35[a]	5.61	1.4228	1.3588	1.4485	1.2055	1784	155.72	108.13	47.59

[a]The parameters are averaged between the s-*cis* and s-*trans* conformations (see Table S3); [b]only the s-*cis* conformation with respect to the exocyclic C=C bond; [c]only *gauche* conformation; [d]only the s-*trans* conformation with respect to the exocyclic C=C bond; [d]only the s-*trans* conformation of the carbonyl groups; [e]$\Delta\delta_{C=C} = \delta C_6 - \delta C_7$

3. Table S3. The calculated E_{π}(MTA) energy (kcal mol^{-1}), bond length (l, Å), C=O vibration frequency (ν, cm^{-1}) and ^{13}C chemical shifts (δ, ppm) for the enones **4**–**6**, **8**, **13**, **18**, **21**–**23**, **27**, **30**, **35** in different conformations[a]

N Comp & substit. conform.	Energy	Bond lengths				Freq	Chemical shifts		
	$-E_{\pi}$(MTA)	l(C_2–C_6)	l(C_6=C_7)	l(C_7–C_8)	l(C_8=O_9)	$\nu_{C=O}$	δC_6	δC_7	$\Delta\delta_{C=C}$[b]
4 *cis*	5.51	1.4167	1.3618	1.4570	1.2211	1736	135.37	114.42	20.95
4 *trans*	5.10	1.4175	1.3611	1.4581	1.2205	1737	135.08	115.25	19.83
6 *cis*	4.80	1.4206	1.3588	1.4600	1.2199	1740	135.98	116.52	19.46
6 *trans*	5.13	1.4177	1.3607	1.4586	1.2202	1739	135.73	115.25	20.48
8 *cis*	4.15	1.4251	1.3570	1.4623	1.2188	1745	136.61	117.57	19.04
8 *trans*	4.26	1.4258	1.3565	1.4625	1.2189	1745	136.24	118.67	17.57
13 *cis*	2.38	1.4334	1.3517	1.4706	1.2153	1750	136.71	123.04	13.67
13 *trans*	2.18	1.4350	1.3508	1.4717	1.2152	1757	136.76	124.78	11.98
18 *cis*	1.84	1.4350	1.3503	1.4737	1.2143	1759	136.86	126.03	10.83
18 *trans*	1.64	1.4360	1.3499	1.4748	1.2139	1760	139.19	127.13	12.06
21 *cis*	2.38	1.4342	1.3479	1.4779	1.2251	1729	138.83	111.40	27.43
21 *trans*	3.01	1.4348	1.3485	1.4753	1.2257	1730	139.37	109.96	29.41
22 *cis*	3.26	1.4312	1.3502	1.4647	1.2124	1774	143.07	109.45	33.62
22 *trans*	3.00	1.4305	1.3504	1.4771	1.2047	1805	144.03	108.38	35.65
23 *cis*	3.21	1.4310	1.3517	1.4769	1.2084	1771	145.14	103.13	42.01
23 *trans*	3.02	1.4327	1.3493	1.4678	1.2131	1757	141.03	112.41	28.62
27 *cis*	3.89	1.4289	1.3533	1.4698	1.2091	1741	137.34	119.06	18.28
27 *trans*	4.06	1.4291	1.3530	1.4657	1.2092	1746	136.20	117.41	18.79
30 *cis*	5.34	1.4247	1.3571	1.4544	1.2243	1720	141.63	110.49	31.14
30 *trans*	4.96	1.4327	1.3582	1.4623	1.2176	1735	144.11	117.43	26.68
35 *cis*	5.84	1.4219	1.3598	1.4469	1.2034	1794	160.43	126.29	34.14
35 *trans*	5.37	1.4238	1.3578	1.4502	1.2077	1774	151.00	89.96	61.04

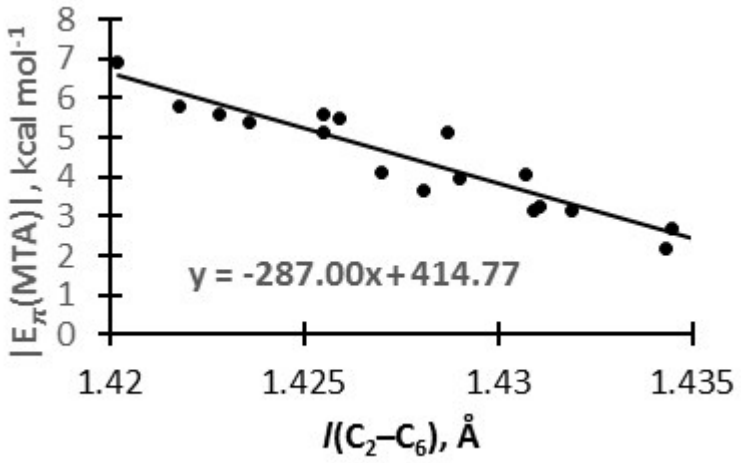
[a]The *cis* and *trans* conformations are defined with respect to the exocyclic C=C bond; [b]$\Delta\delta_{C=C} = \delta C_6 - \delta C_7$.

4. Table S4. The Mulliken charges in the enones **1**, **2**, **17**, **19**, **34**

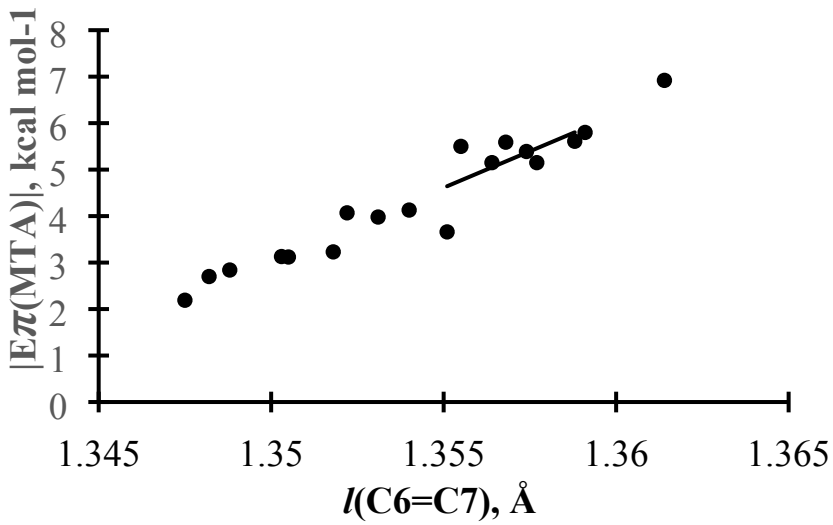
N Comp	Frag ment	charge, *e*								
		$q(N_1)$	$q(C_2)$	$q(C_3)$	$q(C_4)$	$q(C_5)$	$q(C_6)$	$q(C_7)$	$q(C_8)$	$q(O_9)$
1	M	−0.1943	0.0218	0.1197	−0.3609	0.0392	0.0303	0.0933	0.1264	−0.5318
R_1=H	M1	–	–	–	–	–	−0.1074	0.0432	0.2652	−0.5068
R_2=H	M2	−0.1888	0.2786	0.0919	−0.3233	0.0497	−0.0853	−0.3990	–	–
2	M	−0.3314	0.0925	−0.0972	−0.0625	0.2649	0.0495	0.0024	0.0881	−0.5501
R_1=N$(CH_3)_2$	M1	–	–	–	–	–	−0.1031	0.0423	0.2639	−0.5104
R_2=H	M2	−0.3293	0.5015	−0.1153	−0.0426	0.3152	−0.3026	−0.4428	–	–
17	M	−0.2229	0.1176	−0.0403	0.0460	0.1575	−0.0282	0.1103	0.1248	−0.4947
R_1=NO_2								(0.1079)[a]	(0.0367)	(0.0554)
R_2=H	M1	–	–	–	–	–	−0.1108	0.0417	0.2672	−0.5032
								(0.0015)	(0.0033)	(0.0072)
	M2	−0.2508	0.5262	−0.1984	0.3008	−0.0153	−0.2064	−0.3542	–	–
19	M	−0.2040	−0.199	0.1375	−0.3985	0.0304	0.0341	0.0070	0.6848	−0.6639
R_1=H			3							
R_2=N$(CH_3)_2$	M1	–	–	–	–	–	−0.3916	0.3007	0.4674	−0.6632
	M2	−0.1902	0.2789	0.0918	−0.3238	0.0501	−0.0928	−0.3874	–	–
34	M	−0.1894	−0.132	0.1436	−0.3785	0.0575	−0.0498	−0.1247	0.7418	−0.4786
R_1=H			7	(0.0239)[b]	(0.0200)	(0.0274)				
R_2=NO_2	M1	–	–	–	–	–	−0.2680	0.2047	0.4185	−0.4452
	M2	−0.1856	0.2763	0.0930	−0.3234	0.0487	−0.0885	−0.3987	–	–
				(0.0012)	(0.0004)	(0.0014)				

[a]difference between charges in the enones **17** and **2** (**34** and **19)** or their M1 (M2) fragments is given in the parentheses.

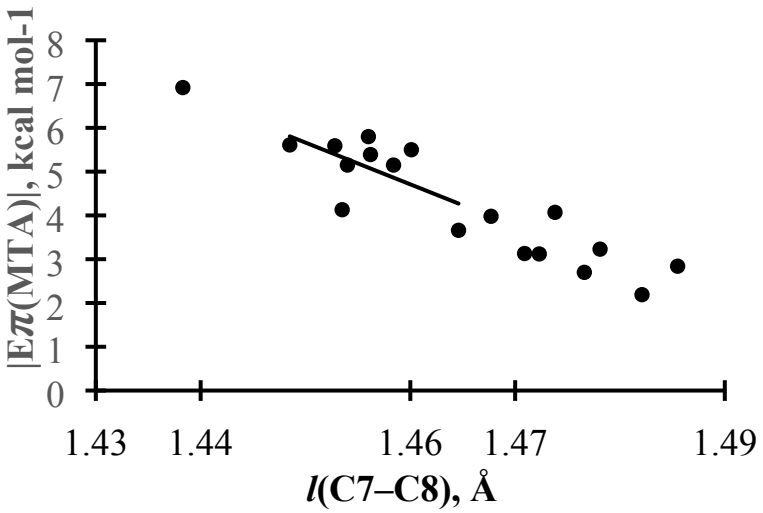
[b]difference between charges in the enones **34** and **1** in this case.



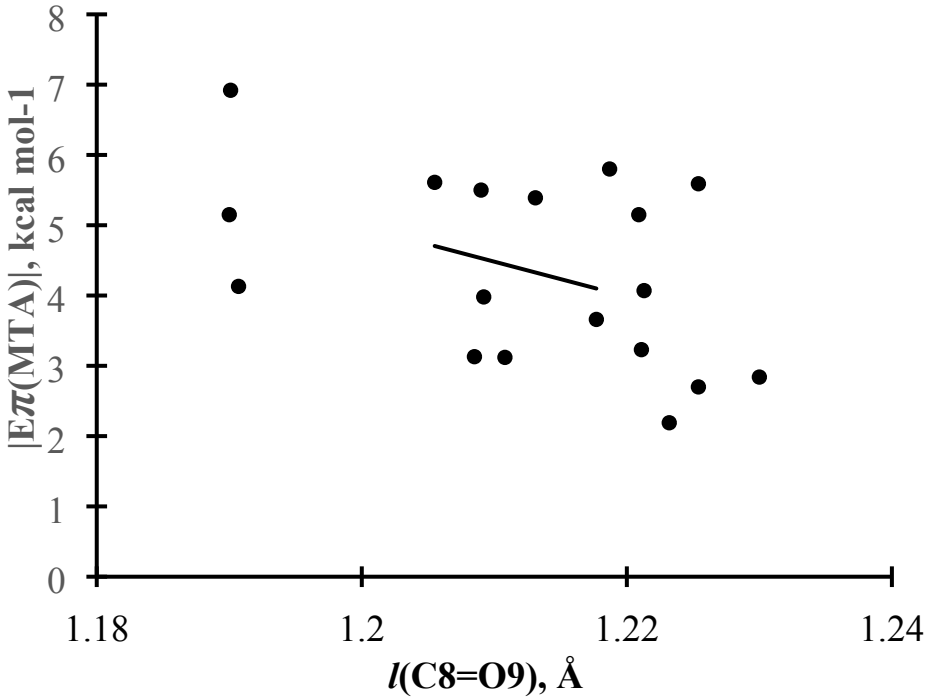
5. Figure S1. Dependence of the E_{π}(MTA) values on the l(C_2–C_6) bond length for the compounds **1**, **19**–**35**



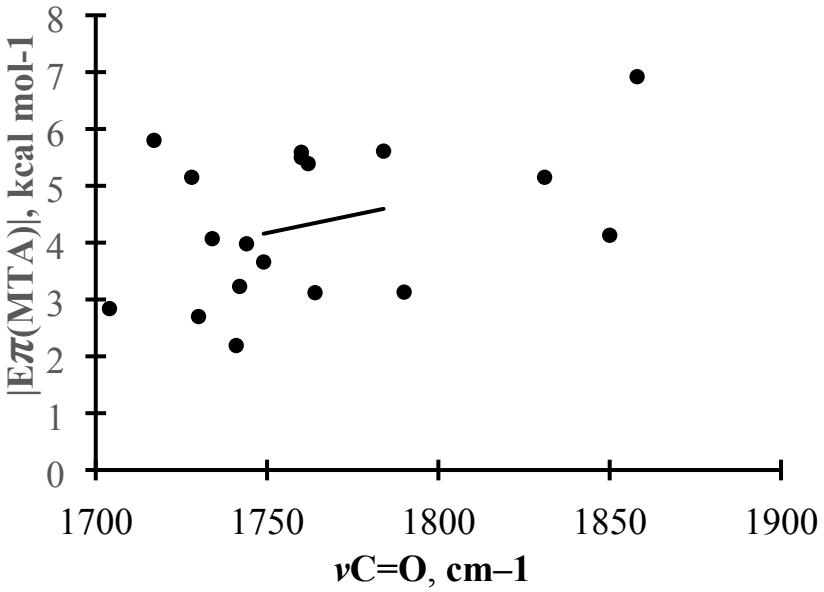
6. Figure S2. Dependence of the E_{π}(MTA) values on the l(C_6=C_7) bond length for the compounds **1**, **19**–**35**



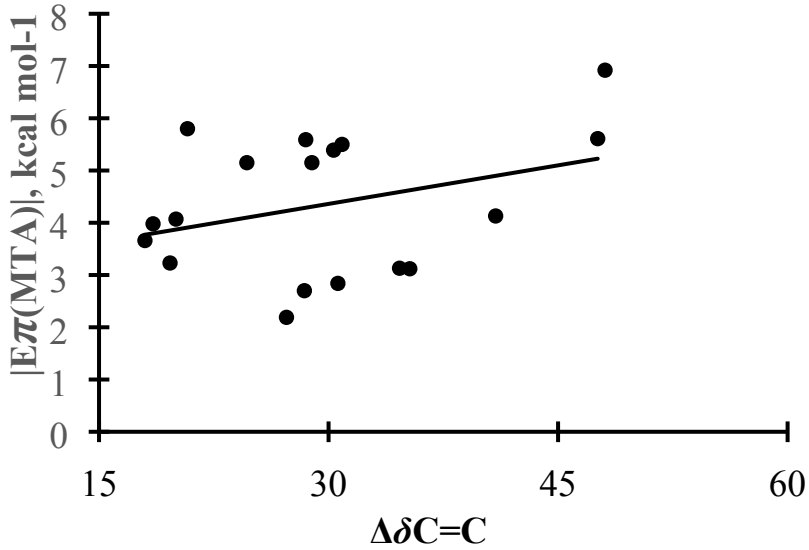
7. Figure S3. Dependence of the E_{π}(MTA) values on the $l(C_7–C_8)$ bond length for the compounds **1**, **19**–**35**



8. Figure S4. Plot of the E_{π}(MTA) values vs the $l(C_8=O_9)$ bond length for the compounds **1**, **19**–**35**



9. Figure S5. Plot of the E_{π}(MTA) values vs the $\nu_{C=O}$ vibrational frequency for the compounds **1**, **19–35**



10. Figure S6. Plot of the E_{π}(MTA) values vs the $\Delta\delta_{C=C}$ ^{13}C chemical shift difference for the compounds **1**, **19–35**

11. Equations (S1) – (S9)

For enones **1**–**18**: $|E_{\pi}(MTA)| = -190.95 \times l(C_2–C_6) + 276.14$; R=0.990, S=0.185, n=18 (S1)
where the $l(C_2–C_6)$ parameter is the $C_2–C_6$ bond length

$|E_{\pi}(MTA)| = 299.25 \times l(C_6=C_7) - 401.95$; R=0.995, S=0.129, n=18 (S2)
where the $l(C_6=C_7)$ parameter is the $C_6=C_7$ bond length

$|E_{\pi}(MTA)| = -217.33 \times l(C_7–C_8) + 322.07$; R=0.996, S=0.110, n=18 (S3)
where the $l(C_7–C_8)$ parameter is the $C_7–C_8$ bond length

$|E_{\pi}(MTA)| = 528.01 \times l(C_8=O_9) - 401.95$; R=0.998, S=0.077, n=18 (S4)
where the $l(C_8=O_9)$ parameter is the $C_8=O_9$ bond length

For enones **1, 19**–**35**: $|E_{\pi}(MTA)| = -287.00 \times l(C_2–C_6) + 414.77$; R=0.946, S=0.453, n=18 (S5)
where the $l(C_2–C_6)$ parameter is the $C_2–C_6$ bond length

$|E_{\pi}(MTA)| = 319.29 \times l(C_6=C_7) - 428.04$; R=0.963, S=0.376, n=18 (S6)
where the $l(C_6=C_7)$ parameter is the $C_6=C_7$ bond length

$|E_{\pi}(MTA)| = -97.66 \times l(C_7–C_8) + 147.29$; R=0.923, S=0.538, n=18 (S7)
where the $l(C_7–C_8)$ parameter is the $C_7–C_8$ bond length

For enones **1**–**18**: $|E_{\pi}(MTA)| = -0.15 \times \nu_{C=O} + 263.41$; R=0.992, S=0.160, n=18 (S8)
where the $\nu_{C=O}$ parameter is the C=O vibrational frequency

$|E_{\pi}(MTA)| = 0.37 \times \Delta\delta_{C=C} - 2.65$; R=0.953, S=0.392, n=18 (S9)
where the $\Delta\delta_{C=C}$ parameter is the ^{13}C chemical shift difference for the olefinic moiety

12. Details of calculations, atom coordinates and total energies for B3LYP/6-311++G(d,p) optimized geometries of studied compounds (1–35)

The calculations were performed with Gaussian 09 program package.[1] All structures were checked by vibrational analysis to verify the absence of imaginary frequencies, and be sure that a true minimum of energy was found. The calculated *v*(C=O) frequencies were identified with the GaussView 5.0.9 package. The ^{13}C shielding constants for the structures under study and TMS as standard were calculated by the GIAO method.[2] The ^{13}C chemical shifts were obtained as the difference between the shielding constant of TMS (184.04) and that of the ^{13}C carbon in interest. The vibrational frequencies and the chemical shifts were calculated with the B3LYP/6-311++G(d,p) protocol.

References

1 Gaussian 09, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2010.

2 K. Wolinski, J. F. Hilton, P. Pulay, *J. Am. Chem. Soc.* 1990**, 112**, 8251–8260.

atom coordinates and total energies

1

E_{total} = -401.017556 Hartree

C	-2.73817	-0.75382	0.00006
C	-2.93038	0.61657	0.00046
C	-1.65273	1.21509	-0.00035
C	-0.69618	0.19964	-0.00003
N	-1.39491	-0.99612	-0.00047
C	0.72741	0.31270	0.00014
C	1.64659	-0.68301	0.00028
C	3.08324	-0.39814	0.00034
O	3.58192	0.71274	-0.00026
H	-3.45197	-1.56207	0.00013
H	-3.88506	1.11790	0.00093
H	-1.42869	2.27080	-0.00047
H	-0.97440	-1.91071	-0.00104
H	1.11070	1.32967	0.00002
H	1.36452	-1.73258	0.00037
H	3.73521	-1.29633	0.00010

2

E_{total} = -535.0243367 Hartree

C	1.61767	0.24864	-0.08717
C	1.45652	1.63820	0.00303
C	0.07471	1.89279	0.04047
C	-0.61068	0.68112	-0.01472
N	0.37052	-0.31360	-0.08683
C	-2.00374	0.43242	0.00875
C	-2.65010	-0.76666	-0.03943
C	-4.10302	-0.85337	-0.00467
O	-4.87400	0.09132	0.06880
N	2.76518	-0.50318	-0.20308
H	2.24794	2.36734	0.03825
H	-0.39789	2.86075	0.11018
H	0.17425	-1.29764	-0.14604
H	-2.63097	1.31778	0.07336
H	-2.11365	-1.70969	-0.10714
H	-4.50569	-1.88758	-0.05392
C	4.02523	0.17763	0.06511
C	2.70629	-1.91979	0.12849
H	4.84799	-0.47064	-0.23758
H	4.08595	1.09238	-0.52590
H	4.14991	0.43681	1.12650
H	3.66790	-2.37609	-0.10567
H	2.48238	-2.10245	1.19021
H	1.95662	-2.43001	-0.48242

3

E_{total} = -456.3934694 Hartree

C	2.36815	-0.24733	-0.00108
C	2.38477	1.14378	0.02092
C	1.04131	1.57067	0.01018
C	0.21530	0.44956	-0.00983
N	1.06809	-0.65899	-0.01189
C	-1.20125	0.37695	-0.00621
C	-1.98843	-0.73247	0.01701
C	-3.44355	-0.63618	0.01248
O	-4.08827	0.39998	-0.01459
N	3.40744	-1.16467	-0.08177
H	3.26856	1.76121	0.05618
H	0.68877	2.59045	0.03803
H	0.77259	-1.61029	-0.16043
H	-1.71372	1.33524	-0.02655
H	-1.57160	-1.73576	0.04563
H	-3.97286	-1.61201	0.03671
H	4.32277	-0.74476	-0.00625
H	3.32507	-1.96822	0.52818

4 *cis*

E_{total} = -511.7241046 Hartree

C	-1.88788	-0.09155	-0.03954
C	-1.84965	1.29809	-0.01417
C	-0.48808	1.66309	-0.00208
C	0.29203	0.50925	-0.01708
N	-0.60742	-0.56427	-0.02900
C	1.70229	0.37484	-0.00323
C	2.44182	-0.76857	0.01394
C	3.89842	-0.73624	0.02285
O	4.58981	0.27027	0.01480
N	-2.96047	-0.96996	-0.12177
H	-2.71304	1.94039	-0.00815
H	-0.09265	2.66708	0.02889
H	-0.34405	-1.52664	-0.16494
H	2.25581	1.31026	-0.00843
H	1.98175	-1.75334	0.02694
H	4.38346	-1.73534	0.04086
N	-4.23036	-0.38352	0.06077
H	-2.81376	-1.85197	0.35907
H	-4.89647	-0.83630	-0.55245
H	-4.54548	-0.44553	1.02564

4 *trans*

E_{total} = -511.7254578 Hartree

C	-2.02138	0.28650	-0.09035
C	-1.85432	1.66449	0.04353
C	-0.46796	1.90463	0.08141
C	0.20339	0.68703	-0.01429
N	-0.78879	-0.29412	-0.11689
C	1.59549	0.42090	0.00917
C	2.22551	-0.78390	-0.05557
C	3.67943	-0.88837	-0.02032
O	4.45821	0.04727	0.06757
N	-3.18506	-0.44875	-0.25483
H	-2.64919	2.39071	0.10660
H	0.01608	2.86336	0.18927
H	-0.61582	-1.27432	-0.26567
H	2.23323	1.29756	0.08750
H	1.67757	-1.71933	-0.13468
H	4.07105	-1.92577	-0.08071
N	-3.28333	-1.76176	0.25660
H	-4.02353	0.08001	-0.06155
H	-2.95838	-2.43236	-0.42982
H	-2.77725	-1.87329	1.13292

5

E_{total} = -476.263707 Hartree

C	2.36487	-0.26759	-0.00019
C	2.40698	1.11823	0.00004
C	1.06167	1.55067	-0.00035
C	0.22984	0.43425	-0.00004
N	1.07365	-0.67926	-0.00023
C	-1.18963	0.37314	0.00013
C	-1.98453	-0.72838	0.00021
C	-3.44090	-0.61747	0.00034
O	-4.07236	0.42600	0.00032
O	3.32866	-1.21347	-0.00022
H	3.29566	1.72948	0.00020
H	0.71561	2.57288	-0.00047
H	0.78893	-1.64556	-0.00027
H	-1.69313	1.33643	0.00015
H	-1.57678	-1.73564	0.00017
H	-3.98059	-1.58749	0.00034
H	4.19462	-0.79267	-0.00009

6 *cis*

E_{total} = -515.5750447 Hartree

C	-1.89009	-0.11397	0.00029
C	-1.86757	1.27555	-0.00007
C	-0.50337	1.64515	0.00031
C	0.27735	0.49274	0.00002
N	-0.61408	-0.58117	0.00041
C	1.69260	0.36942	-0.00022
C	2.43768	-0.76694	-0.00021
C	3.89703	-0.72248	-0.00042
O	4.57627	0.29086	-0.00069
O	-2.88251	-1.01657	0.00042
H	-2.72128	1.93204	-0.00029
H	-0.11149	2.65078	0.00036
H	-0.37395	-1.55928	0.00053
H	2.23823	1.30947	-0.00036
H	1.98446	-1.75464	-0.00003
H	4.39175	-1.71634	-0.00045
C	-4.21197	-0.48990	0.00017
H	-4.87463	-1.35236	0.00031
H	-4.38738	0.11358	0.89540
H	-4.38722	0.11317	-0.89536

6 *trans*

E_{total} = -515.5695891 Hartree

C	2.03207	0.30534	0.00002
C	1.86405	1.68337	-0.00007
C	0.47618	1.91590	0.00005
C	-0.19011	0.69128	-0.00003
N	0.80566	-0.29250	0.00003
C	-1.58162	0.42023	-0.00009
C	-2.20829	-0.78758	-0.00015
C	-3.66307	-0.89281	-0.00021
O	-4.44395	0.04479	0.00026
O	3.20056	-0.35536	0.00005
H	2.66350	2.40541	-0.00015
H	-0.01408	2.87744	0.00006
H	0.62864	-1.28269	0.00014
H	-2.22261	1.29818	-0.00008
H	-1.65848	-1.72536	-0.00017
H	-4.05233	-1.93287	0.00017
C	3.17069	-1.78143	0.00004
H	4.21023	-2.10106	0.00002
H	2.67662	-2.16641	0.89881
H	2.67657	-2.16640	-0.89871

7

E_{total} = -440.3486524 Hartree

C	-2.36623	-0.21022	0.00032
C	-2.35445	1.17781	0.00042
C	-1.00775	1.59655	0.00010
C	-0.20096	0.45993	0.00003
N	-1.06322	-0.62792	0.00010
C	1.22152	0.37304	-0.00016
C	1.99436	-0.74224	-0.00028
C	3.45450	-0.66105	-0.00049
O	4.10603	0.36894	-0.00054
C	-3.50859	-1.17107	0.00047
H	-3.23136	1.80651	0.00063
H	-0.64032	2.61144	0.00003
H	-0.77083	-1.59179	0.00000
H	1.74349	1.32638	-0.00024
H	1.56785	-1.74185	-0.00022
H	3.97416	-1.64202	-0.00052
H	-4.45326	-0.62656	0.00064
H	-3.49504	-1.81732	-0.88378
H	-3.49476	-1.81738	0.88467

8 *cis*

E_{total} = -671.4527124 Hartree

C	-0.13495	-0.25045	-0.00021
C	-0.15955	1.13703	-0.00032
C	1.17738	1.58725	-0.00021
C	2.01295	0.47190	-0.00009
N	1.17838	-0.63731	-0.00004
C	3.43712	0.42051	0.00001
C	4.23765	-0.67516	0.00014
C	5.69523	-0.55784	0.00024
O	6.32107	0.48799	0.00006
C	-1.24569	-1.26478	-0.00029
H	-1.05167	1.74207	-0.00044
H	1.51864	2.61130	-0.00025
H	1.49483	-1.59358	0.00007
H	3.93515	1.38658	-0.00001
H	3.83620	-1.68507	0.00018
H	6.23914	-1.52556	0.00017
C	-2.63059	-0.65191	-0.00007
H	-1.13841	-1.91530	-0.87718
H	-1.13826	-1.91561	0.87635
C	-3.27956	-0.35675	-1.20265
C	-4.54732	0.22233	-1.20464
C	-5.18466	0.51353	0.00031
C	-4.54693	0.22238	1.20507
C	-3.27918	-0.35669	1.20270
H	-2.78898	-0.58070	-2.14456
H	-5.03768	0.44251	-2.14631
H	-6.17231	0.96054	0.00046
H	-5.03699	0.44261	2.14689
H	-2.78830	-0.58058	2.14446

8 *trans*

E_{total} = -671.4544772 Hartree

C	0.28842	1.73225	-0.24424
C	-0.47680	2.79929	0.20843
C	-1.79410	2.33139	0.39243
C	-1.82406	0.97852	0.05469
N	-0.53623	0.64663	-0.33722
C	-2.92356	0.07162	0.09478
C	-2.93801	-1.24408	-0.23526
C	-4.15846	-2.04379	-0.13559
O	-5.24433	-1.63520	0.23810
C	1.73534	1.67309	-0.64550
H	-0.11197	3.80075	0.37733
H	-2.64519	2.89910	0.73665
H	-0.22247	-0.28000	-0.58077
H	-3.86371	0.49881	0.43389
H	-2.04996	-1.76204	-0.58713
H	-4.04288	-3.10658	-0.43433
C	2.43512	0.38399	-0.25112
H	1.81858	1.80509	-1.73097
H	2.24376	2.53018	-0.19478
C	2.82987	-0.54173	-1.22100
C	3.46158	-1.73288	-0.85816
C	3.70713	-2.01105	0.48346
C	3.31788	-1.09324	1.46046
C	2.68604	0.09188	1.09558
H	2.65068	-0.32687	-2.27001
H	3.76389	-2.43759	-1.62477
H	4.19979	-2.93367	0.76830
H	3.50837	-1.30165	2.50735
H	2.38093	0.79799	1.86122

9

E_{total} = -500.2790363 Hartree

C	2.36575	-0.26350	-0.00015
C	2.42729	1.10898	-0.00026
C	1.07903	1.54183	-0.00009
C	0.24444	0.42757	0.00005
N	1.07987	-0.68956	0.00005
C	-1.17948	0.37193	0.00020
C	-1.97555	-0.72493	0.00035
C	-3.43532	-0.60750	0.00053
O	-4.05693	0.43968	-0.00028
F	3.34642	-1.16239	-0.00020
H	3.32353	1.70605	-0.00043
H	0.73525	2.56468	-0.00012
H	0.79371	-1.65556	0.00019
H	-1.67810	1.33774	0.00021
H	-1.57259	-1.73417	0.00034
H	-3.98013	-1.57409	-0.00017

10

E_{total} = -799.2323461 Hartree

C	-1.97551	0.10535	0.00407
C	-1.85465	1.48743	0.00161
C	-0.47817	1.78608	0.00576
C	0.22944	0.58259	0.00134
N	-0.71186	-0.42743	-0.00307
C	1.64551	0.38127	0.00142
C	2.32156	-0.79148	0.00109
C	3.78766	-0.82818	0.00021
O	4.51449	0.14807	0.00076
S	-3.41586	-0.91675	-0.08184
H	-2.67889	2.18219	-0.00222
H	-0.02598	2.76609	0.01066
H	-0.51951	-1.41619	-0.02797
H	2.24180	1.28993	0.00159
H	1.81546	-1.75312	0.00159
H	4.22829	-1.84630	-0.00094
H	-3.59538	-1.08554	1.24917

11

E_{total} = -860.6359811 Hartree

C	1.97490	0.09211	0.00006
C	1.88399	1.46965	-0.00011
C	0.50485	1.77229	0.00024
C	-0.21408	0.57883	-0.00006
N	0.72347	-0.44557	-0.00002
C	-1.62816	0.38427	-0.00008
C	-2.31221	-0.78491	0.00017
C	-3.77748	-0.81106	0.00012
O	-4.49760	0.17052	-0.00022
Cl	3.36946	-0.92073	-0.00002
H	2.71443	2.15580	-0.00014
H	0.06294	2.75680	0.00047
H	0.52431	-1.43298	-0.00069
H	-2.21891	1.29660	-0.00028
H	-1.81264	-1.75005	0.00048
H	-4.22532	-1.82607	0.00038

12

E_{total} = -569.7763316 Hartree

C	-1.69801	0.28906	0.00087
C	-1.51530	1.66056	0.10833
C	-0.13049	1.89756	0.14983
C	0.52530	0.66734	0.05538
N	-0.45492	-0.30168	-0.01237
C	1.93260	0.40807	0.02361
C	2.55571	-0.78950	-0.06737
C	4.02033	-0.89026	-0.09152
O	4.78710	0.05196	-0.03247
C	-2.96739	-0.46276	-0.06393
H	-2.31418	2.38216	0.16364
H	0.36382	2.85234	0.24320
H	-0.28893	-1.26804	-0.24573
H	2.56785	1.28801	0.07866
H	2.00812	-1.72645	-0.12465
H	4.41581	-1.92357	-0.16976
O	-4.01072	0.05666	-0.41626
N	-2.87713	-1.80832	0.25585
H	-3.76717	-2.28624	0.29398
H	-2.20844	-2.09762	0.95498

13 *cis*

E_{total} = -514.3757096 Hartree

C	-2.00118	-0.07228	0.00004
C	-1.93493	1.32060	0.00005
C	-0.58074	1.67502	-0.00001
C	0.17995	0.49641	-0.00001
N	-0.70867	-0.54881	0.00000
C	1.60718	0.36345	-0.00002
C	2.33316	-0.77677	0.00003
C	3.80348	-0.74678	0.00000
O	4.47827	0.26395	-0.00004
C	-3.14672	-0.96960	0.00007
H	-2.79251	1.97401	0.00008
H	-0.16680	2.67175	-0.00002
H	-0.45772	-1.52536	-0.00000
H	2.16046	1.29860	-0.00008
H	1.87136	-1.76053	0.00010
H	4.29177	-1.74219	0.00012
O	-4.30543	-0.60929	-0.00009
H	-2.88975	-2.05220	-0.00013

13 *trans*

E_{total} = -514.3816503 Hartree

C	2.10269	0.21447	-0.00005
C	1.94692	1.60144	0.00005
C	0.56972	1.86427	0.00012
C	-0.10462	0.63435	-0.00000
N	0.85245	-0.34647	0.00012
C	-1.52123	0.40522	-0.00005
C	-2.16352	-0.78309	0.00015
C	-3.63338	-0.85684	0.00011
O	-4.37713	0.10419	-0.00027
C	3.29511	-0.61230	-0.00012
H	2.75053	2.32174	0.00003
H	0.08857	2.83014	0.00017
H	0.70608	-1.34542	0.00025
H	-2.13781	1.29986	-0.00022
H	-1.63199	-1.73056	0.00038
H	-4.05045	-1.88386	0.00040
O	3.26534	-1.83087	-0.00009
H	4.25222	-0.05823	-0.00015

14

E_{total} = -1819.1908418 Hartree

C	0.68335	0.58951	-0.00003
C	0.42284	1.95173	0.00010
C	-0.97672	2.10484	0.00008
C	-1.55359	0.83556	0.00000
N	-0.51631	-0.07198	-0.00016
C	-2.94327	0.48612	0.00001
C	-3.48611	-0.75162	-0.00015
C	-4.94288	-0.94729	-0.00011
O	-5.76632	-0.05287	0.00009
C	1.96353	-0.16017	-0.00008
H	1.16391	2.73266	0.00016
H	-1.52471	3.03418	0.00012
H	-0.61675	-1.07500	0.00007
H	-3.63242	1.32622	0.00016
H	-2.87888	-1.65262	-0.00034
H	-5.27213	-2.00607	-0.00030
Cl	3.36438	0.94911	-0.00013
Cl	2.06782	-1.24173	1.46768
Cl	2.06797	-1.24177	-1.46746

15

E_{total} = -738.1643074 Hartree

C	1.34683	0.37676	-0.03772
C	1.14938	1.74506	-0.01593
C	-0.24449	1.95324	0.00802
C	-0.87239	0.70791	0.00200
N	0.12718	-0.24242	-0.01983
C	-2.27600	0.41579	0.00595
C	-2.87129	-0.79702	-0.00709
C	-4.33571	-0.92894	-0.00171
O	-5.11872	0.00061	0.01514
C	2.60877	-0.40766	-0.00090
H	1.92606	2.49242	-0.01875
H	-0.75670	2.90265	0.02344
H	-0.00999	-1.23997	-0.06678
H	-2.92936	1.28394	0.02169
H	-2.30424	-1.72379	-0.02225
H	-4.71091	-1.97224	-0.01459
F	3.64243	0.29406	-0.49563
F	2.95248	-0.78712	1.25703
F	2.49553	-1.55602	-0.71928

16

E_{total} = -493.2826031 Hartree

N	4.21322	-1.41469	-0.00003
C	2.11821	0.07295	0.00001
C	2.00206	1.45942	0.00035
C	0.62976	1.75709	0.00004
C	-0.08028	0.55366	0.00004
N	0.84981	-0.45957	0.00003
C	-1.50125	0.35983	-0.00002
C	-2.17809	-0.80933	-0.00008
C	-3.64928	-0.83872	-0.00016
O	-4.36304	0.14463	-0.00014
C	3.27134	-0.74248	-0.00004
H	2.82820	2.15184	0.00057
H	0.18029	2.73783	0.00002
H	0.64672	-1.44670	-0.00003
H	-2.09287	1.27121	-0.00004
H	-1.67661	-1.77337	-0.00007
H	-4.09745	-1.85256	-0.00016

17

E_{total} = -605.5796957 Hartree

C	-1.71243	0.22802	0.00005
C	-1.58593	1.60770	0.00018
C	-0.20656	1.86545	-0.00012
C	0.47437	0.63942	-0.00007
N	-0.47741	-0.34939	-0.00009
C	1.89213	0.41342	-0.00008
C	2.53619	-0.77246	0.00027
C	4.00887	-0.84006	0.00018
O	4.74396	0.12621	-0.00021
N	-2.87912	-0.59170	0.00002
H	-2.40157	2.31115	0.00036
H	0.26973	2.83352	-0.00016
H	-0.34050	-1.34982	-0.00039
H	2.50513	1.31050	-0.00041
H	2.00827	-1.72202	0.00066
H	4.43154	-1.86427	0.00054
O	-3.97102	-0.03419	0.00015
O	-2.70004	-1.81457	-0.00027

18 *cis*

E_{total} = -530.3491023 Hartree

C	2.01574	-0.10904	-0.00010
C	1.97329	1.29090	-0.00011
C	0.62650	1.65007	-0.00023
C	-0.14921	0.47197	-0.00003
N	0.72268	-0.57687	0.00001
C	-1.58001	0.36195	0.00006
C	-2.31784	-0.76899	0.00019
C	-3.79068	-0.71971	0.00025
O	-4.44736	0.30169	0.00019
N	3.02872	-1.05703	-0.00009
H	2.83820	1.93389	-0.00014
H	0.21798	2.64926	-0.00034
H	0.49550	-1.56043	0.00010
H	-2.11962	1.30492	-0.00001
H	-1.86706	-1.75756	0.00024
H	-4.29319	-1.70733	0.00035
O	4.17256	-0.61274	-0.00016

18 *trans*

E_{total} = -530.3526752 Hartree

C	2.01574	-0.10904	-0.00010
C	1.97329	1.29090	-0.00011
C	0.62650	1.65007	-0.00023
C	-0.14921	0.47197	-0.00003
N	0.72268	-0.57687	0.00001
C	-1.58001	0.36195	0.00006
C	-2.31784	-0.76899	0.00019
C	-3.79068	-0.71971	0.00025
O	-4.44736	0.30169	0.00019
N	3.02872	-1.05703	-0.00009
H	2.83820	1.93389	-0.00014
H	0.21798	2.64926	-0.00034
H	0.49550	-1.56043	0.00010
H	-2.11962	1.30492	-0.00001
H	-1.86706	-1.75756	0.00024
H	-4.29319	-1.70733	0.00035
O	4.17256	-0.61274	-0.00016

19

E_{total} = -535.0485424 Hartree

C	-3.80576	1.05910	0.04478
C	-4.26948	-0.24139	-0.00062
C	-3.13634	-1.08700	-0.03540
C	-1.99647	-0.28835	-0.01097
N	-2.43797	1.02229	0.03752
C	-0.61941	-0.69185	-0.02982
C	0.47612	0.09468	-0.01128
C	1.82359	-0.53073	-0.01553
O	1.95979	-1.75274	0.01590
H	-4.33935	1.99534	0.08175
H	-5.30561	-0.54057	-0.00750
H	-3.13056	-2.16551	-0.07422
H	-1.84117	1.83174	0.06875
H	-0.44768	-1.76376	-0.06058
H	0.38656	1.17307	0.02911
C	4.24903	-0.26234	0.08321
H	4.88960	0.06024	-0.74401
H	4.71337	0.05154	1.02599
H	4.16282	-1.34559	0.07182
N	2.91608	0.31177	-0.05427
C	2.83996	1.76709	-0.05670
H	3.79440	2.16151	-0.40931
H	2.07124	2.12828	-0.74029
H	2.65386	2.18200	0.94255

20

E_{total} = -456.4206149 Hartree

C	3.11011	-0.91390	-0.01091
C	3.43737	0.42820	0.01200
C	2.22342	1.15294	0.01939
C	1.17226	0.24048	0.00159
N	1.74625	-1.01857	-0.01617
C	-0.23848	0.49926	0.00221
C	-1.24999	-0.39104	-0.00298
C	-2.65563	0.07871	-0.00449
O	-2.97645	1.25885	-0.02530
H	3.73768	-1.79058	-0.02453
H	4.43710	0.83246	0.02187
H	2.10651	2.22568	0.03647
H	1.23664	-1.88592	-0.03890
H	-0.52006	1.54870	0.00666
H	-1.07307	-1.46349	-0.00931
N	-3.60088	-0.92086	-0.00514
H	-4.56611	-0.64723	0.09202
H	-3.35904	-1.88240	0.16639

21 *cis*

E_{total} = -511.7569528 Hartree

C	3.58451	-0.97843	0.00579
C	3.95741	0.35140	-0.03306
C	2.76914	1.11736	-0.03599
C	1.68757	0.24158	-0.00021
N	2.21813	-1.03616	0.02447
C	0.28658	0.54814	0.00765
C	-0.75360	-0.30893	0.02527
C	-2.14024	0.20217	0.03950
O	-2.44140	1.38946	0.06235
H	4.18167	-1.87602	0.02258
H	4.97022	0.72103	-0.05597
H	2.68923	2.19330	-0.06226
H	1.67969	-1.88542	0.06129
H	0.04196	1.60663	-0.00084
H	-0.61347	-1.38673	0.03749
N	-3.10845	-0.78111	0.03978
N	-4.47097	-0.46588	-0.11872
H	-2.86613	-1.71670	-0.24920
H	-4.83972	-0.18953	0.78796
H	-4.53141	0.36001	-0.71222

21 *trans*

E_{total} = -511.753424 Hartree

C	3.33218	1.11996	-0.00004
C	3.84049	-0.16507	0.00009
C	2.73714	-1.04971	0.00008
C	1.57101	-0.28927	-0.00001
N	1.96709	1.03625	-0.00012
C	0.20613	-0.73172	0.00000
C	-0.90401	0.03372	-0.00005
C	-2.23252	-0.60780	-0.00004
O	-2.41435	-1.81990	-0.00002
H	3.83373	2.07447	-0.00011
H	4.88633	-0.42844	0.00015
H	2.76835	-2.12851	0.00015
H	1.33996	1.82354	-0.00014
H	0.06433	-1.80878	0.00006
H	-0.87674	1.11583	-0.00011
N	-3.33214	0.23042	-0.00012
N	-3.25885	1.62888	0.00016
H	-4.22942	-0.24023	0.00004
H	-3.70358	2.01105	-0.82859
H	-3.70341	2.01075	0.82914

22 *cis*

E_{total} = -476.2985694 Hartree

C	-3.09795	-0.91089	0.00005
C	-3.43087	0.43136	0.00005
C	-2.22096	1.15959	0.00001
C	-1.16612	0.24912	0.00001
N	-1.73583	-1.01218	0.00005
C	0.24122	0.50937	-0.00002
C	1.24755	-0.39087	-0.00001
C	2.64237	0.05627	-0.00004
O	3.03892	1.20203	-0.00006
H	-3.72330	-1.78931	0.00007
H	-4.43217	0.83161	0.00006
H	-2.10777	2.23290	-0.00002
H	-1.22280	-1.87832	0.00006
H	0.51866	1.55970	-0.00004
H	1.08479	-1.46235	0.00001
O	3.50404	-1.00225	-0.00002
H	4.39829	-0.63102	-0.00004

22 *trans*

E_{total} = -476.2881517 Hartree

C	3.09866	-0.90470	-0.00038
C	3.42061	0.44000	0.00020
C	2.20512	1.15833	0.00028
C	1.15707	0.24000	-0.00008
N	1.73712	-1.01734	-0.00019
C	-0.25018	0.49686	0.00004
C	-1.26532	-0.39374	0.00052
C	-2.66412	0.08065	0.00058
O	-3.00563	1.23588	-0.00077
H	3.73122	-1.77798	-0.00074
H	4.41862	0.84828	0.00046
H	2.08309	2.23065	0.00066
H	1.23407	-1.88897	-0.00103
H	-0.52947	1.54689	-0.00023
H	-1.08387	-1.46562	0.00096
O	-3.62076	-0.89885	0.00002
H	-3.21349	-1.77255	0.00033

23 *cis*

E_{total} = -515.5938234 Hartree

C	3.32569	1.10496	-0.00014
C	3.81856	-0.18689	0.00022
C	2.70584	-1.05634	0.00024
C	1.54778	-0.28127	-0.00005
N	1.96087	1.04034	-0.00023
C	0.18481	-0.71729	-0.00004
C	-0.93291	0.04291	-0.00002
C	-2.25496	-0.61538	-0.00004
O	-2.41203	-1.81350	-0.00022
H	3.84007	2.05266	-0.00032
H	4.86097	-0.46288	0.00043
H	2.72315	-2.13542	0.00050
H	1.34844	1.83889	-0.00078
H	0.04374	-1.79415	-0.00006
H	-0.87529	1.12379	0.00006
O	-3.37254	0.17151	0.00002
C	-3.30241	1.59842	0.00025
H	-4.33665	1.93891	0.00031
H	-2.80416	1.97838	0.89686
H	-2.80418	1.97867	-0.89625

23 *trans*

E_{total} = -515.6082584 Hartree

C	-3.56624	-0.99540	0.00001
C	-3.95653	0.33085	-0.00010
C	-2.77864	1.11099	-0.00010
C	-1.68581	0.24730	0.00005
N	-2.20039	-1.03700	0.00011
C	-0.28920	0.56681	0.00007
C	0.75342	-0.28966	-0.00004
C	2.13188	0.21457	0.00001
O	2.47324	1.37868	0.00013
H	-4.15259	-1.90020	0.00006
H	-4.97411	0.68769	-0.00019
H	-2.71203	2.18812	-0.00021
H	-1.64958	-1.87943	0.00034
H	-0.05585	1.62769	0.00017
H	0.63618	-1.36726	-0.00018
O	3.02086	-0.81375	-0.00006
C	4.40806	-0.44076	-0.00008
H	4.96158	-1.37752	-0.00197
H	4.64690	0.14773	-0.88735
H	4.64774	0.14450	0.88912

24

E_{total} = -440.3523589 Hartree

C	-3.10605	-0.94353	-0.00021
C	-3.45868	0.39362	-0.00048
C	-2.25956	1.13983	-0.00023
C	-1.19051	0.24568	-0.00012
N	-1.74218	-1.02401	-0.00008
C	0.21265	0.52711	-0.00001
C	1.24150	-0.34977	0.00015
C	2.64352	0.11820	0.00028
O	2.94106	1.30247	0.00020
H	-3.71829	-1.83116	-0.00020
H	-4.46587	0.77894	-0.00071
H	-2.16211	2.21466	-0.00026
H	-1.21572	-1.88178	0.00004
H	0.47521	1.58182	-0.00003
H	1.07892	-1.42438	0.00020
C	3.71146	-0.96122	0.00040
H	4.69965	-0.50375	0.00044
H	3.60447	-1.60271	0.88147
H	3.60459	-1.60281	-0.88060

25

E_{total} = -671.4577817 Hartree

C	-4.09522	-1.79619	-0.27992
C	-4.93793	-0.91776	0.37674
C	-4.19786	0.25816	0.62894
C	-2.91228	0.08059	0.12016
N	-2.88148	-1.18842	-0.43212
C	-1.80864	0.99092	0.13479
C	-0.57431	0.81060	-0.38720
C	0.45499	1.86075	-0.28816
O	0.26991	2.92074	0.28944
H	-4.26881	-2.79649	-0.64317
H	-5.96581	-1.10983	0.64032
H	-4.54503	1.15152	1.12506
H	-2.07544	-1.61026	-0.86302
H	-1.99626	1.94094	0.62800
H	-0.29511	-0.10688	-0.89626
C	1.80082	1.56628	-0.96289
H	1.62423	1.41445	-2.03339
H	2.41408	2.46266	-0.84919
C	2.50458	0.35281	-0.38806
C	2.77776	-0.77125	-1.17374
C	3.42596	-1.88256	-0.63416
C	3.81008	-1.88498	0.70462
C	3.54421	-0.76871	1.49825
C	2.89807	0.33910	0.95659
H	2.49016	-0.77404	-2.22067
H	3.63434	-2.74226	-1.26168
H	4.31541	-2.74647	1.12635
H	3.84257	-0.76054	2.54079
H	2.69538	1.20358	1.58046

26

E_{total} = -500.3148948 Hartree

C	-3.08133	-0.91197	0.00001
C	-3.41982	0.43029	0.00015
C	-2.21451	1.16179	0.00009
C	-1.15514	0.25391	0.00003
N	-1.72091	-1.01014	0.00006
C	0.24645	0.52188	-0.00001
C	1.26093	-0.37491	-0.00004
C	2.64031	0.08339	-0.00007
O	3.08429	1.18826	-0.00009
H	-3.70468	-1.79188	-0.00002
H	-4.42266	0.82634	0.00022
H	-2.10486	2.23547	0.00012
H	-1.20692	-1.87591	0.00005
H	0.51429	1.57459	-0.00001
H	1.10684	-1.44670	-0.00003
F	3.50319	-0.99370	-0.00012

27 *cis*

E_{total} = -799.2473549 Hartree

C	-3.44551	-1.05723	0.00001
C	-3.88680	0.25390	-0.00015
C	-2.74116	1.07769	-0.00013
C	-1.61448	0.25611	0.00006
N	-2.08019	-1.04804	0.00015
C	-0.23689	0.63571	0.00007
C	0.85118	-0.16892	0.00001
C	2.19533	0.42568	0.00009
O	2.43410	1.61099	0.00014
H	-3.99780	-1.98334	0.00006
H	-4.91737	0.57113	-0.00030
H	-2.71542	2.15659	-0.00028
H	-1.50058	-1.87085	0.00064
H	-0.05320	1.70635	0.00015
H	0.76981	-1.24952	-0.00011
S	3.61552	-0.72125	-0.00013
H	2.92463	-1.87957	-0.00002

27 *trans*

E_{total} = -799.2510211 Hartree

C	-3.43468	-1.06406	0.00012
C	-3.88793	0.24313	-0.00013
C	-2.74973	1.07726	-0.00013
C	-1.61582	0.26558	0.00005
N	-2.06969	-1.04250	0.00004
C	-0.24060	0.65430	0.00008
C	0.84904	-0.14779	0.00002
C	2.19618	0.42958	0.00007
O	2.46729	1.60802	0.00009
H	-3.97846	-1.99518	0.00023
H	-4.92136	0.55097	-0.00026
H	-2.73389	2.15636	-0.00027
H	-1.48192	-1.85976	0.00034
H	-0.06301	1.72589	0.00013
H	0.77643	-1.23032	-0.00009
S	3.49644	-0.85591	-0.00013
H	4.50982	0.03189	0.00055

28

E_{total} = -860.6611603 Hartree

C	-3.40798	-1.07519	-0.00012
C	-3.87479	0.22864	0.00008
C	-2.74645	1.07276	-0.00010
C	-1.60371	0.27090	0.00001
N	-2.04517	-1.04215	0.00005
C	-0.23606	0.67298	0.00004
C	0.85945	-0.12682	0.00010
C	2.18653	0.46725	0.00012
O	2.50121	1.61486	-0.00005
H	-3.94384	-2.01097	-0.00017
H	-4.91125	0.52573	0.00016
H	-2.74092	2.15198	-0.00015
H	-1.45032	-1.85460	0.00013
H	-0.07198	1.74651	0.00001
H	0.80500	-1.20680	0.00013
Cl	3.50340	-0.82581	-0.00005

29

E_{total} = -569.7854537 Hartree

C	-3.70767	1.07714	0.00009
C	-4.19818	-0.21859	0.00003
C	-3.08504	-1.08288	-0.00003
C	-1.92750	-0.30152	-0.00000
N	-2.34605	1.01877	0.00004
C	-0.56434	-0.71847	-0.00003
C	0.53746	0.07327	-0.00002
C	1.87127	-0.50262	-0.00005
O	2.13610	-1.69902	-0.00011
H	-4.22657	2.02244	0.00015
H	-5.24002	-0.49660	0.00003
H	-3.09849	-2.16203	-0.00008
H	-1.73266	1.81776	0.00006
H	-0.40556	-1.79367	-0.00007
H	0.49035	1.15532	0.00001
C	3.03328	0.52630	-0.00009
O	2.83588	1.73112	-0.00020
N	4.24660	-0.06690	0.00027
H	5.08139	0.49605	0.00038
H	4.29620	-1.07495	0.00046

30 *cis*

E_{total} = -514.3721488 Hartree

C	-3.26843	1.09344	-0.00008
C	-3.76338	-0.20072	0.00014
C	-2.65368	-1.06857	0.00019
C	-1.49307	-0.29132	0.00001
N	-1.90713	1.03075	-0.00017
C	-0.13326	-0.71654	-0.00002
C	0.97779	0.06274	-0.00022
C	2.30766	-0.52612	-0.00024
O	2.57316	-1.72126	0.00035
H	-3.78436	2.04037	-0.00019
H	-4.80614	-0.47505	0.00025
H	-2.67071	-2.14765	0.00035
H	-1.29246	1.82858	-0.00032
H	0.01681	-1.79300	0.00013
H	0.93666	1.14624	-0.00038
C	3.49338	0.44994	0.00006
O	3.38607	1.65049	-0.00013
H	4.47417	-0.06571	0.00058

30 *trans*

E_{total} = -514.3636872 Hartree

C	3.45563	-1.01827	-0.00001
C	3.86173	0.30645	0.00001
C	2.69608	1.09677	0.00002
C	1.58993	0.24305	-0.00000
N	2.09303	-1.04829	-0.00001
C	0.20706	0.58153	-0.00001
C	-0.86375	-0.25398	-0.00002
C	-2.22756	0.27358	-0.00001
O	-2.52670	1.45381	-0.00002
H	4.03478	-1.92795	-0.00002
H	4.88345	0.65091	0.00001
H	2.63981	2.17450	0.00003
H	1.53596	-1.88682	0.00002
H	-0.00974	1.64678	0.00000
H	-0.74672	-1.33383	-0.00002
C	-3.33864	-0.80215	0.00000
O	-4.50933	-0.54008	0.00003
H	-2.98335	-1.85729	-0.00002

31

E_{total} = -1819.1944568 Hartree

C	-4.63602	-1.09974	-0.00003
C	-5.19821	0.16581	-0.00009
C	-4.13527	1.09144	-0.00002
C	-2.93599	0.37707	0.00007
N	-3.27906	-0.96509	0.00005
C	-1.60124	0.87874	0.00013
C	-0.44991	0.16337	0.00012
C	0.83684	0.85337	0.00019
O	0.99080	2.05255	0.00013
H	-5.10070	-2.07285	-0.00004
H	-6.25392	0.38513	-0.00017
H	-4.20959	2.16814	-0.00006
H	-2.62511	-1.73078	0.00023
H	-1.51249	1.96133	0.00019
H	-0.44698	-0.91904	0.00005
C	2.10985	-0.08125	-0.00002
Cl	2.05699	-1.12878	-1.47462
Cl	3.60491	0.87181	-0.00059
Cl	2.05783	-1.12829	1.47499

32

E_{total} = -738.1648381 Hartree

C	-3.98674	-1.12924	-0.00002
C	-4.51763	0.15057	-0.00002
C	-3.43281	1.04862	0.00000
C	-2.25078	0.30412	0.00001
N	-2.62777	-1.02944	-0.00001
C	-0.90632	0.77223	0.00003
C	0.23224	0.03310	0.00005
C	1.53415	0.68538	0.00007
O	1.74785	1.87953	-0.00004
H	-4.47627	-2.09011	-0.00003
H	-5.56759	0.39577	-0.00003
H	-3.47992	2.12683	0.00001
H	-1.99370	-1.81179	-0.00000
H	-0.79160	1.85267	0.00004
H	0.21804	-1.05090	0.00005
C	2.74746	-0.29268	-0.00000
F	2.70870	-1.09968	1.08960
F	2.70840	-1.09991	-1.08943
F	3.91458	0.34567	-0.00023

33

E_{total} = -493.278863 Hartree

C	-3.27041	-1.09102	-0.00026
C	-3.73195	0.21619	-0.00001
C	-2.60118	1.05394	-0.00011
C	-1.46008	0.24625	0.00002
N	-1.90884	-1.06540	0.00038
C	-0.09465	0.64267	0.00004
C	1.00576	-0.15490	0.00031
C	2.34046	0.42698	0.00035
O	2.61463	1.61440	-0.00038
H	-3.81169	-2.02378	-0.00039
H	-4.76720	0.51736	-0.00003
H	-2.58984	2.13311	-0.00020
H	-1.31851	-1.88127	0.00071
H	0.07741	1.71538	-0.00012
H	0.94419	-1.23787	0.00052
C	3.44188	-0.56571	-0.00002
N	4.30450	-1.33238	-0.00030

34

E_{total} = -605.5871603 Hartree

C	3.64936	-1.09673	0.00029
C	4.15892	0.19356	0.00036
C	3.06033	1.07131	0.00026
C	1.89030	0.30463	0.00012
N	2.29088	-1.02261	0.00026
C	0.54071	0.74677	-0.00006
C	-0.57879	-0.02788	-0.00016
C	-1.87242	0.60079	-0.00030
O	-2.20667	1.74298	-0.00030
H	4.15686	-2.04833	0.00033
H	5.20453	0.45639	0.00046
H	3.08839	2.15021	0.00025
H	1.67055	-1.81647	0.00027
H	0.40812	1.82512	-0.00011
H	-0.55732	-1.10766	-0.00010
N	-3.08253	-0.48450	-0.00012
O	-4.20261	-0.02925	-0.00043
O	-2.78071	-1.67175	0.00009

35 *cis*

E_{total} = -530.3425025 Hartree

C	3.26175	-1.07034	0.02341
C	3.73966	0.22975	-0.02018
C	2.61912	1.08225	-0.03748
C	1.46868	0.29005	-0.00334
N	1.90015	-1.02618	0.03411
C	0.10540	0.70071	-0.00500
C	-0.99913	-0.08723	0.04760
C	-2.32076	0.50960	0.05092
O	-2.63148	1.67117	-0.06159
H	3.79049	-2.00991	0.04667
H	4.77862	0.51748	-0.03729
H	2.62195	2.16098	-0.07008
H	1.29779	-1.83295	0.05656
H	-0.05279	1.77500	-0.05278
H	-0.94911	-1.16788	0.09499
N	-3.50948	-0.45338	0.23147
O	-3.30225	-1.54799	-0.21749

35 *trans*

E_{total} = -530.3431031 Hartree

C	-3.43154	-1.01843	0.00006
C	-3.84797	0.30428	-0.00024
C	-2.68922	1.10242	0.00009
C	-1.57643	0.25553	0.00003
N	-2.07020	-1.03951	0.00010
C	-0.19700	0.60026	0.00001
C	0.87181	-0.24044	-0.00001
C	2.22543	0.27067	0.00001
O	2.62131	1.40710	0.00007
H	-4.00470	-1.93194	0.00008
H	-4.87228	0.64085	-0.00047
H	-2.64073	2.18054	0.00009
H	-1.50642	-1.87402	0.00034
H	0.01331	1.66667	0.00006
H	0.77404	-1.32049	-0.00006
N	3.23740	-0.93105	-0.00006
O	4.37068	-0.55877	-0.00007