BEILSTEIN JOURNAL OF ORGANIC CHEMISTRY

Supporting Information

for

A combinatorial approach to improving the performance of azoarene photoswitches

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Beilstein J. Org. Chem. **2019,** *15,* 2753–2764. doi:10.3762/bjoc.15.266

Theoretical calculations, synthetic methods, experimental characterization and X-ray crystallography data

Additional theoretical data

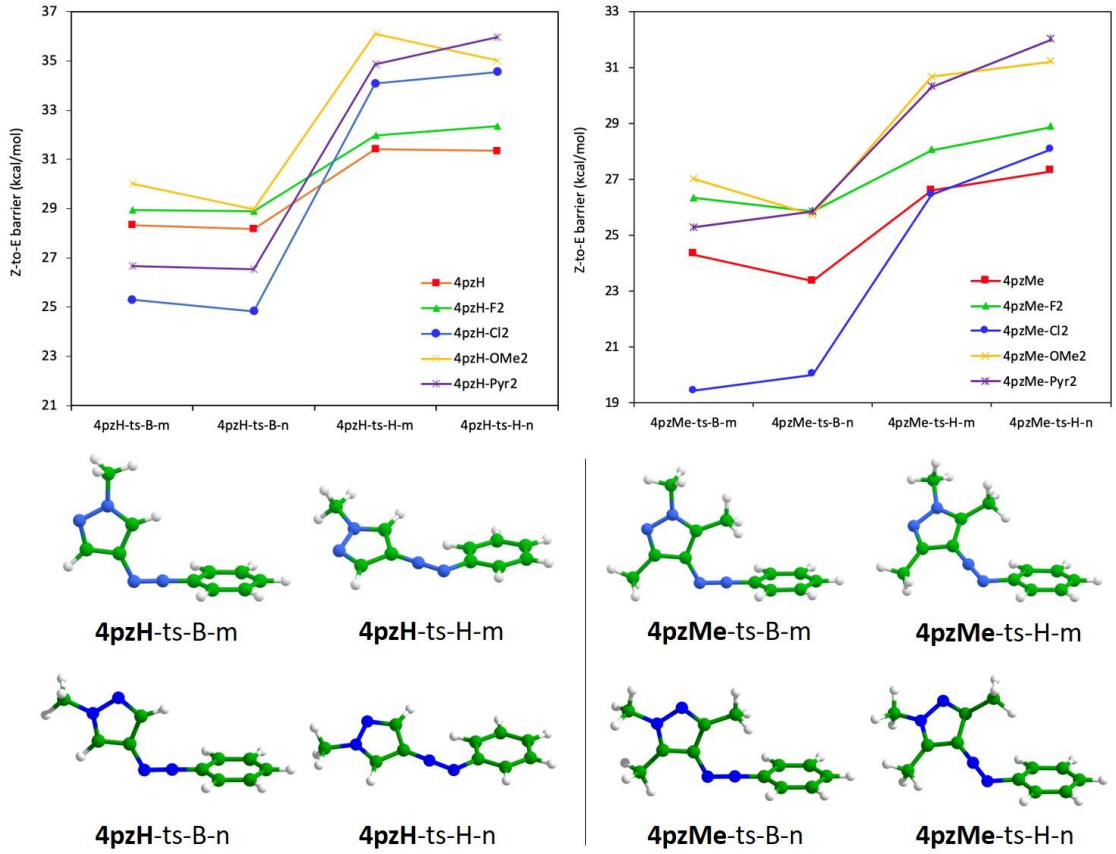


Figure S1: Free-energy barriers calculated for the *Z*–*E* thermal isomerization process in the different pathways considering all possible conformers. Representative transition-state geometries for **4pzH** and **4pzMe** photoswitches are displayed (bottom). "B" and "H" refer to transition states in which the azo N atom is inverted adjacent to the benzene (B) or the heteroring (H) moiety, respectively. The "m" and "n" labels refer to the relative orientation of the heteroring with respect to the benzene moiety: *N*-methyl "m" or =N– atom "n" close to the benzene ring.

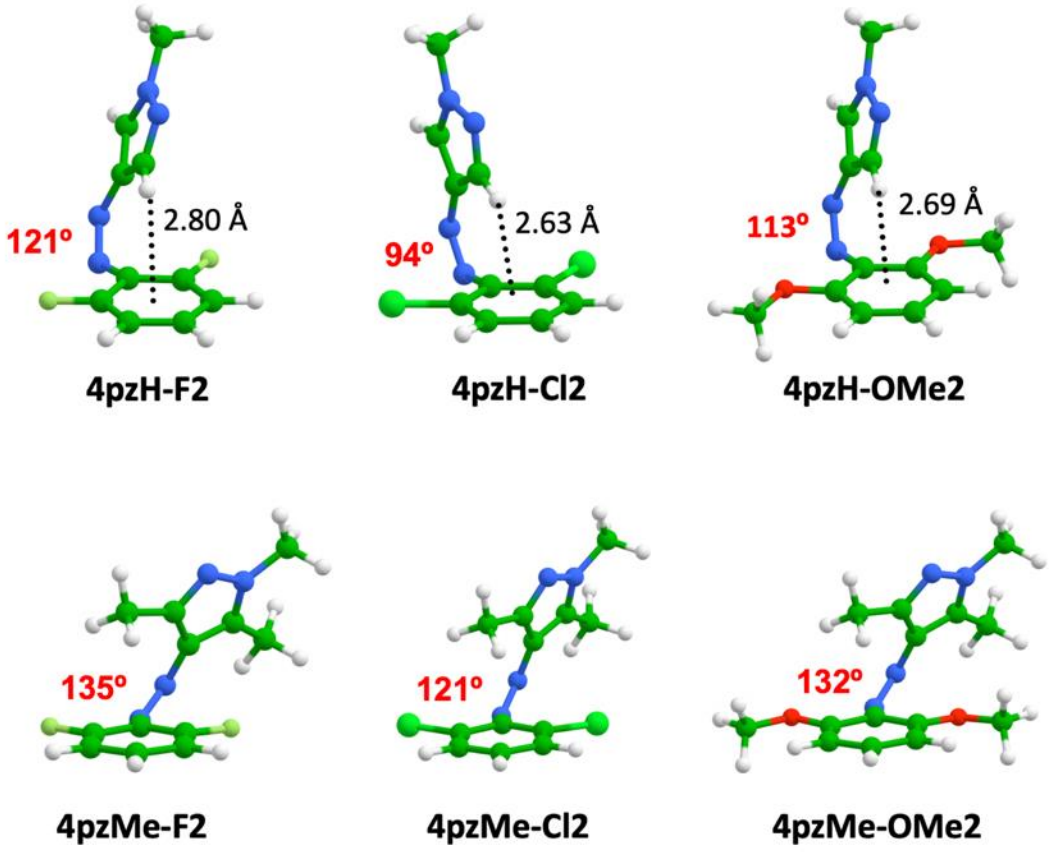


Figure S2: Minimum-energy structure calculated at the PBE0-D3/6-31G** level of theory for representative T-shaped and twisted *Z*-isomers of *ortho*-substituted **4pzH-X** and **4pzMe-X** photoswitches, respectively. Short CH···π distances and tilting dihedral angle θ as defined in Figure 3 are shown.

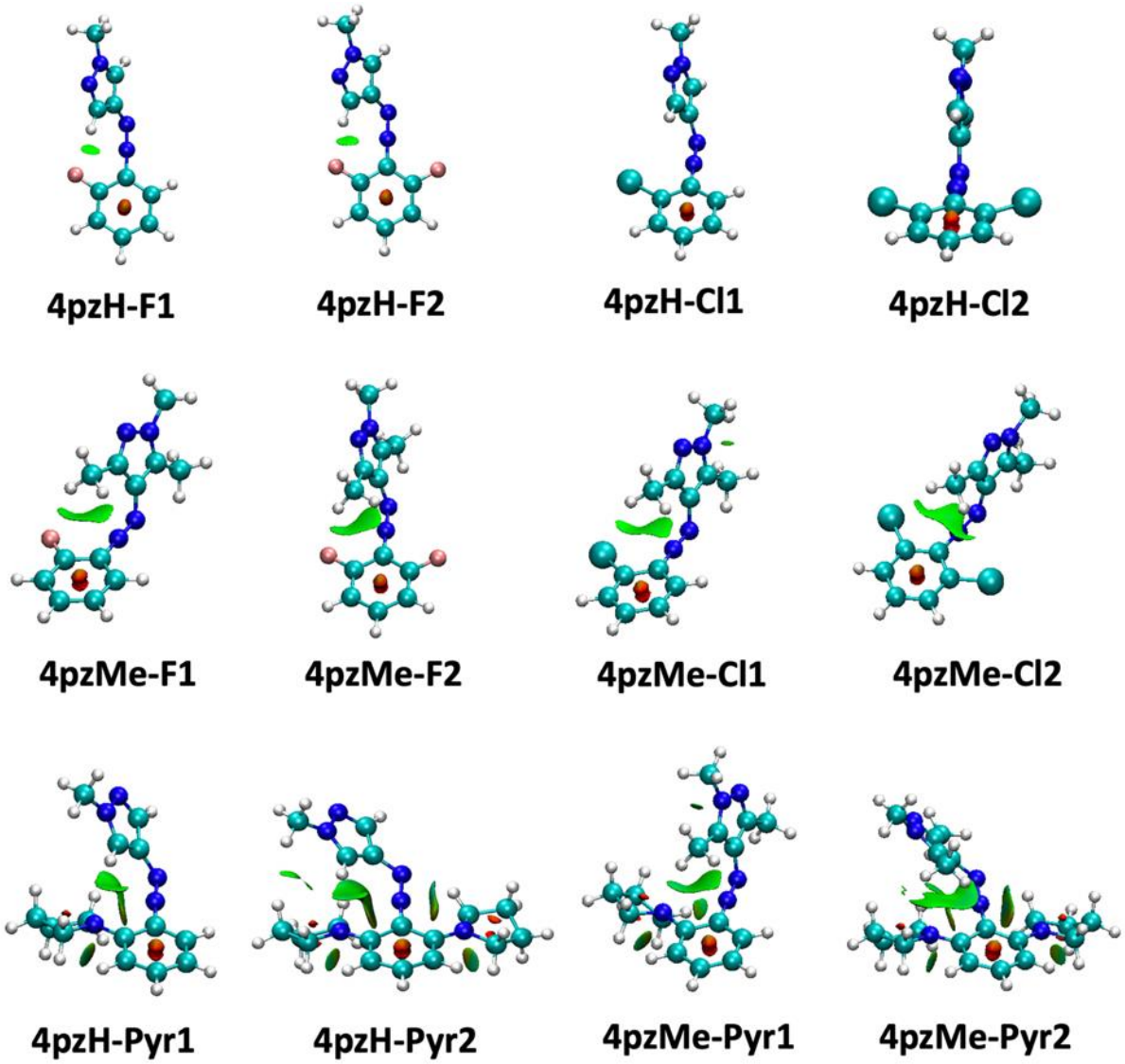


Figure S3. Non-covalent index (NCI) surfaces calculated for representative *ortho*-substituted arylazopyrazoles at the lowest-lying transition-state geometry.

Our previous studies reported a reasonably good correlation between the strength of the N=N azo bond and the half-life time in *Z*-arylazopyrazoles [1]. Thus, analysis of the Wiberg index of the N=N bond was demonstrated to be a diagnostic tool for predicting *Z*-isomer half-life in the heteroarylazo switches. The Wiberg index directly correlates with the azo bond strength and thus with the N=N distance (Figure S4).

However, a quick inspection of the relationship between the computed Wiberg indexes and the theoretical $t_{1/2}$ (Figure S5) for these *ortho*-substituted derivatives, suggests a weaker correlation for our new arylazopyrazoles. The pyrrolidine-substituted photoswitches were the largest outliers and so were removed from the comparison, resulting in an improved correlation between Wiberg index and $t_{1/2}$ (Figure S6). Nonetheless, for the halogen-substituted photoswitches, similar Wiberg indexes are computed (1.837, 1.838, 1.834 and 1.822 for **4pzH-F2**, **4pzH-Cl2**, **4pzMe-F2** and **4pzMe-Cl2**, respectively) whereas very large differences in half-life times are predicted (from 5 days in **4pzH-Cl2** to ca. 4000 days in **4pzH-F2**, or from 2 minutes in **4pzMe-Cl2** to 26 days in **4pzMe-F2**). Thus, it would seem that *ortho*-benzene substitution presents a limitation with respect to the use of the Wiberg index as a parameter to estimate the *Z*-isomer half-life.

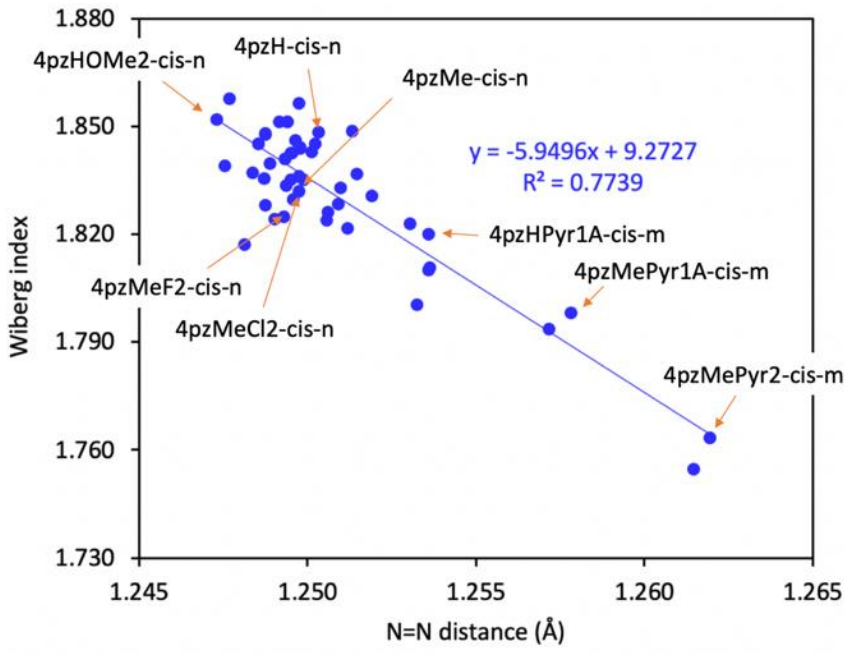


Figure S4: Relationship between the Wiberg index and the azo N=N distance for all the conformers studied.

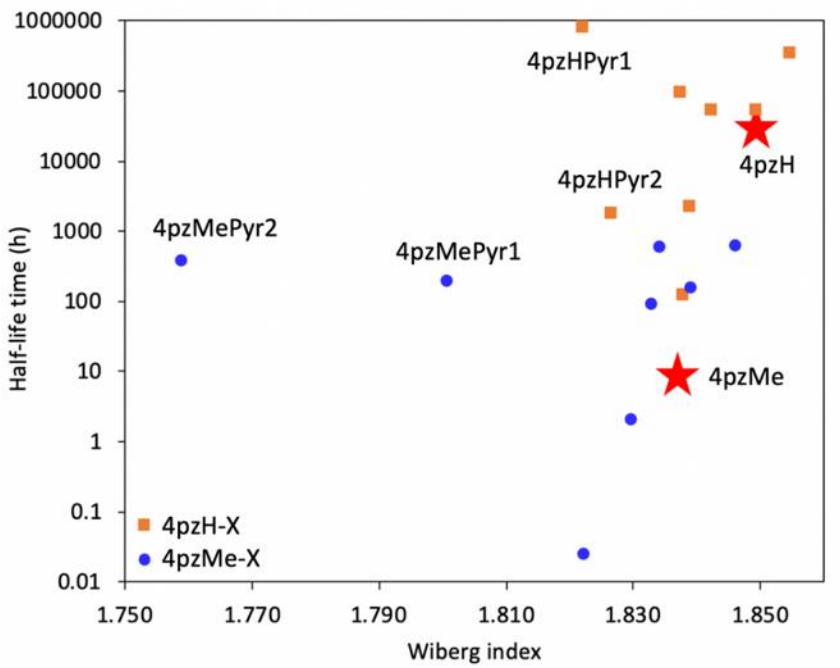


Figure S5: Relationship between the theoretical half-life time and the Wiberg index for the list of photoswitches under study in this paper.

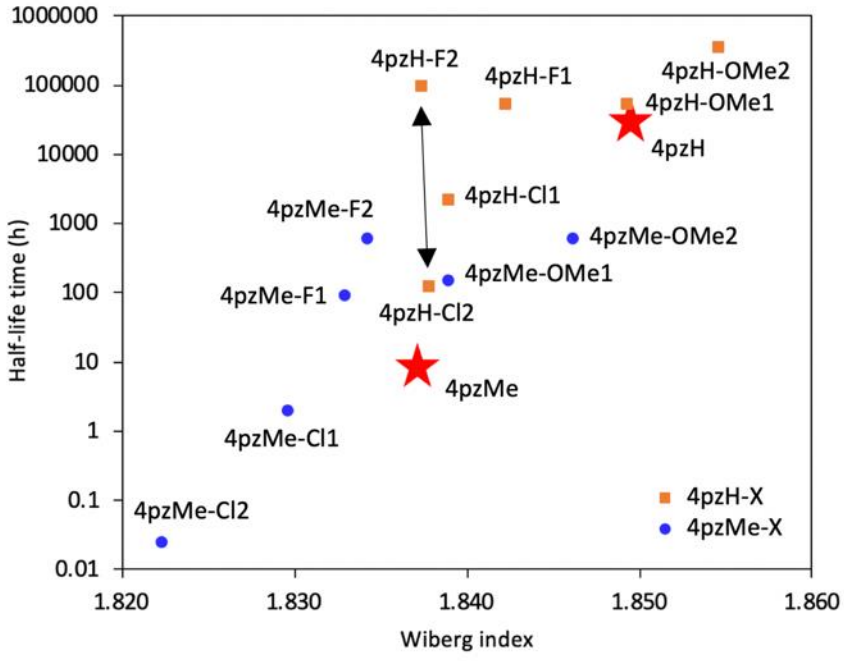


Figure S6: Relationship between the theoretical half-life time and the Wiberg index for the list of photoswitches under study in this paper excluding the pyrrolidine-based derivatives.

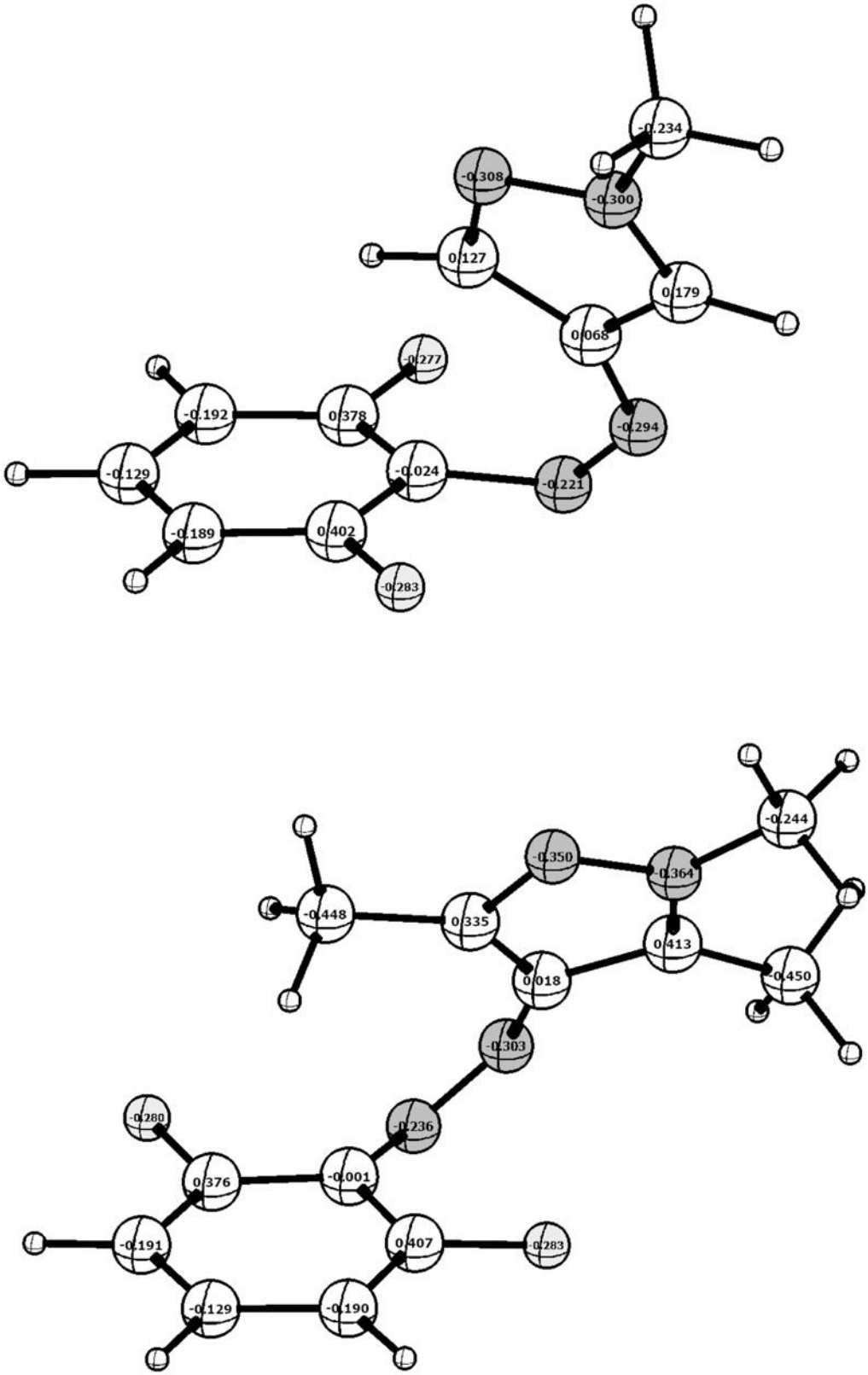


Figure S7: Atomic charges calculated for the *Z*-isomer minimum-energy geometry of **4pzH-F2** (top) and **4pzMe-F2** (bottom).

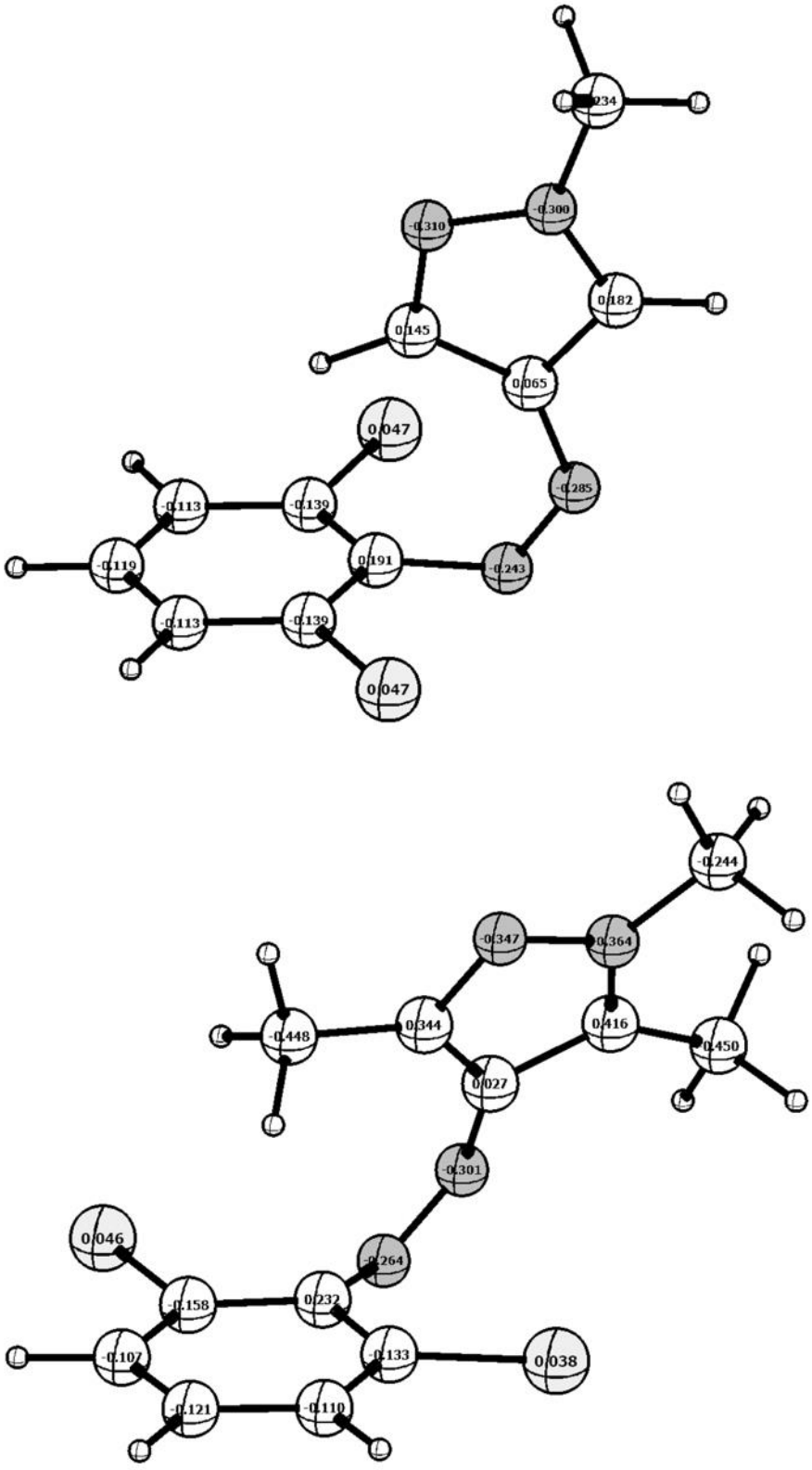


Figure S8: Atomic charges calculated for the *Z*-isomer minimum-energy geometry of **4pzH-Cl2** (top) and **4pzMe-Cl2** (bottom).

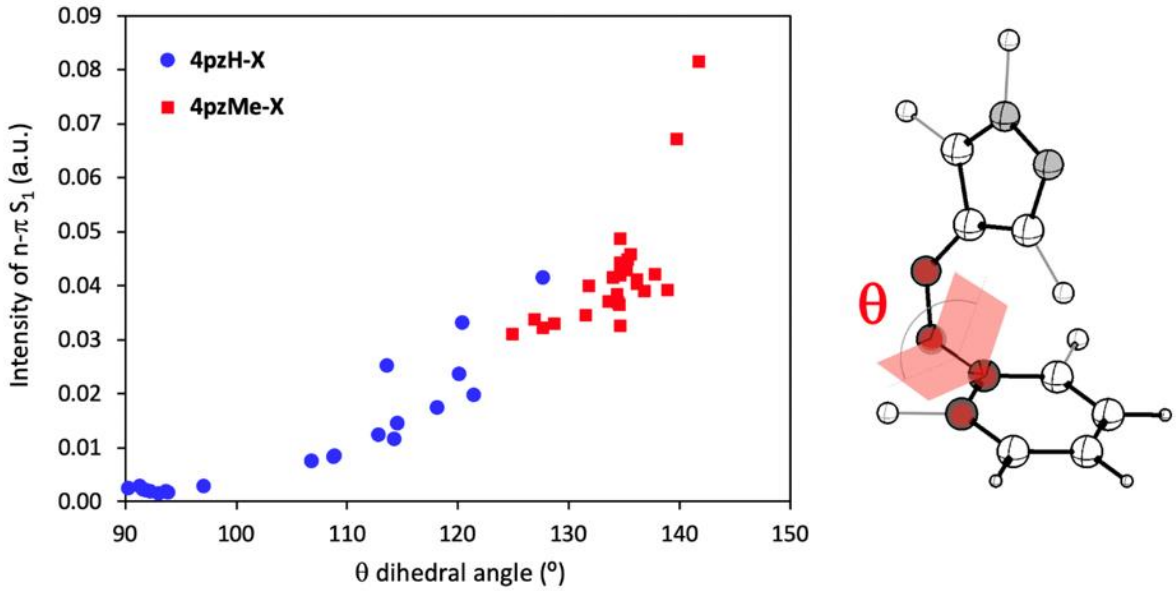


Figure S9: Intensity of the *n*–π* electronic excitation as a function of the CCNN dihedral angle θ between the aryl ring and the azo moiety.

Conformer labelling: “1” and “2” indicate the number of *ortho*-substitutions; “m” and “n” labels refer to the relative orientation of the heteroring with respect to the benzene moiety: N-methyl “m” or =N– atom “n” close to the benzene ring; and “X” and “Y” indicate the target *ortho* position in mono-substituted photoswitches (see Table 1).

Table S1: Excitation energies and oscillator strengths for the characteristic *n*–π* and π–π* transitions in *Z*-isomers.

	n-π* excitation			π-π* excitation[a]		
	E (eV)	E (nm)	f	E (eV)	E (nm)	f
4pzH-m	3.0264	410	0.0020	4.7832	259	0.13
4pzH-n	3.0332	409	0.0019	4.8637	255	0.12
4pzHCl1X-m	3.0311	409	0.0021	4.7692	260	0.15
4pzHCl1X-n	3.0400	408	0.0027	4.9402	251	0.25
4pzHCl1Y-m	3.0318	409	0.0021	4.7510	261	0.15
4pzHCl1Y-n	3.0401	408	0.0027	4.9402	251	0.25
4pzHCl2-m	3.0376	408	0.0018	4.7328	262	0.23
4pzHCl2-n	3.0570	406	0.0017	4.8438	256	0.27
4pzHF1X-m	2.9588	419	0.0084	4.9206	252	0.20
4pzHF1X-n	2.9123	426	0.0174	4.8819	254	0.30
4pzHF1Y-m	2.9595	419	0.0083	4.9206	252	0.20
4pzHF1Y-n	2.9123	426	0.0174	4.8819	254	0.30
4pzHF2-m	2.9441	421	0.0116	4.8062	258	0.23
4pzHF2-n	2.9229	424	0.0197	4.8438	256	0.28
4pzHOMe1X-m	2.9192	425	0.0075	4.8438	256	0.15
4pzHOMe1X-n	2.8829	430	0.0144	4.8819	254	0.30
4pzHOMe1Y-m	2.9194	425	0.0075	4.8438	256	0.15
4pzHOMe1Y-n	2.8827	430	0.0144	4.8819	254	0.30
4pzHOMe2-m	2.9413	422	0.0015	4.8249	257	0.20
4pzHOMe2-n	2.8918	429	0.0122	4.8819	254	0.25
4pzHPyr1X-m	2.6420	469	0.0252	4.5588	272	0.10
4pzHPyr1X-n	2.6557	467	0.0331	4.6269	268	0.13
4pzHPyr1Y-m	2.6267	472	0.0236	4.5091	275	0.10
4pzHPyr1Y-n	2.6334	471	0.0415	4.4765	277	0.12
4pzHPyr2-m	2.7493	451	0.0023	4.6269	268	0.15
4pzHPyr2-n	2.6266	472	0.0052	4.7328	262	0.15
4pzMe-m	2.6610	466	0.0389	4.1751	297	0.10
4pzMe-n	2.6960	460	0.0419	4.3206	287	0.18
4pzMeCl1X-m	2.7119	457	0.0401	4.2177	294	0.10
4pzMeCl1X-n	2.7424	452	0.0418	4.3972	282	0.20
4pzMeCl1Y-m	2.7696	448	0.0327	4.2321	293	0.10
4pzMeCl1Y-n	2.8108	441	0.0336	4.4928	276	0.18
4pzMeCl2-m	2.8094	441	0.0319	4.2177	294	0.10
4pzMeCl2-n	2.8513	435	0.0309	4.5588	272	0.24
4pzMeF1X-m	2.7523	450	0.0426	4.2321	293	0.07
4pzMeF1X-n	2.7552	450	0.0455	4.3972	282	0.19
4pzMeF1Y-m	2.7491	451	0.0388	4.1751	297	0.10
4pzMeF1Y-n	2.7645	448	0.0409	4.3509	285	0.20
4pzMeF2-m	2.8352	437	0.0414	4.2034	295	0.10
4pzMeF2-n	2.8241	439	0.0438	4.3972	282	0.18
4pzMeOMe1X-m	2.7513	451	0.0441	4.3056	288	0.14
4pzMeOMe1X-n	2.7557	450	0.0485	4.4444	279	0.18
4pzMeOMe1Y-m	2.7333	454	0.0324	4.1892	296	0.10
4pzMeOMe1Y-n	2.7409	452	0.0366	4.3816	283	0.19
4pzMeOMe2-m	2.8055	442	0.0344	4.3206	287	0.15
4pzMeOMe2-n	2.7956	443	0.0397	4.4604	278	0.23
4pzMePyr1X-m	2.5757	481	0.0362	4.2177	294	0.10
4pzMePyr1X-n	2.6059	476	0.0383	4.3206	287	0.14
4pzMePyr1Y-m	2.5816	480	0.0670	4.2177	294	0.12
4pzMePyr1Y-n	2.5907	479	0.0814	4.3056	288	0.18
4pzMePyr2-m	2.4752	501	0.0368	4.1892	296	0.10
4pzMePyr2-n	2.5041	495	0.0446	4.3056	288	0.15

[a] Excitation energies and intensities for the π-π* transition in Z isomers were obtained from the simulated absorption spectra through Gaussian convolution of all the computed electronic excitations with a full-width-at-half-maximum of 0.2 eV.

Table S2: Excitation energies and oscillator strengths for the characteristic *n*–π* and π–π* transitions in *E*-isomers.

	n-π* excitation			π-π* excitation		
	E (eV)	E (nm)	f	E (eV)	E (nm)	f
4pzH-m	2.7745	447	0.0000	3.8991	318	0.7770
4pzH-n	2.7727	447	0.0000	3.9699	312	0.8187
4pzH-Cl1X-m	2.6898	461	0.0000	3.7638	329	0.6834
4pzH-Cl1X-n	2.6846	462	0.0000	3.8218	324	0.7107
4pzH-Cl1Y-m	2.7023	459	0.0158	3.9933	310	0.5169
4pzH-Cl1Y-n	2.7101	458	0.0137	4.0524	306	0.5281
4pzH-Cl2-m	2.7320	454	0.0155	4.0759	304	0.5298
4pzH-Cl2-n	2.7443	452	0.0152	4.1463	299	0.5341
4pzH-F1X-m	2.7497	451	0.0000	3.8238	324	0.7652
4pzH-F1X-n	2.7455	452	0.0000	3.8881	319	0.8034
4pzH-F1Y-m	2.6976	460	0.0000	3.9325	315	0.7779
4pzH-F1Y-n	2.6987	459	0.0000	4.0052	310	0.8136
4pzH-F2-m	2.6560	467	0.0000	3.8992	318	0.8221
4pzH-F2-n	2.6529	467	0.0000	3.9732	312	0.8805
4pzH-OMe1X-m	2.7015	459	0.0000	3.5866	346	0.5749
4pzH-OMe1X-n	2.6997	459	0.0000	3.6305	342	0.5899
4pzH-OMe1Y-m	2.6560	467	0.0000	3.7510	331	0.5748
4pzH-OMe1Y-n	2.6613	466	0.0000	3.8121	325	0.5693
4pzH-OMe2-m	2.6218	473	0.0201	3.8302	324	0.6526
4pzH-OMe2-n	2.6415	469	0.0207	3.8951	318	0.6432
4pzH-Pyr1X-m	2.8232	439	0.0603	3.2570	381	0.2066
4pzH-Pyr1X-n	2.8281	438	0.0553	3.2930	377	0.1951
4pzH-Pyr1Y-m	2.7637	449	0.0003	3.0612	405	0.3504
4pzH-Pyr1Y-n	2.7711	447	0.0002	3.0817	402	0.3677
4pzH-Pyr2-m	2.7419	452	0.0594	2.9836	347	0.2708
4pzH-Pyr2-n	2.7484	451	0.0556	2.9991	346	0.2704
4pzMe-m	2.7358	453	0.0000	3.7937	327	0.7551
4pzMe-n	2.8094	441	0.0000	3.9022	318	0.8044
4pzMe-Cl1X-m	2.7086	458	0.0000	3.7014	335	0.6954
4pzMe-Cl1X-n	2.7225	455	0.0000	3.7739	329	0.7471
4pzMe-Cl1Y-m	2.7260	455	0.0193	3.9606	313	0.5769
4pzMe-Cl1Y-n	2.7599	449	0.0148	4.0252	308	0.6282
4pzMe-Cl2-m	2.8101	441	0.0140	4.0196	308	0.5588
4pzMe-Cl2-n	2.7868	445	0.0153	4.0778	304	0.6042
4pzMe-F1X-m	2.7062	458	0.0000	3.7168	334	0.7488
4pzMe-F1X-n	2.7794	446	0.0000	3.8205	325	0.7991
4pzMe-F1Y-m	2.7136	457	0.0031	3.8639	321	0.7665
4pzMe-F1Y-n	2.7365	453	0.0000	3.9432	314	0.8306
4pzMe-F2-m	2.6379	470	0.0017	3.7961	327	0.7816
4pzMe-F2-n	2.7073	458	0.0032	3.9164	317	0.8388
4pzMe-OMe1X-m	2.6593	466	0.0000	3.5322	351	0.6283
4pzMe-OMe1X-n	2.7323	454	0.0000	3.6168	343	0.6602
4pzMe-OMe1Y-m	2.6140	474	0.0000	3.6933	336	0.6396
4pzMe-OMe1Y-n	2.6890	461	0.0000	3.7930	327	0.6481
4pzMe-OMe2-m	2.5953	478	0.0095	3.7048	335	0.6652
4pzMe-OMe2-n	2.6616	466	0.0152	3.8167	325	0.7077
4pzMe-Pyr1X-m	2.7918	444	0.0547	3.2550	381	0.2322
4pzMe-Pyr1X-n	2.8417	436	0.0591	3.3370	372	0.2002
4pzMe-Pyr1Y-m	2.7371	453	0.0885	3.1391	395	0.2328
4pzMe-Pyr1Y-n	2.7794	446	0.0888	3.1711	391	0.2540
4pzMe-Pyr2-m	2.6756	463	0.0884	2.9741	352	0.3585
4pzMe-Pyr2-n	2.6898	461	0.0845	2.9983	349	0.3668

Table S3: Solvent effect on the theoretical half-life time (in days) calculated at the PBE0-D3/6-31G** level in a single-point calculation or including geometry reoptimization, under the PCM model (acetonitrile).[a]

	Gas phase	Single-point PCM	Optimized PCM
4pzH	1300	3200	4000
4pzHF2	4100	40000	46000
4pzHCl2	5.1	810	62
4pzMe	0.38	4.2	4.1
4pzMeF2	26	490	110
4pzMeCl2	0.001	0.10	0.01

[a] In all cases, the most stable transition state conformer is the one in which the azo N atom adjacent to the benzene moiety is inverted (B-type).

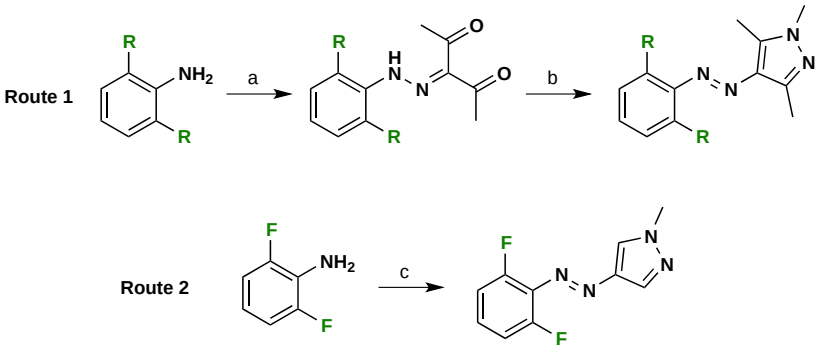
Table S4: Solvent effect (PCM, acetonitrile) on the theoretical energy separation (in nm) of the characteristic electronic excitations calculated at the PBE0-D3/6-31G** level.

	Gas phase	Single-point PCM	Gas phase	Single-point PCM
	n-π*(*E*–*Z*)	n-π*(*E*–*Z*)	π-π* (*E*–*Z*)	π–π* (*E*–*Z*)
4pzH	38	41	58	80
4pzHF2	44	46	58	67
4pzHCl2	46	41	43	50
4pzMe	-15	-10	30	48
4pzMeF2	26	23	33	41
4pzMeCl2	5	7	23	21

General synthetic methods

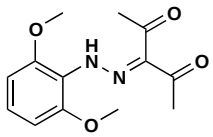
All reagents and solvents were purchased from commercial sources and used as supplied unless otherwise indicated. All reactions were monitored by thin-layer chromatography (TLC) using Merck silica gel 60 F254 plates (0.25 mm). TLC plates were visualised using UV light (254 nm) and/or by using the appropriate TLC stain. Silica column chromatography was performed using Merck Silica Gel 60 (230–400 mesh) treated with a solvent system specified in the individual procedures. Solvents were removed by rotary evaporator at 40 °C or below, in the dark, and the compounds further dried using high vacuum pumps. Infrared spectra were recorded neat on an Agilent Cary 630 FTIR. Reported absorptions are in wavenumbers (cm^{-1}). ^{1}H and ^{13}C NMR were recorded on a Bruker Avance 400 spectrometer at 400 MHz and 100 MHz, respectively. Chemical shifts (δ) are quoted in ppm (parts per million) downfield from tetramethylsilane, referenced to residual solvent signals: ^{1}H δ = 7.26 ($CHCl_3$), 1.94 (MeCN-d_3), ^{13}C δ = 77.16 ($CDCl_3$). The following abbreviations are used to designate multiplicity within ^{1}H NMR analysis; s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br. = broad signal. High-resolution mass spectra (ESI, APCI) were recorded by the Imperial College London Department of Chemistry Mass Spectroscopy Service using a Micromass Autospec Premier and Micromass LCT Premier spectrometer. LCMS analysis of compounds were conducted using a reverse phase LCMS Waters 2767 system equipped with a photodiode array and an ESI mass spectrometer using an XBridge C18 (5 µm, 100 mm × 4.6 mm) column, equipped with an XBridge C18 guard column (5 µm, 4.6 mm × 20 mm). An eluent of MeCN and H_2O was used: 0–10 min 50–98% MeCN, 10–12 min 98% MeCN, 12–13 min 98 to 50% MeCN, 13–17 min 50% MeCN.

Synthetic route



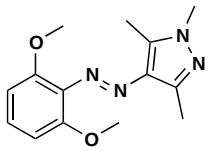
Scheme S1: (a) (i) $NaNO_2$, HCl or AcOH, 0°C (ii) Acetylacetone, NaOAc, H_2O. (b) (i) $MeNHNH_2$, EtOH or MeOH/CH_2Cl_2, reflux. (c) (i) oxone, CH_2Cl_2/H_2O (ii) 1-methyl-1H-pyrazol-4-amine, AcOH, $CHCl_3$.

3-(2-(2,6-Dimethoxyphenyl)hydrazono)pentane-2,4-dione



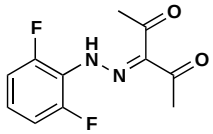
A solution of $NaNO_2$ (169 mg, 2.45 mmol) in water (0.2 mL) was added dropwise to 2,6-dimethoxyaniline (250 mg, 1.63 mmol) in 1 M HCl (5 mL) at 0 °C. The resulting solution was stirred for 0.5 h before being added dropwise to a solution of acetylacetone (0.2 mL, 2.0 mmol) and NaOAc (201 mg, 2.45 mmol) in water (2 mL) at 0 °C. Further NaOAc was added to adjust the pH to 7 resulting in a yellow-green precipitate. After 1 h, the precipitate was filtered, washed with water and dried to yield the desired product as yellow-green solid (375 mg, 1.42 mmol, 87% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 14.67 (s, 1H), 7.11 (t, *J* = 8.4 Hz, 1H), 6.62 (d, *J* = 8.5 Hz, 2H), 3.88 (s, 6H), 2.56 (s, 3H), 2.39 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.8, 196.8, 152.2, 133.6, 126.7, 119.5, 104.9, 56.4, 31.6, 26.5; HRMS (ES) *m/z* calc. for $C_{13}H_{17}N_2O_4$ $[M+H]^+$ 265.1188; found 265.1184; IR: 2964, 2832, 1653, 1517, 1354, 1326, 1255, 1180, 1105, 1095, 1025, 847.

(*E*)-4-((2,6-Dimethoxyphenyl)diazenyl)-1,3,5-trimethyl-1*H*-pyrazole



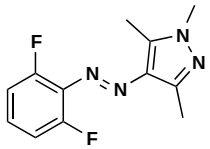
Methylhydrazine (0.10 mL, 2.0 mmol) was added to a solution of 3-(2-(2,6-dimethoxyphenyl)hydrazono)pentane-2,4-dione (350 mg, 1.32 mmol) in CH_2Cl_2 (3 mL) and MeOH (6 mL). The reaction mixture was heated at 50 °C for 1 h. Further methylhydrazine (0.10 mL, 2.0 mmol) was added and heating continued for another 0.75 h. The reaction mixture was allowed to cool to room temperature, diluted with CH_2Cl_2 (30 mL) and washed with 1 M HCl (50 mL). The organic layer was separated and the aqueous layer was extracted with CH_2Cl_2 (2 × 30 mL). The combined organic phases were washed with brine, dried over anhydrous Mg_2SO_4, concentrated in vacuo and subjected to purification by silica gel column chromatography (100% EtOAc). Recrystallization from diethyl ether produced pale orange crystals (329 mg, 1.20 mmol, 91% yield). LCMS (2.76 min); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.16 (t, J = 8.3 Hz, 1H), 6.66 (d, J = 8.4 Hz, 2H), 3.80 (s, 6H), 3.76 (s, 3H), 2.53 (s, 3H), 2.47 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.3, 142.5, 137.9, 136.5, 134.8, 127.9, 105.8, 56.7, 36.0, 13.7, 10.2; HRMS (ES) *m/z* calc. for $C_{14}H_{19}N_4O_2$ $[M+H]^+$ 275.1508; found 275.1508; IR: 2990, 2935, 2836, 1587, 1476, 1433, 1409, 1366, 1251, 1108, 1031, 984, 892.

3-(2-(2,6-Difluorophenyl)hydrazono)pentane-2,4-dione



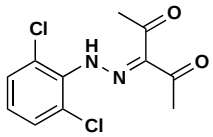
This compound was synthesized according to literature precedent [2]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 14.44 (s, 1H), 7.17 – 7.04 (m, 1H), 7.03 – 6.93 (m, 2H) 2.59 (s, 3H), 2.40 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 198.2, 197.5, 155.5, 155.4, 153.0, 152.9, 135.1, 125.5, 125.5, 125.5, 125.4, 119.8, 112.7, 112.7, 112.6, 112.5, 31.8, 26.6; ^{19}F NMR (377 MHz, $CDCl_3$) δ -124.4; HRMS (ES) *m/z* calc. for $C_{11}H_{11}N_2O_2F_2$ $[M+H]^+$ 241.0789; found 241.0796; IR: 3060, 3003, 1677, 1633, 1520.

(*E*)-4-((2,6-Difluorophenyl)diazenyl)-1,3,5-trimethyl-1*H*-pyrazole



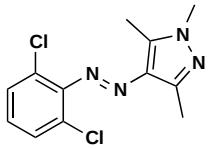
Methylhydrazine (70 µL, 1.2 mmol) was added to a solution of 3-(2-(2,6-difluorophenyl)hydrazono)pentane-2,4-dione (250 mg, 1.04 mmol) in EtOH (10 mL). The reaction mixture was refluxed for 1 h, cooled to room temperature and concentrated in vacuo. EtOAc (50 mL) and H_2O (25 mL) were added and the aqueous layer separated. The aqueous layer was extracted with EtOAc (2 × 10 mL). The combined organic phases were washed with 1 M HCl, saturated $NaHCO_3$, brine, dried over anhydrous Mg_2SO_4, concentrated in vacuo and subjected to purification by silica gel column chromatography (0–10% EtOAc/CH_2Cl_2). The title compound was obtained as orange solid (182 mg, 0.73 mmol, 70% yield). LCMS (5.83 min); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.23 – 7.15 (m, 1H), 7.01 – 6.93 (m, 2H), 3.78 (s, 3H), 2.55 (s, 3H), 2.46 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.2, 157.1, 154.6, 154.6, 142.6, 140.0, 136.8, 132.3, 128.4, 128.3, 128.2, 112.5, 112.4, 112.3, 112.3, 36.2, 13.9, 10.0; HRMS (ES) *m/z* calc. for $C_{12}H_{13}N_4F_2$ $[M+H]^+$ 251.1108; found 251.1108; IR: 2985, 2920, 1610, 1506, 1422.

3-(2-(2,6-Dichlorophenyl)hydrazono)pentane-2,4-dione



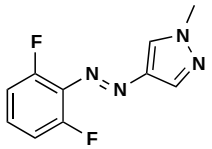
This compound was synthesized according to literature precedent [3]. ^{1}H NMR (400 MHz, $CDCl_3$) δ 14.54 (s, 1H), 7.38 (d, *J* = 8.1 Hz, 2H), 7.10 (dd, *J* = 8.4, 7.8 Hz, 1H), 2.62 (s, 3H), 2.44 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 198.3, 197.6, 135.5, 134.6, 129.8, 129.2, 129.0, 127.6, 126.9, 31.8, 26.9; HRMS (ES) *m/z* calc. for $C_{11}H_{11}N_2O_2Cl_2$ $[M+H]^+$ 273.0198; found 273.0193; IR: 3076, 2999, 2919, 1668, 1631, 1506.

(*E*)-4-((2,6-Dichlorophenyl)diazenyl)-1,3,5-trimethyl-1*H*-pyrazole



Methylhydrazine (93 µL, 1.8 mmol) was added to a solution of 3-(2-(2,6-dichlorophenyl)hydrazono)pentane-2,4-dione (400 mg, 1.47 mmol) in EtOH (10 mL). The reaction mixture was refluxed for 1 h, cooled to room temperature and concentrated in vacuo. EtOAc (50 mL) and H_2O (25 mL) were added and the aqueous layer separated. The aqueous layer was extracted with EtOAc (2 × 10 mL). The combined organic phases were washed with 1 M HCl, saturated $NaHCO_3$, brine, dried over anhydrous Mg_2SO_4, concentrated in vacuo and subjected to purification by silica gel column chromatography (0–10% EtOAc/CH_2Cl_2). The title compound was obtained as orange solid (261 mg, 0.93 mmol, 63% yield). LCMS (7.64 min); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 (d, *J* = 8.1 Hz, 2H), 7.11 (dd, *J* = 8.4, 7.8 Hz, 1H), 3.79 (s, 3H), 2.57 (s, 3H), 2.49 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.9, 142.9, 140.3, 135.9, 129.2, 127.6, 127.4, 36.2, 13.9, 10.1; HRMS (ES) *m/z* calc. for $C_{12}H_{13}N_4Cl_2$ $[M+H]^+$ 283.0517; found 283.0518; IR: 2976, 2919, 1554, 1427, 1392, 1366.

(*E*)-4-((2,6-Difluorophenyl)diazenyl)-1-methyl-1*H*-pyrazole



To a stirred biphasic mixture of 2,6-difluoroaniline (100 mg, 0.78 mmol) in CH_2Cl_2 (10 mL) and H_2O (10 mL) was added a solution of oxone (288 mg, 0.94 mmol) in H_2O (3 mL). The reaction mixture was stirred in the dark at room temperature for 18 h. CH_2Cl_2 (20 mL) and H_2O (5 mL) were added and the aqueous layer separated. The aqueous layer was extracted with CH_2Cl_2 (2 × 15 mL). The combined organic phases were washed with brine, dried over anhydrous Mg_2SO_4 and concentrated in vacuo to yield crude 1,3-difluoro-2-nitrosobenzene as tan solid. This was dissolved in AcOH acid/$CHCl_3$ 4:1 and added to a solution of 1-methyl-1*H*-pyrazol-4-amine (76 mg, 0.78 mmol) in AcOH (1 mL). The reaction mixture was stirred at room temperature for 18 h. Subsequently, the mixture was concentrated in vacuo, using PhMe to azeotrope off any AcOH, and subjected to purification by silica gel column chromatography (0–20% Et_2O/pentane). The title compound was obtained as orange solid (100 mg, 0.45 mmol, 58% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 – 8.01 (m, 2H), 7.29 – 7.22 (m, 1H), 7.05 – 6.96 (m, 2H), 3.98 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 157.1, 157.1, 154.6, 154.5, 142.8, 133.6, 129.6, 129.5, 129.4, 127.5, 112.7, 112.6, 112.5, 112.4, 39.8; HRMS (ES) *m/z* calc. for $C_{10}H_9N_4F_2$ $[M+H]^+$ 223.0795; found 223.0794; IR: 3111, 1534, 1472, 1450, 1386.

UV–vis, photostationary state (PSS) and thermal isomerization kinetics

All samples were irradiated using a Luzchem LZC-4V photoreactor fitted with 12 × 8W LZC-UV A (***E***→***Z***) or LZC-420 nm (***Z***→***E***) lamps. To measure UV–vis spectra, 25 μM solutions of each compound in MeCN were prepared. To determine the PSS, an ≈ 20 mM solution of the relevant compound in MeCN-d_3 was irradiated until no further change was observable by ^{1}H NMR. In order to determine the ***Z***→***E*** thermal isomerization kinetics an ≈ 20 mM solution of the relevant compound in MeCN-d_3 or DMSO-d_6 was irradiated using 12 × 8W LZC-UV A lamps until no further change was observable by ^{1}H NMR. The change in ***Z*** isomer percentage was then followed as a function of time by ^{1}H NMR, through integration of the relevant peaks. In between measurements, NMR samples were kept in the dark and immersed in an oil bath which was held at 25 °C. The natural log of the ***Z*** isomer concentration was plotted against time to yield a straight line, as would be expected from first order kinetics. The gradient of this line was used to calculate the rate constant for ***Z***→***E*** conversion from which the thermal half-life could be calculated:

$$t_{1/2} = \frac{\ln(2)}{k}$$

For the case of **4pzH-F2**, kinetic studies were instead performed at elevated temperatures (vide infra) so as to generate an Eyring plot which in turn allowed determination of the thermal half-life at 25 ºC via extrapolation.

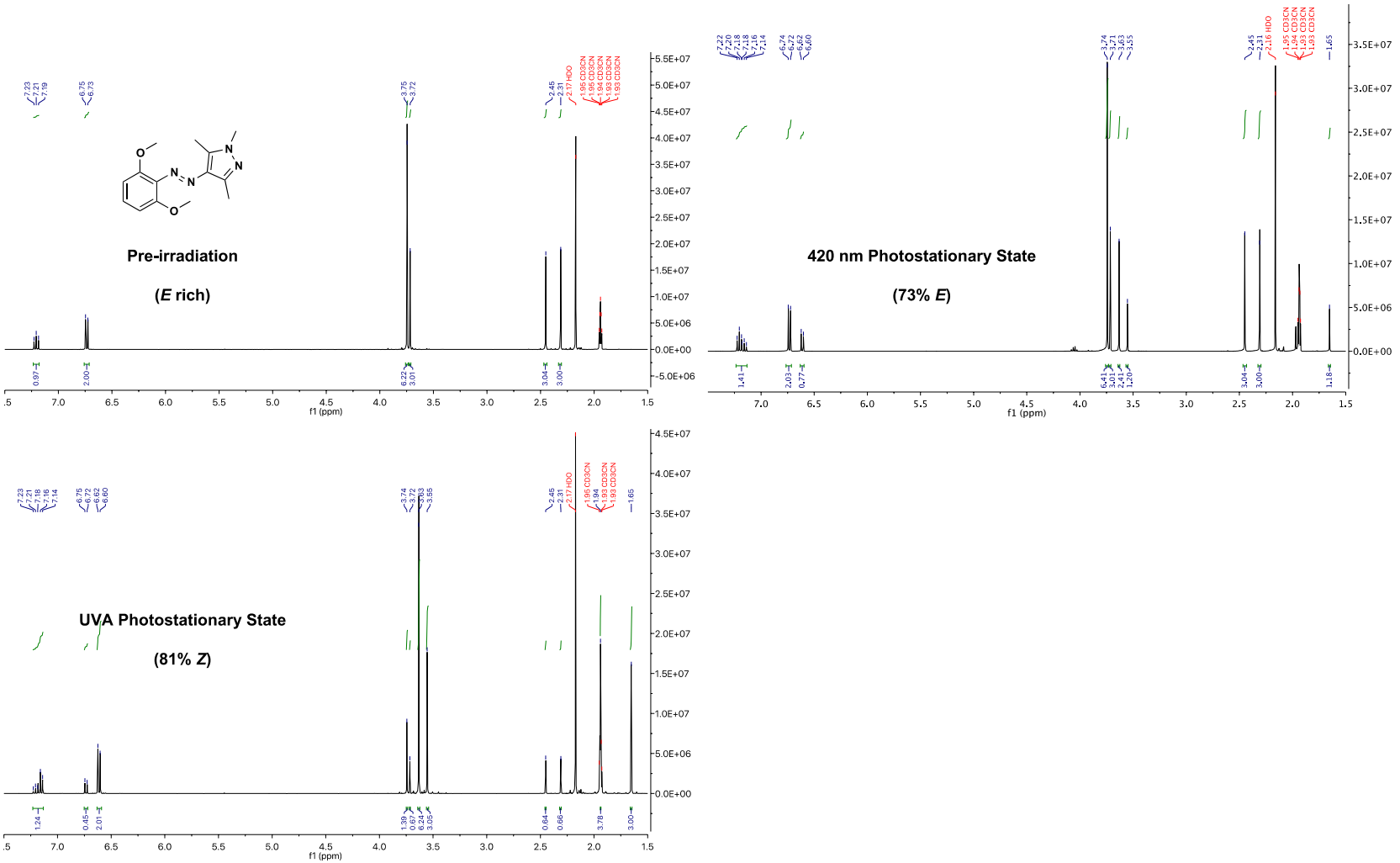


Figure S10. 4pzMe-OMe2 ^{1}H NMR spectra of the ***E***-rich state, UVA PSS and 420 nm PSS in MeCN-d_3 at ≈ 20 mM.

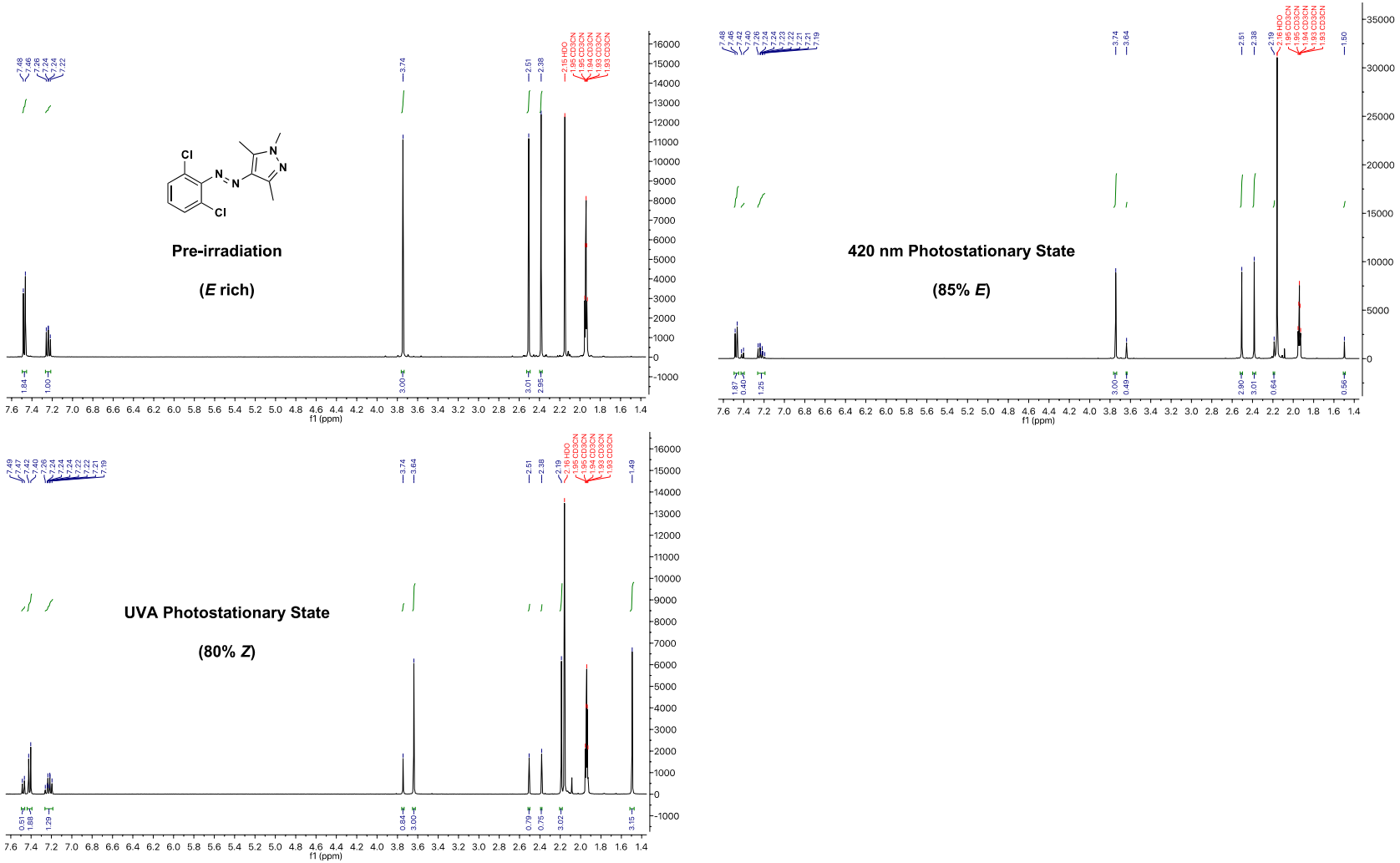


Figure S11. 4pzMe-Cl2 ^{1}H NMR spectra of the ***E***-rich state, UVA PSS and 420 nm PSS in MeCN-d_3 at ≈ 20 mM.

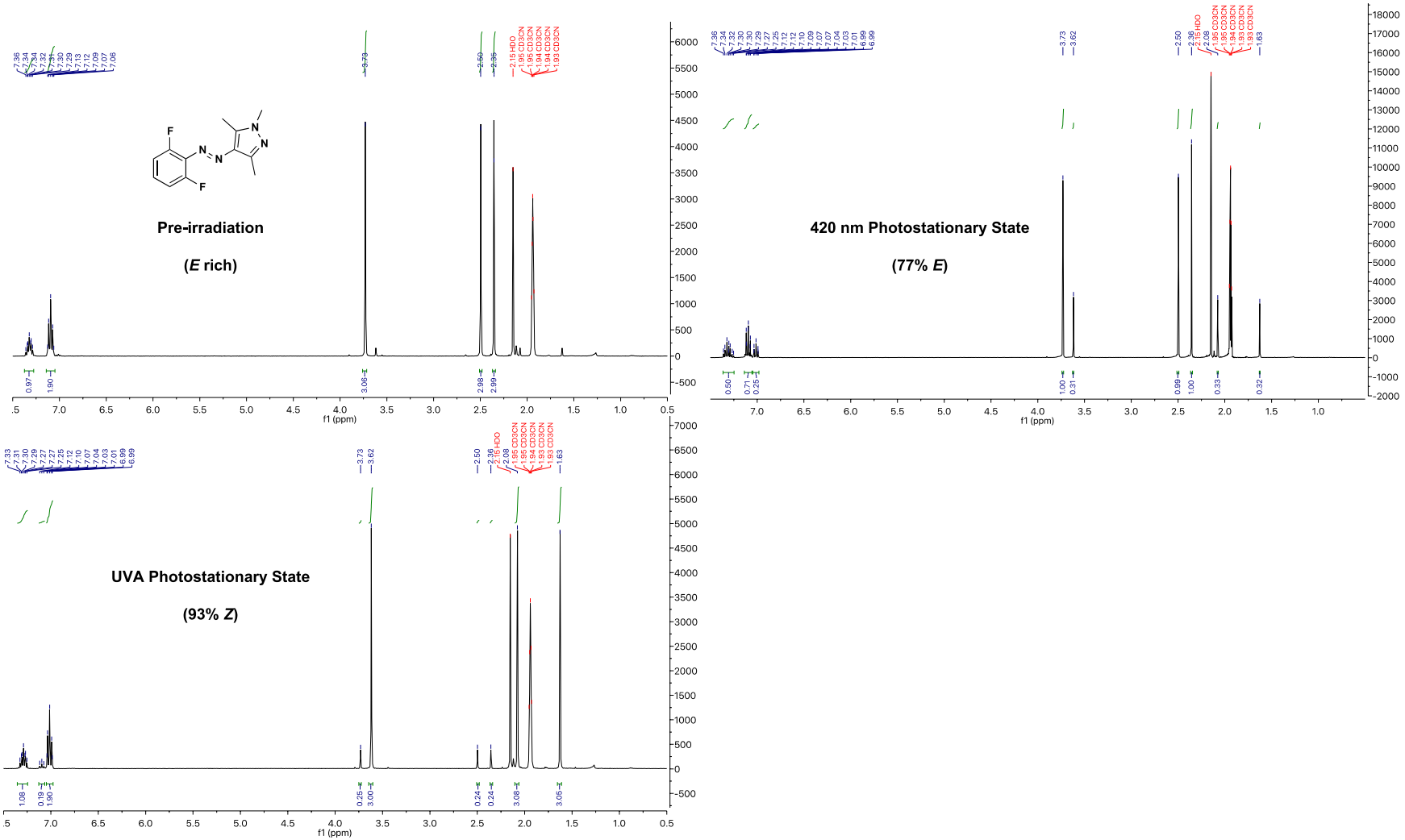


Figure S12. 4pzMe-F2 ^{1}H NMR spectra of the ***E***-rich state, UVA PSS and 420 nm PSS in MeCN-d_3 at ≈ 20 mM.

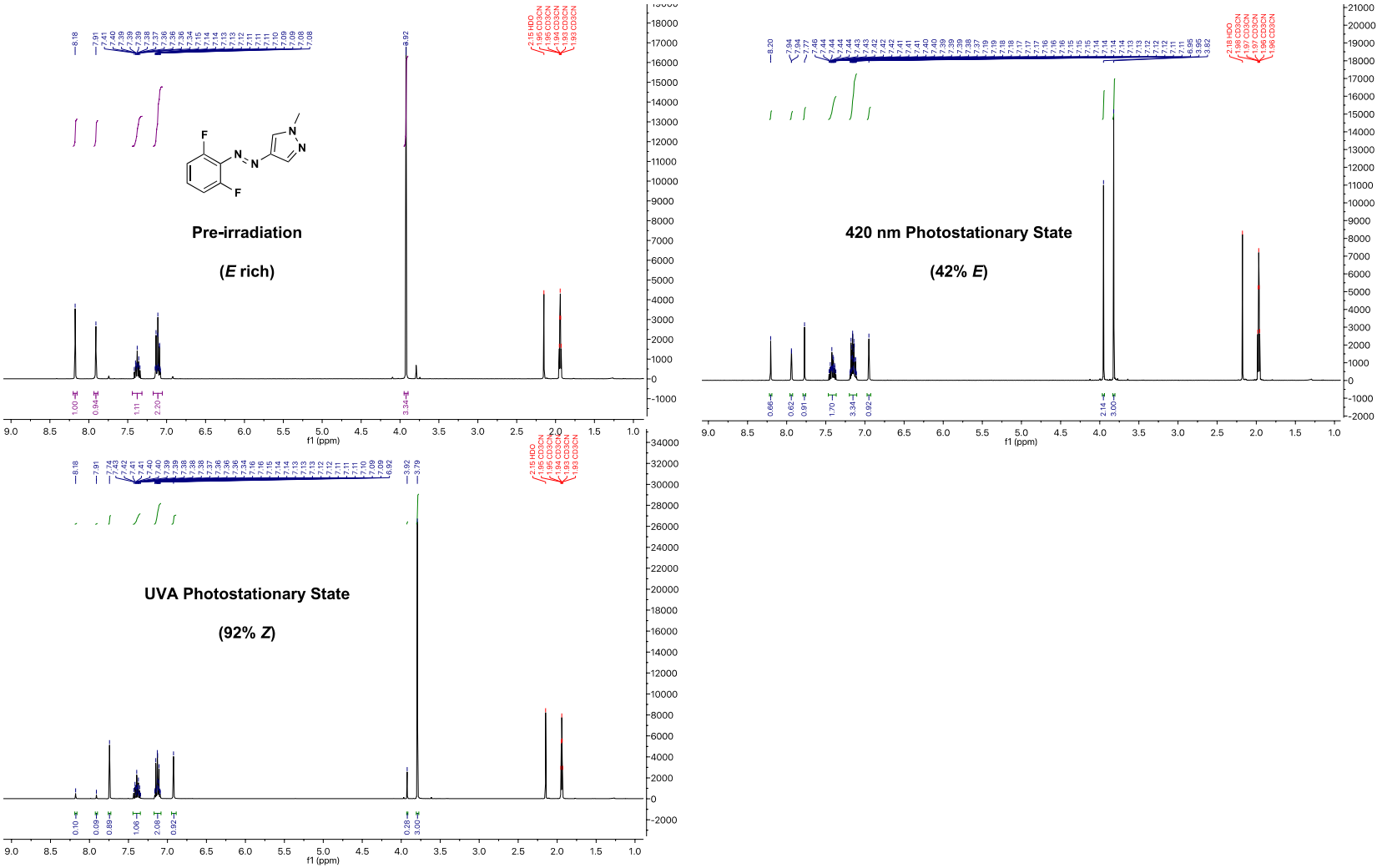


Figure S13. 4pzH-F2 ^{1}H NMR spectra of the ***E***-rich state, UVA PSS and 420 nm PSS in MeCN-d_3 at ≈ 20 mM.

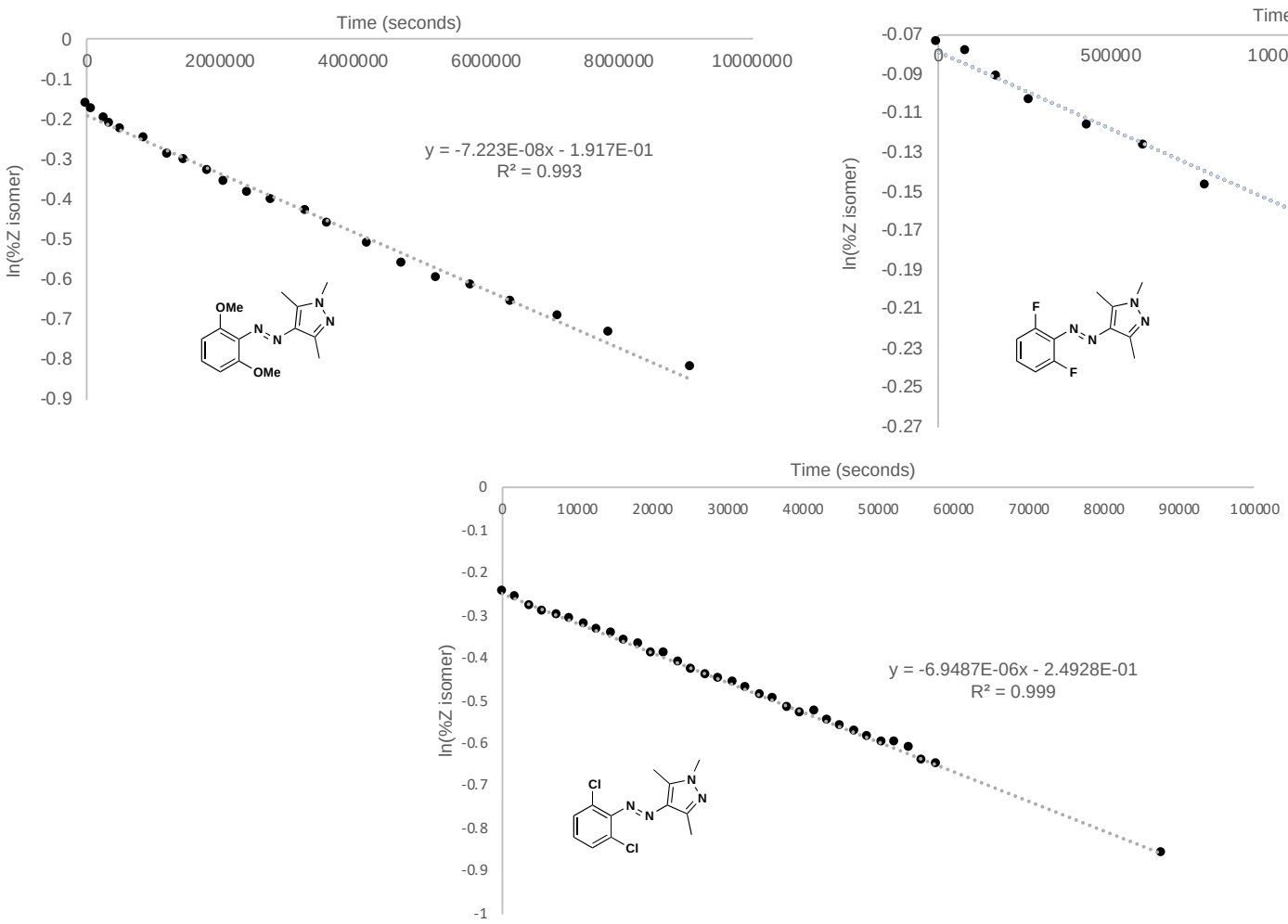


Figure S14. *Z*→*E* thermal isomerisation kinetics of **4pzMe-OMe2**, **4pzMe-F2** and **4pzMe-Cl2** in MeCN-d_3 at ≈ 20 mM.

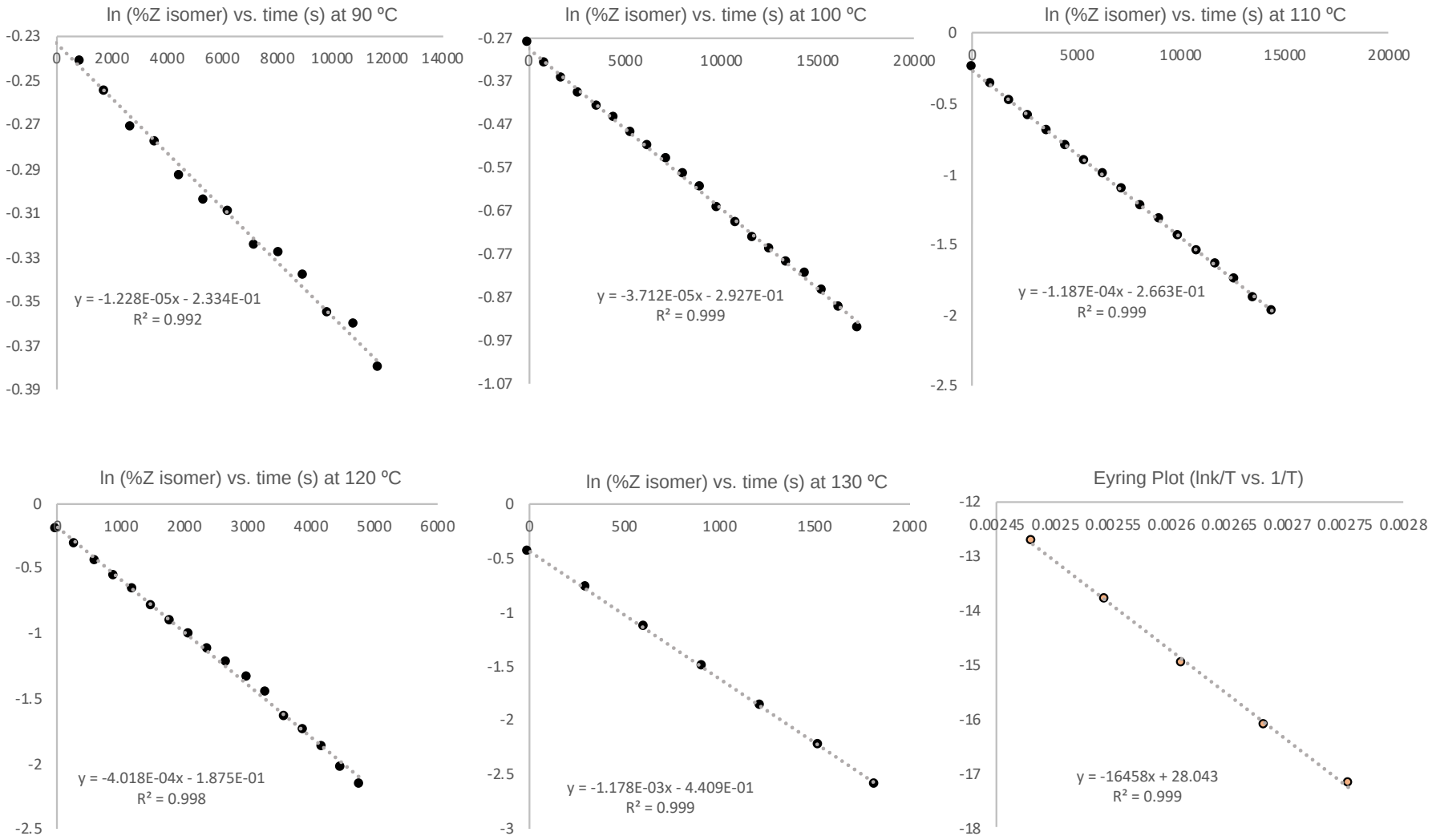


Figure S15. *Z*→*E* thermal isomerisation kinetics of **4pzH-F2** in DMSO-d_6 at ≈ 20 mM for a range of temperatures. An Eyring plot is also included for extrapolation to 25 ºC.

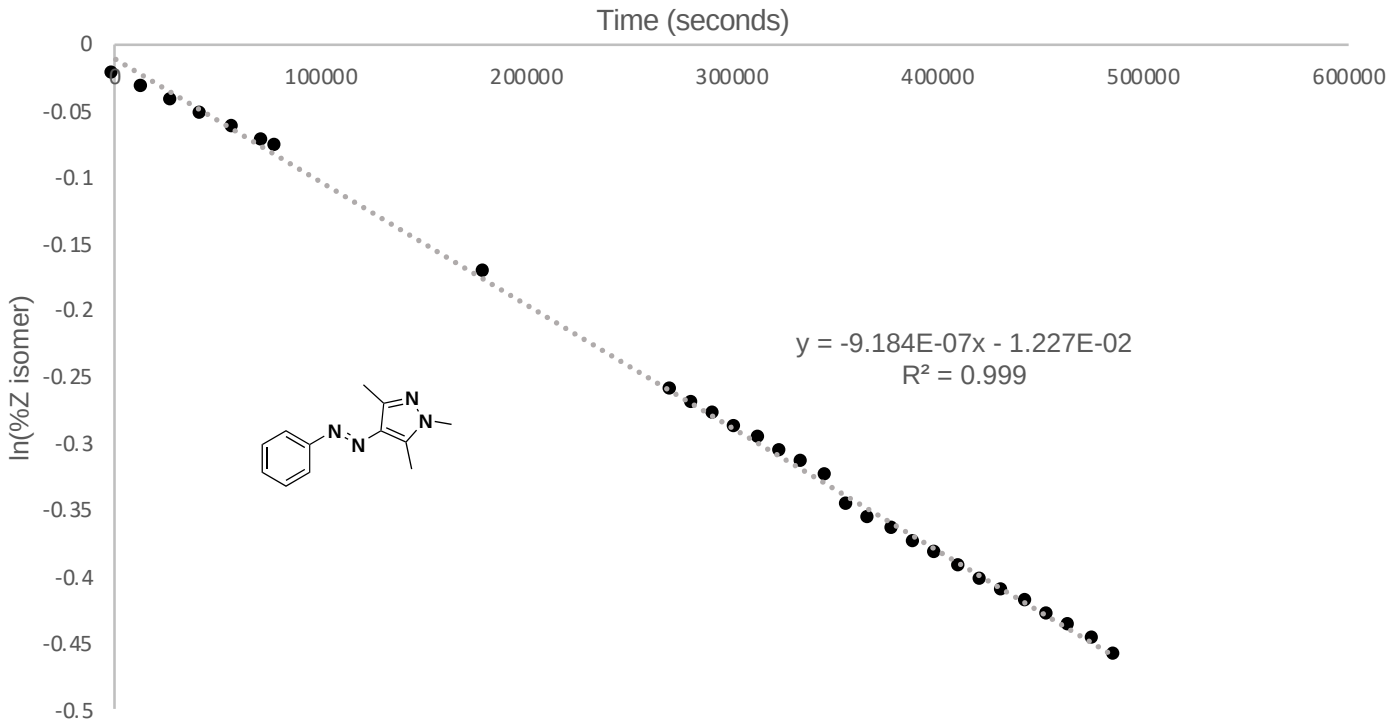


Figure S16 *Z*→*E* thermal isomerisation kinetics of **4pzMe** in DMSO-d_6 at ≈ 20 mM.

X-Ray crystallography

The X-ray crystal structure of 4pzH-F2

Crystal data for **4pzH-F2**: $C_{10}H_8F_2N_4$, M = 222.20, monoclinic, $P2_1/c$ (no. 14), a = 19.826(3), b = 3.9279(4), c = 13.2624(17) Å, β = 109.525(15)°, V = 973.4(2) Å^3, Z = 4, D_c = 1.516 g cm^{-3}, μ(Mo-Kα) = 0.124 mm^{-1}, T = 173 K, yellow tabular needles, Agilent Xcalibur 3 E diffractometer; 2044 independent measured reflections (R_{int} = 0.0207), F^2 refinement [4,5], R_1(obs) = 0.0403, wR_2(all) = 0.1004, 1675 independent observed absorption-corrected reflections [$|F_o| > 4\sigma(|F_o|)$, completeness to θ_{full}(25.2°) = 99.8%], 146 parameters. CCDC 1956314.

The X-ray crystal structure of 4pzMe-F2

Crystal data for **4pzMe-F2**: $C_{12}H_{12}F_2N_4$, M = 250.26, monoclinic, $P2_1/c$ (no. 14), a = 9.8817(7), b = 16.6285(11), c = 7.5309(5) Å, β = 103.152(7)°, V = 1205.00(15) Å^3, Z = 4, D_c = 1.379 g cm^{-3}, μ(Mo-Kα) = 0.109 mm^{-1}, T = 173 K, orange blocky needles, Agilent Xcalibur 3 E diffractometer; 2408 independent measured reflections (R_{int} = 0.0200), F^2 refinement [4,5], R_1(obs) = 0.0439, wR_2(all) = 0.1118, 1835 independent observed absorption-corrected reflections [$|F_o| > 4\sigma(|F_o|)$, completeness to θ_{full}(25.2°) = 99.0%], 167 parameters. CCDC 1941406.

The X-ray crystal structure of 4pzMe-OMe2

Crystal data for **4pzMe-OMe2**: $C_{14}H_{18}N_4O_2$, M = 274.32, monoclinic, $P2_1/c$ (no. 14), a = 7.0910(4), b = 20.3120(9), c = 10.3246(6) Å, β = 103.879(6)°, V = 1443.67(14) Å^3, Z = 4, D_c = 1.262 g cm^{-3}, μ(Mo-Kα) = 0.087 mm^{-1}, T = 173 K, yellow blocky needles, Agilent Xcalibur 3 E diffractometer; 2913 independent measured reflections (R_{int} =

0.0228), F^2 refinement [4,5], R_1(obs) = 0.0483, wR_2(all) = 0.1185, 2211 independent observed absorption-corrected reflections [$|F_o| > 4\sigma(|F_o|)$, completeness to θ_{full}(25.2°) = 99.0%], 186 parameters. CCDC 1941407.

The X-ray crystal structure of 4pzMe-OMe2_diethylether

Crystal data for **4pzMe-OMe2_diethylether**: $C_{14}H_{18}N_4O_2$, M = 274.32, monoclinic, $P2_1/c$ (no. 14), a = 7.0836(4), b = 20.2850(12), c = 10.3061(6) Å, β = 103.825(5)°, V = 1437.99(14) Å^3, Z = 4, D_c = 1.267 g cm^{-3}, μ(Mo-Kα) = 0.088 mm^{-1}, T = 173 K, yellow blocky needles, Agilent Xcalibur 3 E diffractometer; 2881 independent measured reflections (R_{int} = 0.0220), F^2 refinement [4,5], R_1(obs) = 0.0484, wR_2(all) = 0.1223, 2201 independent observed absorption-corrected reflections [$|F_o| > 4\sigma(|F_o|)$, completeness to θ_{full}(25.2°) = 98.7%], 187 parameters. CCDC 1941801.

Crystallization of **4pzMe-OMe2** from diethyl ether rather than ethyl acetate has led to an unchanged structure.

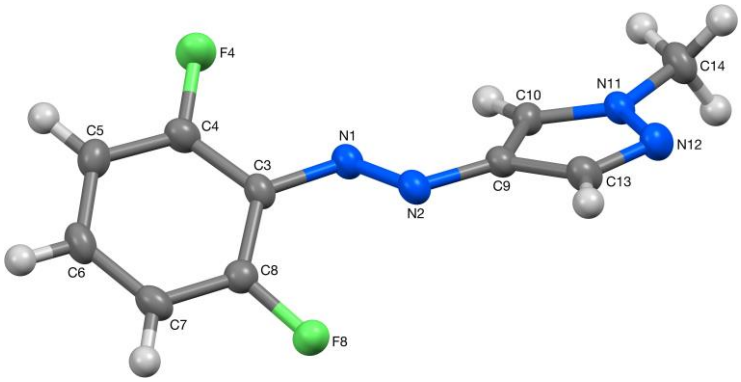


Figure S17. The crystal structure of **4pzH-F2** (50% probability ellipsoids).

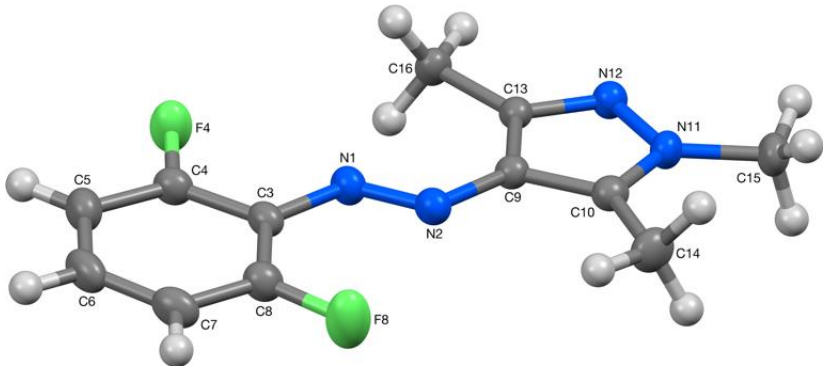


Figure S18. The crystal structure of **4pzMe-F2** (50% probability ellipsoids).

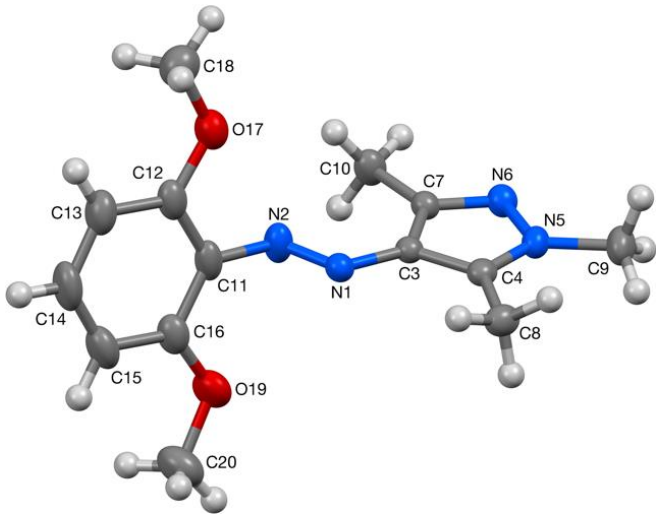


Figure S19. The crystal structure of **4pzMe-OMe2** (50% probability ellipsoids).

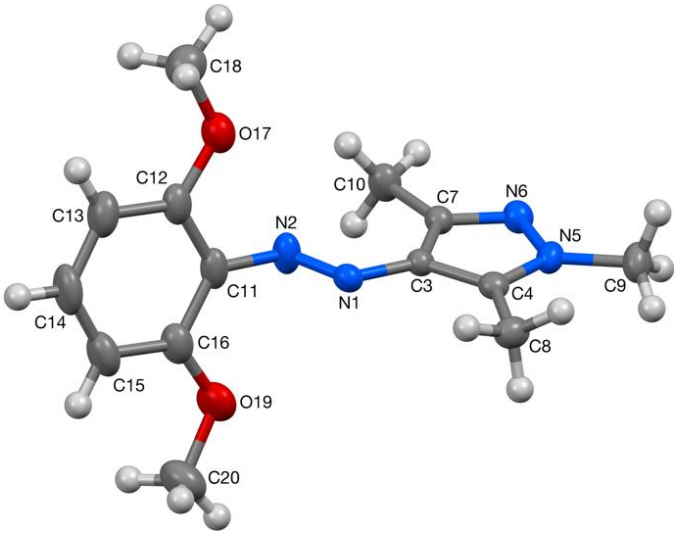


Figure S20. The crystal structure of **4pzMe-OMe2_diethylether** (50% probability ellipsoids).

Cartesian coordinates for all the optimized structures

```
24
4pzH-cis-m ; E = -605.348392323 Hartree
C       -1.882050       -0.345931       -1.210606
C       -2.609669        0.839330       -1.204569
C       -1.498487       -0.925379       -0.000308
H       -2.899926        1.294761       -2.146949
C       -2.967157        1.440902        0.000606
C       -1.881714       -0.346652        1.210447
H       -1.592351       -0.823717        2.141641
C       -2.609355        0.838598        1.205320
H       -2.899370        1.293449        2.148054
H       -1.592949       -0.822459       -2.142157
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N        0.471489       -2.154533       -0.000570
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C        1.042663        0.386039       -0.000188
C        2.670409       -1.120861        0.000455
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H        1.646795        2.926981        0.006830
H        3.165704        2.603615        0.884498
H        0.149380        0.989569       -0.000597
H        3.239996       -2.039995        0.000804
H       -3.536575        2.365166        0.000963
24
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H       -1.724838        0.762578        2.142016
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C        2.529644        0.802747        0.000010
C        0.861890       -0.661579       -0.000140
N        1.980662       -1.365193       -0.000154
N        2.978973       -0.457660       -0.000044
C        4.344546       -0.920264        0.000342
H        4.530393       -1.527250       -0.888416
H        5.011377       -0.057610       -0.000730
H        4.530696       -1.525282        0.890392
H        3.180207        1.664848        0.000034
H       -0.085740       -1.177307       -0.000247
H       -3.932010       -2.248185        0.000196
24
4pzH-trans-m ; E = -605.365368227 Hartree
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C        4.039866       -1.260794        0.000279
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C        4.655875       -0.012829       -0.000226
C        2.496247        1.069078       -0.000471
H        1.873372        1.956774       -0.000721
C        3.879851        1.148596       -0.000599
H        4.363580        2.121200       -0.000974
H        2.141296       -2.304989        0.000801
N        0.479149       -0.391081        0.000236
N       -0.198440        0.669437        0.000425
C       -1.567541        0.464908        0.000281
C       -2.316651       -0.709802       -0.000119
C       -2.533757        1.496361        0.000588
N       -3.764816        1.009933        0.000131
N       -3.604044       -0.328655       -0.000134
C       -4.775045       -1.170094       -0.000603
H       -5.375761       -0.968643       -0.890332
H       -4.461673       -2.214390       -0.000116
H       -5.376753       -0.968105        0.888324
H       -2.006553       -1.743034       -0.000374
H       -2.361118        2.563894        0.000949
H        5.739501        0.059208       -0.000308
24
4pzH-trans-n ; E = -605.365601144 Hartree
C        2.851801        1.236311       -0.000281
C        4.217150        0.975383       -0.000317
C        1.934828        0.183164        0.000006
H        4.926419        1.797532       -0.000619
C        4.671026       -0.340252        0.000012
C        2.392362       -1.141078        0.000356
H        1.662662       -1.943280        0.000578
C        3.754895       -1.394650        0.000348
H        4.112323       -2.420464        0.000589
H        2.464845        2.250522       -0.000550
N        0.575638        0.563024        0.000023
N       -0.231018       -0.402807       -0.000302
C       -1.561103       -0.019630       -0.000040
C       -2.618082       -0.920272       -0.000407
C       -2.184992        1.255032        0.000451
N       -3.501600        1.142243        0.000395
N       -3.743455       -0.185196        0.000005
C       -5.108284       -0.647651       -0.000164
H       -5.625721       -0.281276       -0.889768
H       -5.113355       -1.738105        0.000184
H       -5.626050       -0.280702        0.889004
H       -2.622829       -2.000031       -0.000832
H       -1.709813        2.225065        0.000789
H        5.736954       -0.548248       -0.000004
24
4pzHCl1A-cis-m ; E = -1064.78465959 Hartree
C       -1.784226       -0.314976       -0.487012
C       -2.470328        0.798685       -0.960625
C       -1.282505       -0.341888        0.816935
H       -2.844023        0.795608       -1.979070
C       -2.665124        1.896295       -0.128377
C       -1.506931        0.755408        1.650703
H       -1.130201        0.714532        2.667983
C       -2.186022        1.871835        1.179609
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H       -2.345364        2.721427        1.836219
Cl       -1.512876       -1.666779       -1.539783
N       -0.647686       -1.498819        1.345802
N        0.588864       -1.652370        1.252987
C        1.447330       -0.751057        0.626101
C        1.325995        0.481720       -0.031707
C        2.834236       -1.033983        0.561686
N        3.504942       -0.086958       -0.066113
N        2.566675        0.817783       -0.413985
C        2.972311        2.000288       -1.134369
H        3.434367        1.714386       -2.081676
H        2.093987        2.616902       -1.326638
H        3.694736        2.564210       -0.540494
H        0.484260        1.119698       -0.246977
H        3.335447       -1.905510        0.959458
H       -3.202294        2.762576       -0.500981
24
4pzHCl1A-cis-n ; E = -1064.78460406 Hartree
C        1.875732       -0.557955        0.330287
C        2.695237        0.158929        1.195332
C        1.403068        0.022583       -0.849331
H        3.040351       -0.312651        2.109179
C        3.053825        1.465946        0.882998
C        1.792369        1.325088       -1.165234
H        1.436770        1.758021       -2.095016
C        2.603807        2.047545       -0.299828
H        2.887243        3.064705       -0.551279
Cl        1.407159       -2.178246        0.740004
N        0.637779       -0.721059       -1.790546
N       -0.605898       -0.787711       -1.702967
C       -1.356329       -0.164116       -0.704983
C       -2.732733       -0.373228       -0.692254
C       -1.134505        0.711437        0.402452
N       -2.269778        0.994764        1.015376
N       -3.224761        0.324560        0.337134
C       -4.593487        0.417901        0.781622
H       -4.904095        1.464538        0.796373
H       -5.228389       -0.142566        0.094979
H       -4.687413        0.003263        1.787831
H       -3.344224       -0.971970       -1.350928
H       -0.216655        1.144977        0.767767
H        3.691404        2.023201        1.561675
24
4pzHCl1A-trans-m ; E = -1064.80116010 Hartree
C        2.479229       -0.700889        0.000050
C        3.849626       -0.459842       -0.000050
C        1.561033        0.359315       -0.000013
H        4.535227       -1.299880        0.000005
C        4.318338        0.847653       -0.000252
C        2.057091        1.670430       -0.000224
H        1.331706        2.476892       -0.000285
C        3.419150        1.914870       -0.000346
H        3.786064        2.936567       -0.000531
Cl        1.927198       -2.345592        0.000266
N        0.192422        0.035431        0.000127
N       -0.574792        1.033313        0.000438
C       -1.917174        0.704675        0.000186
C       -2.548857       -0.538131       -0.000378
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C       -2.978160        1.638845        0.000304
N       -4.155480        1.035104        0.000435
N       -3.865532       -0.282727       -0.000133
C       -4.950224       -1.233392       -0.000523
H       -5.567366       -1.089777       -0.890114
H       -4.537320       -2.242375       -0.000418
H       -5.567905       -1.089803        0.888691
H       -2.137274       -1.535441       -0.000770
H       -2.910378        2.717960        0.000616
H        5.388235        1.031854       -0.000317
24
4pzHCl1A-trans-n ; E = -1064.80090683 Hartree
C       -2.618272       -0.555208       -0.000023
C       -3.942204       -0.125984       -0.000052
C       -1.562412        0.368599        0.000027
H       -4.737408       -0.863161       -0.000095
C       -4.225827        1.233593       -0.000012
C       -1.872779        1.735626        0.000077
H       -1.043049        2.434253        0.000132
C       -3.187789        2.166390        0.000058
H       -3.410049        3.229026        0.000109
Cl       -2.299187       -2.259066       -0.000067
N       -0.251635       -0.141439        0.000044
N        0.644820        0.742080       -0.000023
C        1.927623        0.228484       -0.000008
C        3.071351        1.017302       -0.000090
C        2.417115       -1.104200        0.000178
N        3.737654       -1.125654        0.000160
N        4.114354        0.171097        0.000026
C        5.519912        0.490200       -0.000146
H        5.996052        0.071888       -0.889815
H        5.637699        1.574243        0.000320
H        5.996380        0.071084        0.888961
H        3.186500        2.090901       -0.000219
H        1.843397       -2.019393        0.000302
H       -5.260020        1.563877       -0.000044
24
4pzHCl1B-cis-m ; E = -1064.78465960 Hartree
C       -1.505810        0.755838       -1.650777
C       -2.184374        1.872647       -1.179748
C       -1.282422       -0.341686       -0.817049
H       -2.342960        2.722430       -1.836295
C       -2.663869        1.897273        0.128066
C       -1.784616       -0.314588        0.486687
Cl       -1.514481       -1.666823        1.539417
C       -2.470100        0.799422        0.960300
H       -2.844103        0.796478        1.978621
H       -1.128719        0.714868       -2.667918
N       -0.647926       -1.498928       -1.345772
N        0.588634       -1.652548       -1.252834
C        1.447085       -0.751280       -0.625837
C        1.326014        0.481373        0.032177
C        2.833990       -1.034430       -0.561582
N        3.504917       -0.087645        0.066304
N        2.566763        0.817168        0.414479
C        2.972754        1.999626        1.134715
H        3.693603        2.564555        0.539863
H        2.094269        2.615387        1.329000
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H        3.436795        1.713520        2.080978
H        0.484351        1.119445        0.247658
H        3.334861       -1.906099       -0.959537
H       -3.200535        2.763903        0.500591
24
4pzHCl1B-cis-n ; E = -1064.78460407 Hartree
C       -1.792413        1.324891       -1.165414
C       -2.603676        2.047510       -0.299958
C       -1.403099        0.022434       -0.849363
H       -2.887093        3.064651       -0.551519
C       -3.053513        1.466120        0.883020
C       -1.875609       -0.557901        0.330432
Cl       -1.407045       -2.178300        0.740285
C       -2.694951        0.159116        1.195497
H       -3.039963       -0.312325        2.109452
H       -1.436967        1.757711       -2.095302
N       -0.637867       -0.721378       -1.790508
N        0.605808       -0.788048       -1.702879
C        1.356199       -0.164256       -0.705010
C        2.732570       -0.373581       -0.692018
C        1.134446        0.712025        0.401877
N        2.269674        0.995454        1.014800
N        3.224615        0.324569        0.337089
C        4.593272        0.417845        0.781774
H        4.686873        0.003893        1.788294
H        5.228183       -0.143272        0.095664
H        4.904151        1.464411        0.795849
H        3.343966       -0.972831       -1.350313
H        0.216631        1.145960        0.766798
H       -3.690970        2.023507        1.561703
24
4pzHCl1B-trans-m ; E = -1064.79441682 Hartree
C       -2.226575        1.839027        0.122927
C       -3.605701        1.934387        0.212002
C       -1.578960        0.603895       -0.006731
H       -4.077582        2.904109        0.333080
C       -4.376619        0.777991        0.130064
C       -2.372916       -0.553111       -0.109835
Cl       -1.705359       -2.126682       -0.406136
C       -3.760483       -0.455249       -0.044849
H       -4.350644       -1.360603       -0.137627
H       -1.593527        2.719745        0.166225
N       -0.175572        0.693309       -0.087876
N        0.449098       -0.286122        0.392843
C        1.824758       -0.186782        0.278805
C        2.628922        0.789275       -0.306628
C        2.738320       -1.142950        0.777194
N        3.989948       -0.794420        0.527124
N        3.894378        0.379658       -0.130579
C        5.104671        1.036563       -0.559173
H        5.655489        0.387741       -1.243701
H        4.843826        1.965802       -1.066287
H        5.732931        1.255554        0.306963
H        2.370295        1.704904       -0.815371
H        2.512240       -2.060346        1.302645
H       -5.459388        0.831444        0.185154
24
4pzHCl1B-trans-n ; E = -1064.79503623 Hartree
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C        2.458437        1.738206       -0.093570
C        3.831529        1.671111       -0.264339
C        1.673523        0.585366        0.036154
H        4.410234        2.581512       -0.382447
C        4.459375        0.428562       -0.267113
C        2.325603       -0.661218        0.052608
Cl        1.490388       -2.155647        0.338622
C        3.708637       -0.728078       -0.094306
H        4.188577       -1.700427       -0.066591
H        1.935565        2.689086       -0.068319
N        0.298890        0.841255        0.205465
N       -0.467492       -0.039704       -0.260202
C       -1.810186        0.227811       -0.060611
C       -2.825238       -0.604862       -0.513531
C       -2.489047        1.293766        0.585040
N       -3.798342        1.126858        0.530121
N       -3.980546       -0.030813       -0.140627
C       -5.323401       -0.502309       -0.369008
H       -5.883166        0.235764       -0.947854
H       -5.280218       -1.441582       -0.921142
H       -5.828429       -0.663501        0.586046
H       -2.778673       -1.536737       -1.057033
H       -2.059166        2.154411        1.075994
H        5.535720        0.354162       -0.386477
24
4pzHCl2-cis-m ; E = -1524.21983515 Hartree
C       -1.564851       -1.198326       -0.079181
C       -2.272919       -1.206711       -1.275136
C       -1.188916        0.000054        0.537176
H       -2.542378       -2.155285       -1.725966
C       -2.623860       -0.000322       -1.871112
C       -1.564942        1.198229       -0.079488
Cl       -1.104570        2.700598        0.651619
C       -2.273013        1.206252       -1.275443
H       -2.542559        2.154671       -1.726546
Cl       -1.104349       -2.700460        0.652260
N       -0.578397        0.000190        1.819840
N        0.662931        0.000254        1.952250
C        1.564234        0.000171        0.894234
C        1.482408        0.000076       -0.506060
C        2.957323        0.000296        1.153154
N        3.666760        0.000285        0.041170
N        2.747980        0.000199       -0.947098
C        3.200142       -0.000673       -2.317476
H        3.801575       -0.892415       -2.506028
H        2.332411        0.003024       -2.977452
H        3.808070        0.886915       -2.504567
H        0.652405       -0.000076       -1.193761
H        3.434976        0.000487        2.123075
H       -3.181440       -0.000437       -2.801846
24
4pzHCl2-cis-n ; E = -1524.22011144 Hartree
C        1.703410       -1.198416        0.052264
C        2.531352       -1.207649        1.168087
C        1.265434       -0.000140       -0.520308
H        2.842707       -2.156281        1.590688
C        2.942768       -0.001602        1.724174
C        1.704996        1.197360        0.052630
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Cl        1.173458        2.700341       -0.629038
C         2.532902        1.205160        1.168500
H         2.845464        2.153241        1.591445
Cl        1.170023       -2.700522       -0.629881
N         0.528327        0.000511       -1.735765
N        -0.719181        0.000821       -1.743558
C        -1.508724        0.000707       -0.597239
C        -2.893063        0.000746       -0.748187
C        -1.319362        0.000739        0.819156
N        -2.479283        0.000762        1.449751
N        -3.419133        0.000745        0.480642
C        -4.811251        0.000611        0.858118
H        -5.032874        0.889997        1.451734
H        -5.423160        0.001100       -0.044172
H        -5.033004       -0.889334        1.450856
H        -3.487181        0.000756       -1.649973
H        -0.407745        0.000768        1.396065
H         3.590732       -0.002148        2.594309
24
4pzHCl2-trans-m ; E = -1524.22919333 Hartree
C        -2.231681        1.223758        0.044216
C        -3.616174        1.156148        0.095017
C        -1.430266        0.075239       -0.054405
H        -4.191662        2.069467        0.192566
C        -4.236575       -0.084985        0.018452
C        -2.089189       -1.163679       -0.137343
Cl       -1.209849       -2.640081       -0.364977
C        -3.477832       -1.241160       -0.106729
H        -3.951428       -2.213173       -0.185248
Cl       -1.463253        2.776284        0.148704
N        -0.042431        0.267273       -0.179616
N         0.654075       -0.508563        0.521223
C         2.016782       -0.340496        0.357232
C         2.737666        0.543059       -0.444660
C         3.004637       -1.090292        1.034899
N         4.222617       -0.710684        0.686673
N         4.030776        0.280660       -0.209835
C         5.183890        0.922751       -0.792199
H         5.786473        0.185116       -1.326500
H         4.848105        1.693662       -1.486062
H         5.790264        1.376132       -0.005175
H         2.402382        1.305944       -1.130286
H         2.855012       -1.884386        1.753106
H        -5.319204       -0.151080        0.048247
24
4pzHCl2-trans-n ; E = -1524.22941741 Hartree
C         2.399324        1.082976       -0.075032
C         3.756514        0.850902       -0.243760
C         1.474461        0.035912        0.065344
H         4.429508        1.691430       -0.368140
C         4.224979       -0.457414       -0.247732
C         1.981724       -1.274848        0.063218
Cl        0.949402       -2.642584        0.329865
C         3.343262       -1.517854       -0.085888
H         3.699236       -2.541722       -0.069461
Cl        1.819868        2.717959       -0.079902
N         0.134739        0.386754        0.312763
N        -0.702504       -0.270756       -0.353954
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C       -2.016681        0.049871       -0.068961
C       -3.098735       -0.556120       -0.694789
C       -2.600533        0.979843        0.830358
N       -3.918356        0.943815        0.759398
N       -4.199259        0.004811       -0.171059
C       -5.578134       -0.278201       -0.482680
H       -6.067874        0.625616       -0.851746
H       -5.616751       -1.052836       -1.249045
H       -6.097651       -0.624648        0.413457
H       -3.132081       -1.326072       -1.451120
H       -2.096932        1.655895        1.505667
H        5.285523       -0.651806       -0.369478
24
4pzHF1A-cis-m ; E = -704.489806843 Hartree
C       -1.618915       -0.268511       -0.929200
C       -2.366425        0.876757       -1.139204
C       -1.416494       -0.789089        0.349940
H       -2.489471        1.244522       -2.152377
C       -2.934712        1.526414       -0.044982
C       -2.018152       -0.147806        1.431201
H       -1.881154       -0.569205        2.422230
C       -2.760336        1.014165        1.237916
H       -3.211378        1.512079        2.090301
F       -1.043781       -0.881993       -1.970051
N       -0.717125       -2.015032        0.535597
N        0.529164       -2.059720        0.453752
C        1.343404       -0.946713        0.246856
C        1.178474        0.444781        0.270246
C        2.730417       -1.119289        0.016407
N        3.360082        0.034315       -0.105646
N        2.397918        0.964111        0.061007
C        2.758761        2.359636        0.000312
H        3.182879        2.588857       -0.979642
H        1.866031        2.964057        0.162867
H        3.499570        2.583188        0.770960
H        0.321648        1.078320        0.434399
H        3.260755       -2.057774       -0.067175
H       -3.521255        2.426110       -0.201019
24
4pzHF1A-cis-n ; E = -704.490084156 Hartree
C        1.627235        0.064769        0.967894
C        2.478239        1.155228        0.974319
C        1.546948       -0.799412       -0.125878
H        2.497174        1.800386        1.846132
C        3.277954        1.398182       -0.140113
C        2.381576       -0.564561       -1.217567
H        2.341204       -1.255897       -2.053514
C        3.227701        0.539765       -1.235196
H        3.856051        0.722326       -2.100982
F        0.839267       -0.162082        2.026846
N        0.756559       -1.982065       -0.077930
N       -0.491475       -1.931787       -0.050873
C       -1.229353       -0.752992       -0.173046
C       -2.595758       -0.783706        0.085714
C       -0.996108        0.583217       -0.616517
N       -2.115036        1.286011       -0.614268
N       -3.069941        0.441356       -0.174505
C       -4.415876        0.931344       -0.008826
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H       -4.734213        1.428091       -0.926935
H       -5.077187        0.090008        0.200447
H       -4.460447        1.645070        0.817703
H       -3.214380       -1.596816        0.435461
H       -0.081688        1.045004       -0.956345
H        3.943982        2.254970       -0.145265
24
4pzHF1A-trans-m ; E = -704.507068932 Hartree
C       -2.559657        1.027647        0.000121
C       -3.939131        0.887783        0.000050
C       -1.703904       -0.079762       -0.000015
H       -4.556897        1.779082        0.000185
C       -4.487448       -0.389167       -0.000187
C       -2.280076       -1.357426       -0.000264
H       -1.609484       -2.209831       -0.000390
C       -3.656631       -1.511846       -0.000346
H       -4.089606       -2.507200       -0.000542
F       -2.038957        2.256660        0.000362
N       -0.323462        0.188307        0.000058
N        0.396270       -0.845320        0.000328
C        1.754069       -0.581756        0.000165
C        2.448656        0.626488       -0.000232
C        2.766215       -1.568420        0.000374
N        3.973371       -1.026083        0.000258
N        3.751381        0.304320       -0.000101
C        4.882932        1.198327       -0.000441
H        5.492127        1.024070       -0.890101
H        4.522125        2.227143       -0.000078
H        5.492863        1.023698        0.888634
H        2.090073        1.644158       -0.000537
H        2.642863       -2.642588        0.000688
H       -5.566517       -0.508247       -0.000257
24
4pzHF1A-trans-n ; E = -704.506971171 Hartree
C        2.730435        0.902208       -0.000064
C        4.079637        0.581733       -0.000051
C        1.736597       -0.083328        0.000001
H        4.809038        1.384222       -0.000101
C        4.455518       -0.756103        0.000024
C        2.140224       -1.425529        0.000077
H        1.363552       -2.182528        0.000129
C        3.484454       -1.759945        0.000084
H        3.782976       -2.803577        0.000141
F        2.376596        2.188162       -0.000118
N        0.403328        0.364086        0.000019
N       -0.444885       -0.566738       -0.000106
C       -1.754787       -0.123162        0.000002
C       -2.852799       -0.973850       -0.000047
C       -2.318186        1.179674        0.000193
N       -3.638326        1.128046        0.000177
N       -3.942106       -0.187033        0.000032
C       -5.327366       -0.584548       -0.000153
H       -5.826637       -0.194085       -0.889856
H       -5.384009       -1.673531        0.000420
H       -5.827056       -0.193127        0.888886
H       -2.907975       -2.052243       -0.000173
H       -1.797298        2.125883        0.000316
H        5.509606       -1.015902        0.000045
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24
4pzHF1B-cis-m ; E = -704.489806906 Hartree
C       -2.016656       -0.145788       -1.431857
C       -2.758468        1.016276       -1.237756
C       -1.416383       -0.788732       -0.350806
H       -3.208505        1.515551       -2.089880
C       -2.933762        1.527039        0.045620
C       -1.619769       -0.269675        0.928800
F       -1.045932       -0.884794        1.969458
C       -2.366842        0.875755        1.139564
H       -2.490566        1.242308        2.153088
H       -1.878914       -0.565949       -2.423304
N       -0.717230       -2.014632       -0.537241
N        0.529037       -2.059444       -0.455420
C        1.343296       -0.946565       -0.247414
C        1.178400        0.444949       -0.269485
C        2.730210       -1.119425       -0.016711
N        3.359871        0.034088        0.106817
N        2.397766        0.964001       -0.059049
C        2.758950        2.359494        0.000819
H        3.491098        2.585639       -0.777398
H        1.864265        2.964045       -0.150050
H        3.193859        2.585895        0.976622
H        0.321591        1.078668       -0.432969
H        3.260592       -2.057923        0.066299
H       -3.519995        2.426867        0.202078
24
4pzHF1B-cis-n ; E = -704.490084127 Hartree
C       -2.381598       -0.564910       -1.217352
C       -3.227753        0.539390       -1.235232
C       -1.546925       -0.799471       -0.125629
H       -3.856114        0.721659       -2.101073
C       -3.278000        1.398080       -0.140364
C       -1.627122        0.065042        0.967896
F       -0.839103       -0.161465        2.026738
C       -2.478175        1.155462        0.974067
H       -2.497090        1.800870        1.845700
H       -2.341253       -1.256450       -2.053134
N       -0.756507       -1.982074       -0.077375
N        0.491532       -1.931806       -0.050525
C        1.229341       -0.753088       -0.173055
C        2.595736       -0.783741        0.085706
C        0.996089        0.583110       -0.616683
N        2.114958        1.285963       -0.614455
N        3.069868        0.441281       -0.174623
C        4.415758        0.931364       -0.008924
H        4.460391        1.644636        0.817995
H        5.077234        0.090005        0.199744
H        4.733790        1.428664       -0.926835
H        3.214332       -1.596872        0.435481
H        0.081634        1.044866       -0.956629
H       -3.944060        2.254839       -0.145625
24
4pzHF1B-trans-m ; E = -704.503169403 Hartree
C       -2.401749        1.575520        0.000529
C       -3.787166        1.627979        0.000763
C       -1.704932        0.359420       -0.000040
H       -4.296240        2.586141        0.001308
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C       -4.516689        0.441479        0.000268
C       -2.469446       -0.821925       -0.000555
F       -1.887631       -2.019287       -0.001357
C       -3.854980       -0.782255       -0.000433
H       -4.394563       -1.723396       -0.000888
H       -1.799228        2.478319        0.000832
N       -0.307050        0.492331       -0.000261
N        0.351845       -0.582170        0.000631
C        1.722255       -0.387772        0.000497
C        2.484655        0.778832       -0.000575
C        2.677074       -1.430102        0.001499
N        3.913257       -0.957455        0.001031
N        3.767445        0.383333       -0.000202
C        4.948152        1.211038       -0.001099
H        5.546643        1.001827       -0.890549
H        4.647151        2.258981       -0.001410
H        5.547378        1.002559        0.888019
H        2.187188        1.815766       -0.001523
H        2.490845       -2.495052        0.002492
H       -5.602016        0.462864        0.000400
24
4pzHF1B-trans-n ; E = -704.503728670 Hartree
C        2.633390        1.465419       -0.000554
C        4.013659        1.335107       -0.000983
C        1.782848        0.351379        0.000086
H        4.644197        2.218084       -0.001591
C        4.581021        0.063102       -0.000594
C        2.385600       -0.920123        0.000525
F        1.651097       -2.031442        0.001462
C        3.764349       -1.063178        0.000218
H        4.175641       -2.067057        0.000627
H        2.154303        2.439315       -0.000740
N        0.414873        0.668198        0.000459
N       -0.379721       -0.310072       -0.000765
C       -1.710702        0.069179       -0.000172
C       -2.760602       -0.840038       -0.001291
C       -2.344972        1.338865        0.001483
N       -3.660624        1.215430        0.001362
N       -3.891430       -0.114282       -0.000275
C       -5.252527       -0.587835       -0.000887
H       -5.772788       -0.224737       -0.890172
H       -5.248468       -1.678255       -0.001576
H       -5.773108       -0.225857        0.888658
H       -2.754181       -1.919832       -0.002629
H       -1.879337        2.313253        0.002702
H        5.659794       -0.058106       -0.000893
24
4pzHF2-cis-m ; E = -803.630444827 Hartree
C       -2.070201       -0.356790       -0.951910
C       -2.815924        0.809126       -1.038839
C       -1.301632       -0.668086        0.168066
H       -3.380567        1.007470       -1.942724
C       -2.826116        1.682335        0.044510
C       -1.351065        0.227320        1.237947
F       -0.626558       -0.054127        2.325034
C       -2.093589        1.395096        1.193927
H       -2.090768        2.054825        2.054188
F       -2.047648       -1.203006       -1.984252
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N       -0.656884       -1.933337        0.275398
N        0.588678       -2.024422        0.272440
C        1.459694       -0.956898        0.074229
C        1.344380        0.375940       -0.342852
C        2.855664       -1.144931        0.225126
N        3.535905       -0.048893       -0.053424
N        2.596518        0.853310       -0.402161
C        3.013665        2.178922       -0.790418
H        3.666530        2.119477       -1.663874
H        2.131393        2.772356       -1.031386
H        3.558332        2.648464        0.031351
H        0.499454        0.990494       -0.608280
H        3.356843       -2.051578        0.534529
H       -3.412158        2.593879       -0.005325
24
4pzHF2-cis-n ; E = -803.631039952 Hartree
C        2.331504       -0.799197        0.514605
C        3.179329        0.121998        1.108907
C        1.394749       -0.437295       -0.452698
H        3.870598       -0.214079        1.873210
C        3.122369        1.449908        0.697042
C        1.382114        0.902267       -0.847369
F        0.505825        1.272365       -1.787050
C        2.223379        1.848770       -0.288634
H        2.162748        2.875547       -0.630820
F        2.374989       -2.077615        0.897386
N        0.657525       -1.440314       -1.141921
N       -0.590341       -1.472935       -1.109365
C       -1.379976       -0.641241       -0.317686
C       -2.759338       -0.652206       -0.500662
C       -1.189835        0.240768        0.788088
N       -2.344181        0.716533        1.219080
N       -3.281349        0.170055        0.417413
C       -4.664077        0.531637        0.609996
H       -4.817202        1.584045        0.358852
H       -5.286673       -0.090997       -0.033046
H       -4.938601        0.369841        1.653882
H       -3.355193       -1.190330       -1.222805
H       -0.280111        0.525911        1.293553
H        3.784211        2.181478        1.148165
24
4pzHF2-trans-m ; E = -803.643917587 Hartree
C       -2.345366        1.279608        0.000231
C       -3.728974        1.287039        0.000384
C       -1.578415        0.100515       -0.000112
H       -4.251147        2.236591        0.000717
C       -4.401508        0.070181        0.000113
C       -2.308718       -1.104621       -0.000400
F       -1.673135       -2.271876       -0.000886
C       -3.694201       -1.127369       -0.000315
H       -4.194425       -2.089169       -0.000575
F       -1.703137        2.447695        0.000524
N       -0.192508        0.288123       -0.000398
N        0.505681       -0.762614        0.000382
C        1.865694       -0.510906        0.000337
C        2.574455        0.689543       -0.000421
C        2.866408       -1.509382        0.001245
N        4.079611       -0.981092        0.000858
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N        3.873057        0.352261       -0.000173
C        5.015260        1.232588       -0.000943
H        5.622387        1.050462       -0.890455
H        4.666949        2.265711       -0.001099
H        5.623085        1.050966        0.888187
H        2.228183        1.711414       -0.001186
H        2.729094       -2.581817        0.002060
H       -5.486386        0.053547        0.000218
24
4pzHF2-trans-n ; E = -803.644114247 Hartree
C        2.553349        1.148672       -0.000091
C        3.924827        0.963566       -0.000388
C        1.630439        0.086976        0.000173
H        4.573531        1.831592       -0.000640
C        4.422115       -0.334607       -0.000372
C        2.186831       -1.207480        0.000199
F        1.395517       -2.276170        0.000524
C        3.555589       -1.422591       -0.000051
H        3.917588       -2.444488       -0.000008
F        2.080107        2.393547       -0.000168
N        0.283833        0.465590        0.000567
N       -0.552284       -0.479017        0.000073
C       -1.863207       -0.038675        0.000042
C       -2.955763       -0.896599       -0.000682
C       -2.435195        1.260778        0.000356
N       -3.754830        1.200512        0.000482
N       -4.049801       -0.117143       -0.000148
C       -5.432438       -0.523710       -0.000368
H       -5.934259       -0.136035       -0.889855
H       -5.481751       -1.613020       -0.000308
H       -5.934525       -0.135918        0.888911
H       -3.001916       -1.975290       -0.001235
H       -1.921226        2.210698        0.000807
H        5.494239       -0.501502       -0.000601
28
4pzHOMe1A-cis-m ; E = -719.750479204 Hartree
C        1.605746       -0.493443        0.336936
C        2.331574        0.434324        1.080237
C        1.287391       -0.206485       -1.004489
H        2.578414        0.233537        2.116536
C        2.741051        1.633839        0.494087
C        1.733310        0.972754       -1.585435
C        2.447538        1.906623       -0.835084
H        2.777399        2.833235       -1.293576
N        0.600106       -1.170208       -1.798330
N       -0.632672       -1.333331       -1.677334
C       -1.441852       -0.579717       -0.823952
C       -1.297941        0.588386       -0.064671
C       -2.797977       -0.940890       -0.634991
N       -3.429695       -0.100916        0.164879
N       -2.499531        0.819439        0.489079
C       -2.874365        1.920720        1.341476
H       -3.268867        1.537218        2.284745
H       -1.993997        2.534188        1.535277
H       -3.642606        2.525762        0.854274
H       -0.467800        1.256622        0.099721
H       -3.305433       -1.795301       -1.061146
H        3.303789        2.347729        1.087845
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H        1.495230        1.154252       -2.629129
O        1.136669       -1.670789        0.809425
C        1.398098       -1.986591        2.155869
H        2.475359       -2.054885        2.353627
H        0.953819       -1.248716        2.836569
H        0.938450       -2.959329        2.331902
28
4pzHOMe1A-cis-n ; E = -719.750440189 Hartree
C        1.634812       -0.642014       -0.229605
C        2.499666       -0.888486        0.833860
C        1.459782        0.678647       -0.686302
H        2.636954       -1.897445        1.205411
C        3.187680        0.166173        1.435564
C        2.183365        1.711685       -0.104777
C        3.033939        1.465370        0.971213
H        3.576000        2.283930        1.433363
N        0.654760        0.955024       -1.829314
N       -0.589714        0.859580       -1.789964
C       -1.316588        0.559310       -0.634122
C       -2.680067        0.312685       -0.750066
C       -1.077293        0.492893        0.771289
N       -2.190933        0.223726        1.431195
N       -3.148884        0.109982        0.488827
C       -4.492679       -0.220334        0.891967
H       -4.824544        0.480485        1.660329
H       -5.150819       -0.150447        0.025335
H       -4.528737       -1.235263        1.296032
H       -3.301390        0.273431       -1.632450
H       -0.161209        0.648801        1.320080
H        3.852889       -0.042642        2.267786
H        2.052528        2.714541       -0.499781
O        0.907074       -1.586684       -0.870219
C        0.988669       -2.908449       -0.393799
H        2.007257       -3.307960       -0.479202
H        0.659974       -2.979775        0.650932
H        0.320197       -3.497239       -1.022613
28
4pzHOMe1A-trans-m ; E = -719.765917403 Hartree
C        2.417427        0.585195        0.000100
C        3.780820        0.277760        0.000098
C        1.469511       -0.463274        0.000064
H        4.521534        1.068359        0.000196
C        4.197040       -1.049353        0.000024
C        1.914935       -1.788408        0.000000
C        3.267967       -2.087514       -0.000032
H        3.599799       -3.120865       -0.000093
N        0.116032       -0.084966        0.000094
N       -0.691554       -1.051828       -0.000028
C       -2.021023       -0.663665        0.000007
C       -2.599249        0.603396        0.000225
C       -3.121131       -1.550468       -0.000229
N       -4.273375       -0.897582       -0.000166
N       -3.927981        0.405222        0.000123
C       -4.969701        1.401718        0.000014
H       -5.594892        1.285418        0.888204
H       -4.513083        2.391832        0.002205
H       -5.592373        1.288197       -0.890329
H       -2.145060        1.582041        0.000358
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H       -3.099204       -2.631507       -0.000350
H        5.260685       -1.269149        0.000032
H        1.159062       -2.566408       -0.000028
O        1.930485        1.843948        0.000181
C        2.855320        2.905390       -0.000336
H        3.492124        2.890089        0.893459
H        3.492064        2.889262       -0.894153
H        2.262112        3.820543       -0.000730
28
4pzHOMe1A-trans-n ; E = -719.765974238 Hartree
C        2.545172        0.460967        0.000297
C        3.857314       -0.020944        0.000524
C        1.469288       -0.456102       -0.000539
H        4.694042        0.667218        0.001248
C        4.097956       -1.390721       -0.000183
C        1.739436       -1.827668       -0.001277
C        3.042239       -2.299892       -0.001102
H        3.237563       -3.367532       -0.001801
N        0.176840        0.095805       -0.001198
N       -0.749835       -0.757465        0.001320
C       -2.014769       -0.193898        0.000195
C       -3.188442       -0.935285        0.002529
C       -2.451675        1.156104       -0.003249
N       -3.771483        1.231861       -0.002980
N       -4.199121       -0.047430        0.000471
C       -5.615220       -0.312279        0.001516
H       -6.076826        0.120681       -0.889045
H       -5.774292       -1.391139        0.004859
H       -6.076465        0.126140        0.889583
H       -3.346910       -2.003378        0.005434
H       -1.840903        2.046859       -0.005757
H        5.124169       -1.746528       -0.000069
H        0.889183       -2.501273       -0.002075
O        2.225152        1.770843        0.001044
C        3.277803        2.705803        0.001483
H        3.906996        2.608607        0.895510
H        3.907363        2.609038       -0.892330
H        2.805451        3.688662        0.001630
28
4pzHOMe1B-cis-m ; E = -719.750479207 Hartree
C        1.733134       -0.973101       -1.585299
C        2.447375       -1.906856       -0.834835
C        1.287333        0.206281       -1.004535
H        2.777130       -2.833588       -1.293160
C        2.741003       -1.633851        0.494275
C        1.605798        0.493445        0.336810
C        2.331651       -0.434207        1.080235
H        2.578631       -0.233214        2.116460
N        0.600111        1.169932       -1.798470
N       -0.632658        1.333130       -1.677445
C       -1.441825        0.579677       -0.823918
C       -1.297968       -0.588349       -0.064484
C       -2.797927        0.940949       -0.634981
N       -3.429699        0.101094        0.164977
N       -2.499570       -0.819269        0.489265
C       -2.874501       -1.920601        1.341565
H       -3.642427       -2.525806        0.854070
H       -1.994088       -2.533889        1.535748
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H       -3.269456       -1.537104        2.284642
H       -0.467815       -1.256504        0.100126
H       -3.305363        1.795324       -1.061208
H        3.303773       -2.347661        1.088098
O        1.136757        1.670888        0.809135
C        1.398377        1.986913        2.155488
H        0.954280        1.249103        2.836380
H        2.475662        2.055346        2.353060
H        0.938655        2.959631        2.331444
H        1.494982       -1.154755       -2.628945
28
4pzHOMe1B-cis-n ; E = -719.750440194 Hartree
C        2.183500       -1.711868       -0.104102
C        3.034350       -1.465087        0.971563
C        1.459795       -0.679081       -0.685925
H        3.576450       -2.283473        1.433979
C        3.188282       -0.165687        1.435268
C        1.635001        0.641785       -0.229845
C        2.500157        0.888729        0.833255
H        2.637636        1.897870        1.204245
N        0.654609       -0.955896       -1.828711
N       -0.589855       -0.860285       -1.789373
C       -1.316743       -0.559367       -0.633748
C       -2.680346       -0.313479       -0.749882
C       -1.077483       -0.491507        0.771622
N       -2.191224       -0.222237        1.431285
N       -3.149259       -0.109860        0.488806
C       -4.493164        0.220346        0.891672
H       -4.529809        1.235987        1.293902
H       -5.151479        0.148437        0.025339
H       -4.824337       -0.479305        1.661389
H       -3.301703       -0.275356       -1.632326
H       -0.161326       -0.646423        1.320580
H        3.853757        0.043495        2.267184
O        0.907115        1.586203       -0.870686
C        0.988868        2.908167       -0.394840
H        0.660570        2.979923        0.649986
H        2.007416        3.307660       -0.480802
H        0.320134        3.496684       -1.023632
H        2.052572       -2.714878       -0.498641
28
4pzHOMe1B-trans-m ; E = -719.761466839 Hartree
C        2.008300       -1.974804       -0.000590
C        3.375635       -2.202784       -0.001194
C        1.462714       -0.685889        0.000006
H        3.765678       -3.215048       -0.001836
C        4.233519       -1.109083       -0.000859
C        2.350395        0.424877        0.000420
C        3.728022        0.187592        0.000057
H        4.419311        1.021722        0.000499
N        0.061068       -0.685896        0.000608
N       -0.521082        0.432196       -0.001602
C       -1.904002        0.323121       -0.001074
C       -2.738266       -0.792068        0.001466
C       -2.792100        1.422090       -0.003676
N       -4.056976        1.028990       -0.002434
N       -3.995612       -0.317106        0.000473
C       -5.224579       -1.070411        0.002735
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H       -5.811654       -0.826629       -0.885684
H       -4.988183       -2.134864        0.002727
H       -5.809038       -0.826111        0.892770
H       -2.506160       -1.845536        0.003818
H       -2.539840        2.473427       -0.006075
H        5.309716       -1.255398       -0.001195
O        1.819495        1.660244        0.001515
C        2.696016        2.762982        0.002216
H        3.331431        2.776065        0.896802
H        3.332568        2.776197       -0.891536
H        2.058268        3.647294        0.001899
H        1.296246       -2.794101       -0.000651
28
4pzHOMe1B-trans-n ; E = -719.761672894 Hartree
C       -2.298287       -1.872682        0.000155
C       -3.684143       -1.905411        0.000491
C       -1.576460       -0.673589       -0.000029
H       -4.212899       -2.852632        0.000693
C       -4.379212       -0.701845        0.000533
C       -2.298571        0.551046       -0.000065
C       -3.695813        0.510700        0.000231
H       -4.262933        1.433734        0.000206
N       -0.189052       -0.873556       -0.000339
N        0.546550        0.149925        0.000427
C        1.898070       -0.162249        0.000100
C        2.902415        0.795711        0.000827
C        2.594193       -1.398772       -0.001132
N        3.903364       -1.212554       -0.001012
N        4.069293        0.125781        0.000234
C        5.404766        0.665722        0.000724
H        5.943544        0.331282       -0.888989
H        5.346955        1.754746        0.001970
H        5.943690        0.329254        0.889581
H        2.844950        1.873923        0.001853
H        2.175332       -2.394179       -0.001982
H       -5.465292       -0.694860        0.000802
O       -1.598958        1.700667       -0.000481
C       -2.313712        2.914055       -0.000713
H       -2.942078        3.015796       -0.894659
H       -2.941852        3.016212        0.893347
H       -1.559867        3.701946       -0.000965
H       -1.708449       -2.783838        0.000082
32
4pzHOMe2-cis-m ; E = -834.151747414 Hartree
C        1.482879       -1.211640       -0.073012
C        2.184128       -1.213372        1.135860
C        1.118492        0.000143       -0.670210
H        2.465182       -2.143983        1.613550
C        2.523155        0.000547        1.724209
C        1.482280        1.212133       -0.073070
C        2.183531        1.214268        1.135804
H        2.464111        2.145044        1.613450
N        0.486155       -0.000059       -1.950325
N       -0.758288       -0.000256       -2.040137
C       -1.625116       -0.000311       -0.944580
C       -1.504879       -0.000275        0.451176
C       -3.024425       -0.000482       -1.162092
N       -3.705601       -0.000548       -0.030541
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N       -2.760032       -0.000417        0.930161
C       -3.169658       -0.000488        2.312677
H       -3.768226       -0.889887        2.522135
H       -2.281398       -0.000210        2.945159
H       -3.768729        0.888590        2.522045
H       -0.655155       -0.000145        1.114375
H       -3.529010       -0.000550       -2.118407
H        3.069416        0.000704        2.662475
O        1.073053        2.321610       -0.731341
C        1.421278        3.571049       -0.184720
H        0.977146        3.716161        0.808717
H        2.509482        3.692131       -0.112335
H        1.021365        4.320441       -0.868287
O        1.074221       -2.321355       -0.731241
C        1.423039       -3.570596       -0.184544
H        2.511304       -3.691169       -0.112201
H        0.979019       -3.715845        0.808922
H        1.023440       -4.320218       -0.868041
32
4pzHOMe2-cis-n ; E = -834.151756590 Hartree
C        2.124501       -0.736719        0.002965
C        2.904145       -0.249226        1.055393
C        1.182238        0.091785       -0.617475
H        3.621726       -0.886942        1.556665
C        2.749081        1.072128        1.457304
C        1.051952        1.425903       -0.207754
C        1.835290        1.918014        0.837691
H        1.737143        2.944438        1.169012
N        0.497250       -0.385112       -1.774117
N       -0.727531       -0.620177       -1.753351
C       -1.525257       -0.531005       -0.608177
C       -2.897155       -0.711895       -0.741964
C       -1.342131       -0.351736        0.795824
N       -2.496112       -0.414818        1.438608
N       -3.426719       -0.628430        0.486417
C       -4.813294       -0.716809        0.868850
H       -5.161865        0.244582        1.254642
H       -5.405261       -0.994342       -0.003895
H       -4.930349       -1.475137        1.645527
H       -3.485529       -0.888637       -1.630109
H       -0.433048       -0.195975        1.355589
H        3.354730        1.452921        2.273869
O        0.122355        2.146695       -0.878295
C       -0.093095        3.476008       -0.469788
H       -0.428237        3.527220        0.573989
H        0.810004        4.088047       -0.588510
H       -0.877510        3.866683       -1.118743
O        2.172052       -2.004512       -0.467975
C        3.124979       -2.873920        0.095278
H        4.146227       -2.492839       -0.031556
H        2.935907       -3.044837        1.163009
H        3.025060       -3.818064       -0.441111
32
4pzHOMe2-trans-m ; E = -834.161134033 Hartree
C       -2.060221       -1.267658       -0.049874
C       -3.454425       -1.240424       -0.031859
C       -1.305850       -0.070441       -0.025938
H       -4.030295       -2.156136       -0.069322
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C       -4.104108       -0.014558        0.032692
C       -1.999430        1.162747        0.046498
C       -3.397272        1.178594        0.080427
H       -3.934018        2.116897        0.138804
N        0.079315       -0.247891        0.036230
N        0.789319        0.701284       -0.391746
C        2.149518        0.460330       -0.249809
C        2.833368       -0.628193        0.284292
C        3.169831        1.346654       -0.660048
N        4.374480        0.856651       -0.406067
N        4.141363       -0.340989        0.165834
C        5.263274       -1.149769        0.571006
H        5.865676       -0.609766        1.305209
H        4.892012       -2.074548        1.013675
H        5.885925       -1.384170       -0.295579
H        2.464333       -1.544897        0.717241
H        3.054552        2.314906       -1.127179
H       -5.189642        0.011582        0.046542
O       -1.254880        2.281787        0.123587
C       -1.914033        3.504381        0.353871
H       -2.568875        3.775814       -0.483721
H       -2.504243        3.481337        1.278819
H       -1.126204        4.252625        0.446374
O       -1.338245       -2.407287       -0.114452
C       -2.038314       -3.628138       -0.109075
H       -2.644536       -3.746184        0.798195
H       -2.687058       -3.728321       -0.988671
H       -1.278002       -4.409672       -0.136328
32
4pzHOMe2-trans-n ; E = -834.161208341 Hartree
C       -2.277943       -1.099185       -0.056882
C       -3.651031       -0.860785       -0.112917
C       -1.352673       -0.029401       -0.012936
H       -4.356694       -1.679871       -0.165435
C       -4.108694        0.450369       -0.102858
C       -1.852484        1.295379        0.002240
C       -3.231397        1.523730       -0.037666
H       -3.621319        2.533534       -0.022751
N       -0.015377       -0.411643        0.131434
N        0.849089        0.398966       -0.296331
C        2.147128       -0.038540       -0.069607
C        3.273774        0.669060       -0.462704
C        2.664040       -1.204092        0.552204
N        3.986619       -1.208379        0.539509
N        4.336795       -0.063223       -0.080689
C        5.733850        0.238402       -0.258102
H        6.213352       -0.544450       -0.850626
H        5.827412        1.193592       -0.776058
H        6.229776        0.301853        0.713482
H        3.366946        1.615750       -0.973524
H        2.107627       -2.017302        0.994419
H       -5.176894        0.640935       -0.146484
O       -0.950214        2.291411        0.101741
C       -1.428245        3.601461        0.293393
H       -1.993140        3.958947       -0.576896
H       -2.059879        3.678388        1.187545
H       -0.542640        4.224740        0.422405
O       -1.734413       -2.334420       -0.065510
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C       -2.608679       -3.437427       -0.062343
H       -3.265545       -3.433335        0.816832
H       -3.224929       -3.469702       -0.970034
H       -1.972807       -4.322879       -0.031120
36
4pzHPyr1A-cis-m ; E = -816.520560386 Hartree
C       -0.532170       -2.719224        1.025498
C       -0.803629       -3.513653       -0.082511
C       -0.670223       -1.334894        0.978861
H       -0.656942       -4.587621       -0.038724
C       -1.260913       -2.898877       -1.243180
C       -1.213674       -0.703389       -0.170299
C       -1.475372       -1.526181       -1.283155
H       -1.854204       -1.081804       -2.195966
N       -0.277862       -0.634056        2.160876
N        0.713497        0.133164        2.151481
C        1.547357        0.334585        1.049009
C        1.764424       -0.295547       -0.182402
C        2.540790        1.344338        1.090757
N        3.286809        1.354537        0.000937
N        2.800609        0.343815       -0.748300
C        3.422540        0.051503       -2.016025
H        4.457007       -0.264775       -1.862064
H        2.865399       -0.746707       -2.507365
H        3.413603        0.945065       -2.643631
H        1.285366       -1.130062       -0.669275
H        2.710830        2.053144        1.889673
H       -1.478635       -3.491344       -2.127238
C       -2.552585        2.627035        0.367227
C       -1.675492        1.509547        0.922158
N       -1.430104        0.652447       -0.237233
C       -1.900767        1.271883       -1.464762
C       -2.081955        2.733934       -1.080245
H       -3.607187        2.329896        0.395608
H       -2.151682        0.945009        1.729674
H       -1.178930        1.128653       -2.278215
H       -1.119762        3.255743       -1.127696
H       -2.860608        0.837593       -1.791623
H       -2.785793        3.253291       -1.735149
H       -2.447427        3.556677        0.931889
H       -0.735440        1.913088        1.321872
H       -0.156233       -3.151562        1.948306
36
4pzHPyr1A-cis-n ; E = -816.519600928 Hartree
C       -2.200692       -2.128670        0.736211
C       -2.982623       -2.405606       -0.376884
C       -1.432967       -0.967873        0.816302
H       -3.540833       -3.333645       -0.440152
C       -3.025151       -1.472225       -1.408107
C       -1.543400        0.032975       -0.182888
C       -2.332594       -0.272722       -1.308340
H       -2.404568        0.443256       -2.118414
N       -0.624736       -0.858637        1.986219
N        0.623124       -0.757582        1.922134
C        1.368330       -0.810335        0.739286
C        2.731110       -0.535189        0.807511
C        1.166525       -1.179400       -0.624946
N        2.298108       -1.125537       -1.306398
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N        3.233086       -0.724042       -0.420292
C        4.587455       -0.528222       -0.871586
H        4.639803        0.318070       -1.561568
H        5.225295       -0.333724       -0.008698
H        4.932616       -1.427287       -1.385588
H        3.331561       -0.230175        1.651875
H        0.262602       -1.495755       -1.121983
H       -3.621659       -1.663559       -2.295403
C       -0.571235        3.379999        0.816617
C       -0.545782        1.894901        1.164665
N       -0.880299        1.235684       -0.096378
C       -0.909759        2.182875       -1.198454
C       -0.153786        3.385399       -0.651214
H       -1.588700        3.775393        0.915277
H       -1.259060        1.619429        1.948296
H       -0.447173        1.752015       -2.094182
H        0.925817        3.219976       -0.739130
H       -1.943160        2.468455       -1.458027
H       -0.402997        4.310442       -1.176848
H        0.084596        3.969752        1.462075
H        0.450498        1.595913        1.517352
H       -2.122194       -2.833213        1.559090
36
4pzHPyr1A-trans-m ; E = -816.530527678 Hartree
C        1.340975       -2.699847       -0.368021
C        2.601855       -3.210790       -0.124639
C        1.031003       -1.344775       -0.177097
H        2.805115       -4.269301       -0.246090
C        3.594181       -2.333264        0.313097
C        2.079964       -0.421366        0.125455
C        3.343315       -0.976598        0.429004
H        4.151759       -0.322459        0.731835
N       -0.347128       -1.106021       -0.245942
N       -0.792869       -0.156435        0.456744
C       -2.174223       -0.017515        0.373742
C       -3.120822       -0.715986       -0.369243
C       -2.929882        0.931467        1.097497
N       -4.224475        0.831804        0.830804
N       -4.313422       -0.175433       -0.057323
C       -5.604192       -0.515598       -0.601244
H       -5.934369        0.244311       -1.315269
H       -5.536545       -1.481075       -1.104057
H       -6.328439       -0.577128        0.212493
H       -3.007438       -1.531268       -1.066513
H       -2.567693        1.666192        1.803566
H        4.589351       -2.704133        0.542112
C        1.611341        2.950098       -1.094377
C        0.948308        1.618915       -0.754517
N        1.928010        0.938167        0.083790
C        3.027186        1.825124        0.433793
C        2.476895        3.212268        0.134179
H        2.245922        2.845757       -1.982133
H        0.714094        1.014636       -1.638910
H        3.318069        1.692528        1.482155
H        1.856928        3.559303        0.968000
H        3.915266        1.623598       -0.188278
H        3.268498        3.946799       -0.032812
H        0.880363        3.738147       -1.291754
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H        0.009662        1.759328       -0.204735
H        0.513219       -3.342608       -0.651895
36
4pzHPyr1A-trans-n ; E = -816.530453350 Hartree
C       -1.717715       -2.621785        0.353916
C       -3.009560       -2.964589        0.000806
C       -1.219484       -1.319707        0.198862
H       -3.358494       -3.987055        0.097296
C       -3.838729       -1.966971       -0.511697
C       -2.109124       -0.268926       -0.184924
C       -3.404322       -0.654677       -0.595840
H       -4.092549        0.098407       -0.959778
N        0.167436       -1.261430        0.388658
N        0.791751       -0.391678       -0.280035
C        2.166521       -0.436822       -0.074220
C        3.071050        0.374875       -0.743322
C        2.972760       -1.226042        0.784837
N        4.254367       -0.923901        0.652139
N        4.292818        0.050741       -0.276714
C        5.569402        0.560495       -0.707615
H        6.059403       -0.140799       -1.389684
H        5.422042        1.515015       -1.215067
H        6.204073        0.707095        0.167438
H        2.915386        1.131284       -1.498257
H        2.650015       -1.981920        1.485325
H       -4.851097       -2.205613       -0.825598
C       -1.307113        3.011040        1.105001
C       -0.796448        1.605466        0.803343
N       -1.783075        1.059833       -0.121595
C       -2.728600        2.081612       -0.544146
C       -2.030685        3.385617       -0.184729
H       -2.019067        2.987988        1.938144
H       -0.716667        0.974697        1.696533
H       -2.951030        1.991070       -1.613624
H       -1.306836        3.651824       -0.962869
H       -3.681638        1.994554        0.004106
H       -2.732203        4.215786       -0.071650
H       -0.499304        3.697728        1.370289
H        0.195274        1.622951        0.335111
H       -1.008113       -3.365478        0.703478
36
4pzHPyr1B-cis-m ; E = -816.518559927 Hartree
C        1.463717        0.854665       -0.102699
C        1.789800        1.972823        0.691590
C        0.336586        0.976212       -0.951054
H        2.641777        1.918982        1.359140
C        1.048466        3.145319        0.639970
C       -0.394557        2.163208       -0.993810
C       -0.054228        3.252437       -0.202854
H       -0.626369        4.172505       -0.260501
N        0.048089       -0.017397       -1.934008
N       -1.027356       -0.656262       -1.920794
C       -1.952819       -0.612874       -0.871867
C       -2.002083       -0.059528        0.414898
C       -3.140479       -1.381268       -0.953153
N       -3.855826       -1.311786        0.154967
N       -3.140130       -0.509568        0.968314
C       -3.648276       -0.219383        2.286636
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H       -3.757860       -1.146423        2.853812
H       -2.948820        0.442633        2.797778
H       -4.622768        0.267608        2.208669
H       -1.339538        0.602728        0.947974
H       -3.470718       -1.974929       -1.794484
H        1.342551        3.983269        1.265403
C        2.613629       -2.561488        0.468046
C        1.699222       -1.634629       -0.332328
N        2.215845       -0.294475       -0.041104
C        3.421863       -0.353676        0.764815
C        3.919417       -1.775676        0.548309
H        2.210089       -2.712184        1.475894
H        1.746578       -1.849890       -1.404253
H        4.142470        0.407707        0.444037
H        4.585174       -2.112935        1.346658
H        0.651883       -1.724291       -0.020554
H        2.721167       -3.542983       -0.000156
H        4.461774       -1.840347       -0.401218
H        3.208945       -0.180094        1.834538
H       -1.232229        2.218208       -1.683362
36
4pzHPyr1B-cis-n ; E = -816.518113843 Hartree
C        1.701090        0.760023       -0.074592
C        2.226548        1.836344        0.667067
C        0.491210        0.987119       -0.774591
H        3.150054        1.702550        1.217939
C        1.589229        3.068531        0.709903
C       -0.136830        2.232076       -0.717815
C        0.397716        3.277868        0.021119
H       -0.096529        4.243434        0.041630
N        0.034997        0.042971       -1.738530
N       -1.119286       -0.437298       -1.707158
C       -2.000254       -0.285483       -0.627065
C       -3.286614       -0.803686       -0.737437
C       -1.928653        0.156370        0.728789
N       -3.064720       -0.073045        1.365623
N       -3.876618       -0.648635        0.456424
C       -5.227531       -0.980477        0.833949
H       -5.811116       -0.070882        0.998332
H       -5.685582       -1.567176        0.036966
H       -5.212191       -1.564761        1.755722
H       -3.776812       -1.261107       -1.584093
H       -1.108482        0.621545        1.253137
H        2.033240        3.872125        1.290254
C        2.547231       -2.748653        0.408505
C        1.656701       -1.736015       -0.310429
N        2.341571       -0.456340       -0.105588
C        3.618094       -0.640866        0.561713
C        3.931280       -2.111143        0.323737
H        2.245328       -2.839259        1.458179
H        1.565108       -1.966637       -1.376269
H        4.376200        0.033643        0.146712
H        4.642949       -2.510583        1.050622
H        0.644990       -1.705577        0.111363
H        2.494318       -3.742327       -0.043391
H        4.352044       -2.246225       -0.678672
H        3.546062       -0.434891        1.644064
H       -1.046480        2.370520       -1.295007
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36
4pzHPyr1B-trans-m ; E = -816.536534834 Hartree
C       -2.166021       -0.360742       -0.014315
C       -3.444689       -0.970205       -0.050077
C       -1.038664       -1.233987        0.032704
H       -4.329961       -0.347770       -0.084423
C       -3.599087       -2.341849       -0.017213
C       -1.230714       -2.625017        0.077235
C       -2.488004       -3.188806        0.053123
H       -2.612656       -4.266302        0.083539
N        0.236190       -0.662257        0.002785
N        1.200014       -1.477726        0.016883
C        2.443385       -0.866867       -0.011301
C        2.809228        0.477164       -0.015422
C        3.674634       -1.560804       -0.028938
N        4.706053       -0.729242       -0.044878
N        4.155443        0.498601       -0.031430
C        5.017166        1.651686       -0.100037
H        5.394801        1.793546       -1.116938
H        4.457055        2.536566        0.205423
H        5.861148        1.502253        0.574785
H        2.212032        1.375599       -0.003590
H        3.828205       -2.631019       -0.025402
H       -4.602325       -2.758442       -0.038322
C       -1.500969        3.201679        0.536560
C       -0.915681        1.818194        0.270716
N       -2.086119        1.004333       -0.041222
C       -3.269260        1.826314       -0.252932
C       -2.714970        3.238992       -0.384593
H       -1.820934        3.279137        1.581988
H       -0.211925        1.830210       -0.572285
H       -3.814334        1.504206       -1.148019
H       -3.450072        4.001249       -0.115003
H       -0.372289        1.407234        1.125397
H       -0.781413        4.001811        0.344115
H       -2.399289        3.421229       -1.417852
H       -3.962345        1.755280        0.600985
H       -0.334904       -3.235265        0.117568
36
4pzHPyr1B-trans-n ; E = -816.537343706 Hartree
C       -2.181474       -0.511461       -0.011215
C       -3.362935       -1.293960       -0.043785
C       -0.943342       -1.219826        0.037650
H       -4.326182       -0.800817       -0.079239
C       -3.324868       -2.673395       -0.005820
C       -0.940368       -2.623856        0.087229
C       -2.106715       -3.357605        0.066491
H       -2.080406       -4.441884        0.100968
N        0.238960       -0.476046        0.003899
N        1.307517       -1.148554        0.020247
C        2.449104       -0.363901       -0.011838
C        3.736628       -0.882087       -0.032257
C        2.640680        1.042336       -0.034337
N        3.926731        1.353065       -0.067216
N        4.574221        0.172336       -0.071415
C        6.014397        0.160642       -0.041244
H        6.385484        0.390228        0.962125
H        6.371241       -0.825497       -0.341868
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H        6.388184        0.911405       -0.738880
H        4.083149       -1.904687       -0.026836
H        1.888401        1.817399       -0.032851
H       -4.260463       -3.225560       -0.024404
C       -2.015644        3.110949        0.521474
C       -1.244355        1.821148        0.261094
N       -2.292307        0.850060       -0.041970
C       -3.578017        1.499318       -0.256846
C       -3.224566        2.974459       -0.396951
H       -2.341479        3.149052        1.567302
H       -0.551982        1.925724       -0.584075
H       -4.073826        1.099599       -1.149344
H       -4.057994        3.628908       -0.129986
H       -0.646830        1.495129        1.115833
H       -1.413502        4.001230        0.323104
H       -2.938569        3.192905       -1.431816
H       -4.253907        1.337668        0.598524
H        0.031683       -3.103378        0.128761
48
4pzHPyr2-cis-m ; E = -1027.68676191 Hartree
C       -1.265612       -0.936145        0.794309
C       -1.245377       -0.864406        2.197880
C       -0.030751       -0.920673        0.112287
H       -2.175441       -0.841736        2.752413
C       -0.035835       -0.824364        2.879305
C        1.196174       -0.963407        0.803576
C        1.176255       -0.903108        2.205535
H        2.105539       -0.918246        2.762305
N       -0.015824       -0.802908       -1.313132
N        0.030676        0.339139       -1.826632
C        0.061319        1.529007       -1.100803
C        0.041265        1.909744        0.248247
C        0.123287        2.761330       -1.798366
N        0.141011        3.797722       -0.980963
N        0.089579        3.250921        0.252185
C        0.090491        4.119770        1.402698
H       -0.777962        4.781575        1.369213
H        0.051172        3.509047        2.305199
H        0.999278        4.725781        1.408969
H       -0.003567        1.353283        1.171328
H        0.155247        2.895624       -2.870937
H       -0.039439       -0.768707        3.964285
C        4.044099       -1.619909       -1.453147
C        2.629256       -1.943547       -0.954431
N        2.389266       -0.947016        0.087678
C        3.646424       -0.764077        0.782463
C        4.658291       -0.718323       -0.360564
H        4.620883       -2.536594       -1.601650
H        2.588845       -2.959194       -0.526019
H        3.627426        0.154207        1.377785
H        4.752055        0.308047       -0.725210
C       -4.027740       -1.218664       -1.579753
C       -2.718101       -1.776366       -1.044544
N       -2.457656       -0.893927        0.086430
C       -3.713115       -0.695953        0.787423
C       -4.791088       -0.805958       -0.309005
H       -3.814426       -0.342751       -2.199501
H       -2.838895       -2.820892       -0.706865
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H       -3.879116       -1.468318        1.558218
H       -5.326989        0.136393       -0.446520
H       -1.896840       -1.745144       -1.762995
H       -4.575806       -1.941138       -2.189802
H       -5.532259       -1.561026       -0.032310
H       -3.709645        0.275301        1.294676
H        3.869826       -1.605590        1.464979
H        5.649724       -1.049640       -0.041018
H        4.010835       -1.097908       -2.412616
H        1.864742       -1.879604       -1.731552
48
4pzHPyr2-cis-n ; E = -1027.68684943 Hartree
C       -0.652704       -1.427841        0.659667
C       -0.539653       -1.729926        2.021788
C        0.452815       -0.858655       -0.004859
H       -1.382040       -2.148005        2.559203
C        0.656095       -1.479070        2.685137
C        1.698820       -0.701791        0.636978
C        1.767207       -0.993359        2.014167
H        2.694487       -0.842264        2.552912
N        0.287251       -0.406901       -1.354402
N       -0.278762        0.689635       -1.565312
C       -0.724724        1.554876       -0.561923
C       -1.422398        2.693108       -0.954699
C       -0.644540        1.679252        0.859670
N       -1.240723        2.784622        1.272762
N       -1.710669        3.381682        0.157094
C       -2.444884        4.615130        0.279780
H       -1.840231        5.350849        0.814173
H       -2.678769        4.990253       -0.717143
H       -3.372371        4.448224        0.833224
H       -1.711269        3.017310       -1.943576
H       -0.176571        1.029631        1.583666
H        0.732918       -1.697857        3.746377
C        4.572893       -0.321700       -1.568930
C        3.052685       -0.434158       -1.450863
N        2.792524       -0.191300       -0.029204
C        4.013102        0.133306        0.685105
C        4.944681        0.610743       -0.419337
H        5.036472       -1.302461       -1.412202
H        2.678625       -1.416370       -1.756722
H        3.824447        0.894816        1.450921
H        4.712866        1.649349       -0.679955
C       -3.356038       -2.104704       -1.721159
C       -1.911774       -2.315589       -1.278415
N       -1.857286       -1.567528       -0.028035
C       -3.066764       -1.899652        0.696538
C       -4.142958       -1.961624       -0.399287
H       -3.425261       -1.183639       -2.306520
H       -1.705410       -3.386073       -1.099868
H       -2.986526       -2.879357        1.202360
H       -4.748532       -1.051814       -0.403255
H       -1.174814       -1.941215       -1.992042
H       -3.718656       -2.925514       -2.345325
H       -4.821233       -2.802097       -0.229316
H       -3.268970       -1.145739        1.463855
H        4.443362       -0.748737        1.191546
H        5.998184        0.555646       -0.133507
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H        4.887518        0.044471       -2.549551
H        2.544269        0.309040       -2.075735
48
4pzHPyr2-trans-m ; E = -1027.69725120 Hartree
C        0.787205       -2.106889        0.207035
C        1.908693       -2.865438        0.598821
C        0.917315       -0.675177        0.179464
H        1.826847       -3.936889        0.717603
C        3.105461       -2.244251        0.909021
C        2.219110       -0.078016        0.319839
C        3.284793       -0.879183        0.763863
H        4.258926       -0.446383        0.947295
N       -0.279068        0.013946        0.105944
N       -0.331390        1.174700        0.614274
C       -1.595604        1.745254        0.512236
C       -2.745793        1.324616       -0.149824
C       -1.973268        2.965398        1.117175
N       -3.238467        3.270899        0.861559
N       -3.683643        2.264590        0.090948
C       -5.045438        2.291408       -0.378205
H       -5.218546        3.190648       -0.974287
H       -5.226105        1.408494       -0.992402
H       -5.734279        2.290665        0.470089
H       -2.933532        0.460902       -0.768352
H       -1.363131        3.613618        1.731178
H        3.941109       -2.853158        1.243574
C        2.721734        2.914345       -1.637992
C        1.699621        1.969048       -1.016212
N        2.461816        1.225669       -0.022316
C        3.782731        1.807536        0.164317
C        3.664219        3.186010       -0.469909
H        3.265203        2.414168       -2.448257
H        1.241784        1.283268       -1.738703
H        4.049202        1.839901        1.226923
H        3.202121        3.887272        0.233585
C       -2.609624       -3.469322       -0.314503
C       -1.708530       -2.237999       -0.313616
N       -0.375148       -2.781317       -0.074222
C       -0.365946       -4.233895       -0.197675
C       -1.698753       -4.562215       -0.856618
H       -2.913651       -3.708811        0.710921
H       -1.750445       -1.706121       -1.274752
H        0.487056       -4.566144       -0.800268
H       -2.038629       -5.575475       -0.627725
H       -1.981607       -1.512748        0.455399
H       -3.516052       -3.319104       -0.907155
H       -1.607534       -4.472429       -1.944967
H       -0.282118       -4.718466        0.788474
H        4.552842        1.213934       -0.355548
H        4.634264        3.590603       -0.769269
H        2.257541        3.815779       -2.046084
H        0.882479        2.519713       -0.533883
48
4pzHPyr2-trans-n ; E = -1027.69767461 Hartree
C       -2.309146        0.081621        0.272291
C       -3.381079       -0.688260        0.769410
C       -1.014945       -0.540424        0.190171
H       -4.348056       -0.232868        0.931953
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C       -3.192988       -2.011601        1.124835
C       -0.897241       -1.961531        0.383172
C       -1.986271       -2.662103        0.927620
H       -1.906576       -3.717794        1.149270
N        0.039475        0.336414        0.013894
N        1.175663        0.000424        0.466271
C        2.136961        0.985288        0.264259
C        3.418330        0.930581        0.793770
C        2.117005        2.201387       -0.466872
N        3.279353        2.833295       -0.387188
N        4.054612        2.046329        0.379157
C        5.376466        2.492450        0.736298
H        5.345795        3.172180        1.593841
H        5.996045        1.628547        0.983315
H        5.806362        3.016835       -0.117719
H        3.889195        0.189999        1.422970
H        1.310951        2.609275       -1.058968
H       -4.030124       -2.567558        1.538597
C        1.591997       -3.554282       -1.689167
C        1.105666       -2.242447       -1.082793
N        0.218690       -2.656540       -0.003783
C        0.315177       -4.089708        0.228966
C        1.601105       -4.486530       -0.481952
H        0.878649       -3.919581       -2.437272
H        0.570212       -1.603976       -1.795057
H        0.325440       -4.312165        1.302159
H        2.466726       -4.272965        0.154912
C       -2.445839        3.709980       -0.419206
C       -1.603835        2.438078       -0.408793
N       -2.557848        1.390700       -0.052427
C       -3.929287        1.881965       -0.113346
C       -3.818730        3.211021       -0.848401
H       -2.498435        4.130157        0.591726
H       -1.153986        2.242773       -1.391924
H       -4.573271        1.169043       -0.640758
H       -4.635523        3.893533       -0.599969
H       -0.781015        2.480409        0.306609
H       -2.029533        4.475159       -1.079492
H       -3.836812        3.039706       -1.930616
H       -4.348733        2.021747        0.896057
H       -0.543453       -4.621228       -0.213844
H        1.621585       -5.547638       -0.742688
H        2.567006       -3.451443       -2.172402
H        1.937864       -1.649417       -0.683753
30
4pzMe-cis-m ; E = -683.903377388 Hartree
C       -2.809900       -0.470705       -0.926639
C       -3.724585        0.389703       -0.331275
C       -1.671354       -0.876998       -0.227442
H       -4.596557        0.718532       -0.888861
C       -3.535335        0.810719        0.982826
C       -1.492301       -0.475748        1.101229
H       -0.628203       -0.824482        1.656750
C       -2.425978        0.361653        1.698581
H       -2.287446        0.665353        2.732197
H       -2.954561       -0.834477       -1.939410
N       -0.831386       -1.838067       -0.856698
N        0.416798       -1.774790       -0.827334
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C        1.141242       -0.671497       -0.360565
C        0.988719        0.706016       -0.544756
C        2.397978       -0.827715        0.282761
N        2.952076        0.350182        0.520989
N        2.094568        1.256724        0.003908
C        2.466206        2.649447        0.016027
H        2.719253        3.003533       -0.988929
H        1.657665        3.263999        0.420231
H        3.342953        2.735857        0.656017
C       -0.043753        1.510267       -1.246766
H        0.385994        2.418021       -1.679219
H       -0.486803        0.927554       -2.056169
H       -0.859242        1.796535       -0.572234
C        3.035079       -2.103823        0.703373
H        2.577081       -2.499816        1.616284
H        2.908325       -2.860331       -0.076100
H        4.098209       -1.946944        0.894819
H       -4.257168        1.470412        1.454447
30
4pzMe-cis-n ; E = -683.904412835 Hartree
C       -2.967972        0.633401        0.779835
C       -3.907787       -0.276279        0.311824
C       -1.793260        0.857625        0.058894
H       -4.807546       -0.466419        0.889403
C       -3.706751       -0.928252       -0.903024
C       -1.600247        0.223394       -1.173088
H       -0.703962        0.429877       -1.748406
C       -2.559168       -0.662378       -1.648389
H       -2.408597       -1.151118       -2.606547
H       -3.118017        1.171728        1.710544
N       -0.918439        1.872618        0.527589
N        0.323115        1.734792        0.564909
C        1.006599        0.529145        0.364652
C        2.312662        0.572240       -0.124086
C        0.790896       -0.838685        0.729741
N        1.871635       -1.553768        0.453154
N        2.764312       -0.694920       -0.084775
C        4.046239       -1.186941       -0.519218
H        4.179769       -1.039711       -1.595377
H        4.859574       -0.684109        0.012573
H        4.071452       -2.251861       -0.292954
C        3.092906        1.732129       -0.617941
H        3.175726        1.738751       -1.711050
H        2.579533        2.645858       -0.310575
H        4.107778        1.739525       -0.207298
C       -0.353406       -1.492506        1.423000
H       -0.718408       -0.875793        2.248727
H       -1.196660       -1.662558        0.746984
H       -0.021522       -2.453846        1.820277
H       -4.447749       -1.628733       -1.275634
30
4pzMe-trans-m ; E = -683.923838401 Hartree
C       -3.022466       -1.360107        0.000263
C       -4.403766       -1.204314        0.000210
C       -2.187387       -0.240737        0.000040
H       -5.047736       -2.078666        0.000386
C       -4.957807        0.072396       -0.000070
C       -2.746015        1.044124       -0.000243
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H       -2.079593        1.899629       -0.000416
C       -4.124068        1.192837       -0.000295
H       -4.558007        2.188763       -0.000516
H       -2.562439       -2.343575        0.000482
N       -0.801748       -0.510983        0.000121
N       -0.077809        0.520132       -0.000011
C        1.285234        0.314287        0.000020
C        2.079003       -0.841955       -0.000042
C        2.204833        1.399839        0.000084
N        3.450883        0.959829        0.000075
N        3.348370       -0.392462       -0.000004
C        4.550224       -1.186329       -0.000135
H        5.389375       -0.492509        0.000430
H        4.600633       -1.820920        0.890006
H        4.601091       -1.819994       -0.890917
C        1.743178       -2.288602       -0.000156
H        2.152471       -2.791366        0.884120
H        0.660019       -2.399060       -0.000747
H        2.153562       -2.791497       -0.883845
C        1.890801        2.853632        0.000193
H        1.300576        3.126683       -0.879585
H        1.301351        3.126739        0.880476
H        2.816740        3.431556       -0.000218
H       -6.036494        0.198176       -0.000116
30
4pzMe-trans-n ; E = -683.925382155 Hartree
C       -3.180892        1.157125       -0.000430
C       -4.535487        0.845674       -0.000463
C       -2.223575        0.139981        0.000030
H       -5.274455        1.641373       -0.000843
C       -4.941345       -0.485701        0.000006
C       -2.633511       -1.199611        0.000518
H       -1.876181       -1.975663        0.000899
C       -3.985930       -1.504137        0.000503
H       -4.304158       -2.542904        0.000897
H       -2.832807        2.185455       -0.000770
N       -0.879937        0.572200        0.000020
N       -0.035756       -0.364221       -0.000120
C        1.281443        0.033150       -0.000018
C        2.324807       -0.894446       -0.000292
C        1.913422        1.315294        0.000153
N        3.227447        1.171075       -0.000005
N        3.455553       -0.165360       -0.000340
C        4.819097       -0.626622        0.000272
H        5.335699       -0.263740        0.892320
H        4.831742       -1.716698       -0.006098
H        5.339175       -0.253230       -0.885300
C        2.258024       -2.376725       -0.000372
H        2.736238       -2.808015        0.885737
H        1.206577       -2.668965       -0.000464
H        2.736308       -2.807950       -0.886486
C        1.295148        2.666369        0.000397
H        0.651785        2.799191       -0.873988
H        0.652000        2.798972        0.874974
H        2.078520        3.427340        0.000412
H       -5.998789       -0.733139        0.000005
52
4pzMeAmid2-cis-m ; E = -1478.16512866 Hartree
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C        2.035439        1.335751       -0.337922
C        2.148596        2.711376       -0.142908
C        0.767755        0.749886       -0.580195
H        3.117955        3.129477        0.090298
C        1.013829        3.507545       -0.263346
C       -0.347039        1.586171       -0.758175
C       -0.219331        2.966425       -0.594383
H       -1.094798        3.590823       -0.717230
N        0.808593       -0.645143       -0.826174
N        0.009082       -1.505130       -0.373996
C       -1.014627       -1.295845        0.532813
C       -1.280424       -0.399380        1.586136
C       -2.127398       -2.188712        0.516897
N       -3.023639       -1.841133        1.420100
N       -2.483844       -0.774685        2.058825
C       -3.258606       -0.097133        3.069495
H       -2.728102       -0.079011        4.025844
H       -3.471715        0.926820        2.748179
H       -4.187197       -0.654518        3.180074
C       -0.518300        0.701240        2.228536
H       -0.615067        0.649480        3.317476
H        0.539273        0.647463        1.975954
H       -0.899360        1.673370        1.894690
C       -2.337257       -3.340752       -0.398618
H       -2.480430       -3.003540       -1.429547
H       -1.462985       -3.997416       -0.394525
H       -3.219905       -3.902404       -0.087396
H        1.103568        4.579765       -0.120089
N        3.106737        0.450181       -0.277544
H        2.870499       -0.496047       -0.562771
N       -1.583643        1.031266       -1.121819
H       -1.568038        0.179055       -1.664554
C        4.410870        0.725924        0.025516
O        4.850279        1.818432        0.357052
C       -2.762342        1.323415       -0.485672
O       -2.896579        2.195957        0.364138
C        6.638545       -0.556531        0.159342
C        6.966877       -1.920482       -0.082467
C        5.802936       -2.531828       -0.437503
O        4.781354       -1.647969       -0.432424
C        5.298889       -0.441771       -0.066841
H        7.289908        0.249760        0.460796
H        7.937596       -2.387709       -0.004407
H        5.548663       -3.544249       -0.711106
C       -5.185447        0.471127       -0.447777
C       -5.828273       -0.595717       -1.135164
C       -4.881134       -1.150617       -1.940381
O       -3.702000       -0.504136       -1.803920
C       -3.894878        0.484999       -0.886570
H       -5.602637        1.148150        0.282121
H       -6.856379       -0.913288       -1.043432
H       -4.890359       -1.972275       -2.639764
52
4pzMeAmid2-cis-n ; E = -1478.16360202 Hartree
C        2.023987        1.370093       -0.136164
C        2.158129        2.685677        0.307646
C        0.746345        0.853027       -0.438948
H        3.137903        3.051646        0.580829
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C        1.023920        3.486672        0.391169
C       -0.371418        1.704422       -0.417057
C       -0.230366        3.023871        0.014619
H       -1.104353        3.659505        0.059222
N        0.716250       -0.471540       -0.945063
N       -0.084758       -1.354669       -0.538616
C       -0.927175       -1.222850        0.555741
C       -2.112925       -1.965723        0.581914
C       -0.863727       -0.574320        1.836722
N       -1.938412       -0.882568        2.542790
N       -2.689232       -1.692952        1.762654
C       -3.998434       -2.091288        2.211991
H       -4.775685       -1.552818        1.659503
H       -4.140033       -3.166779        2.078083
H       -4.065163       -1.842148        3.269972
C       -2.686467       -2.878754       -0.435345
H       -3.641788       -2.512284       -0.825110
H       -1.980372       -2.966921       -1.262727
H       -2.857566       -3.875851       -0.014693
C        0.219707        0.220652        2.478348
H        1.205125       -0.189922        2.242733
H        0.208631        1.263108        2.148448
H        0.076251        0.198200        3.560377
H        1.126820        4.509789        0.738977
N        3.082527        0.475431       -0.266397
H        2.831306       -0.404422       -0.705774
N       -1.597834        1.209930       -0.876112
H       -1.560243        0.425003       -1.510893
C        4.399221        0.678930        0.042823
O        4.865188        1.693203        0.542111
C       -2.824276        1.504474       -0.344494
O       -3.036754        2.323443        0.533939
C        6.606830       -0.636204       -0.105211
C        6.905019       -1.943835       -0.582689
C        5.722076       -2.471415       -1.002905
O        4.716325       -1.587912       -0.820255
C        5.264199       -0.467501       -0.271110
H        7.279542        0.098948        0.309829
H        7.869121       -2.430004       -0.611568
H        5.443438       -3.419746       -1.435942
C       -5.242885        0.648692       -0.573481
C       -5.847535       -0.271885       -1.478407
C       -4.857747       -0.681807       -2.319218
O       -3.685412       -0.088083       -1.995256
C       -3.929041        0.725201       -0.929354
H       -5.700186        1.199255        0.234837
H       -6.882347       -0.580420       -1.509762
H       -4.829584       -1.351542       -3.164988
52
4pzMeAmid2-trans-m ; E = -1478.18685783 Hartree
C        1.349149       -2.178837       -0.029898
C        1.365650       -3.568806        0.035038
C        0.115115       -1.467658       -0.079163
H        2.313096       -4.087036        0.069428
C        0.151882       -4.245914        0.051867
C       -1.108631       -2.195212       -0.061077
C       -1.071319       -3.591624        0.007379
H       -2.004237       -4.135852        0.026719
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N        0.279183       -0.090523       -0.089314
N       -0.726867        0.650943       -0.298299
C       -0.490624        2.006034       -0.196399
C        0.503999        2.701756        0.501211
C       -1.318539        3.004310       -0.777067
N       -0.869356        4.211024       -0.473883
N        0.222072        4.005329        0.299828
C        0.898410        5.147472        0.861788
H        0.707904        5.235006        1.936505
H        1.976187        5.079620        0.693190
H        0.505952        6.028380        0.356044
C        1.613917        2.227675        1.365140
H        1.833027        2.939769        2.166042
H        1.346620        1.266303        1.809415
H        2.532790        2.060924        0.792676
C       -2.488910        2.809134       -1.674033
H       -2.165404        2.587826       -2.696921
H       -3.098906        1.967888       -1.338840
H       -3.094785        3.717279       -1.700798
H        0.159305       -5.330917        0.099120
N        2.500094       -1.401570       -0.065052
H        2.308060       -0.407833       -0.138681
N       -2.295155       -1.477218       -0.079093
H       -2.163026       -0.466850       -0.184590
C        3.802126       -1.811194       -0.008803
O        4.188445       -2.965825        0.102147
C       -3.567678       -1.965313        0.070520
O       -3.884294       -3.143848        0.149807
C        6.138802       -0.741435       -0.066966
C        6.572614        0.607001       -0.212495
C        5.442794        1.356993       -0.324544
O        4.342229        0.572311       -0.257512
C        4.776710       -0.711573       -0.099806
H        6.736990       -1.632947        0.045249
H        7.588729        0.972694       -0.234329
H        5.262053        2.412825       -0.455964
C       -5.957256       -1.041565        0.258898
C       -6.469768        0.285301        0.312844
C       -5.390363        1.110602        0.227091
O       -4.250089        0.391440        0.123356
C       -4.603595       -0.924319        0.141960
H       -6.497944       -1.974862        0.302128
H       -7.502220        0.589018        0.404932
H       -5.271246        2.183297        0.226064
52
4pzMeAmid2-trans-n ; E = -1478.18769106 Hartree
C        1.606692       -2.060472       -0.063518
C        1.731104       -3.447063       -0.094121
C        0.320409       -1.445857       -0.067752
H        2.716565       -3.889736       -0.094239
C        0.576022       -4.217804       -0.126097
C       -0.840744       -2.269835       -0.102790
C       -0.694752       -3.659866       -0.128747
H       -1.581981       -4.275588       -0.148250
N        0.373424       -0.060936        0.008001
N       -0.689414        0.605730       -0.166452
C       -0.563354        1.970989       -0.010082
C       -1.509531        2.873656       -0.497193
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C        0.412842        2.769159        0.660337
N        0.081280        4.047960        0.584156
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C       -1.669535        5.367222       -0.418714
H       -1.669016        5.566519       -1.494997
H       -2.698483        5.408853       -0.049257
H       -1.072496        6.123039        0.089249
C       -2.729447        2.651648       -1.310637
H       -2.600816        3.017981       -2.335764
H       -2.950326        1.585052       -1.353963
H       -3.596883        3.168419       -0.885353
C        1.621636        2.347619        1.416554
H        1.401654        1.490630        2.059672
H        2.428772        2.040995        0.745860
H        1.974154        3.179571        2.030256
H        0.669373       -5.299527       -0.151994
N        2.696944       -1.200634       -0.045958
H        2.434617       -0.220550       -0.033308
N       -2.083212       -1.650905       -0.077852
H       -2.031543       -0.628574       -0.106155
C        4.026465       -1.520976       -0.050581
O        4.492028       -2.651671       -0.041620
C       -3.311174       -2.250448        0.015845
O       -3.532710       -3.453221        0.010457
C        6.284279       -0.291897       -0.052502
C        6.621171        1.090792       -0.096504
C        5.440384        1.766412       -0.141286
O        4.399550        0.902946       -0.128628
C        4.922732       -0.354824       -0.072331
H        6.944350       -1.145047       -0.011625
H        7.608959        1.527752       -0.095656
H        5.182673        2.813565       -0.183288
C       -5.771872       -1.550235        0.231001
C       -6.400856       -0.279179        0.354841
C       -5.398562        0.641259        0.327109
O       -4.197655        0.033828        0.194293
C       -4.433612       -1.307127        0.135955
H       -6.227139       -2.528821        0.215551
H       -7.456616       -0.073894        0.454717
H       -5.377528        1.717948        0.393744
30
4pzMeCl1A-cis-m ; E = -1143.34071795 Hartree
C       -2.484252       -0.156319       -0.115080
C       -3.238630        0.889535        0.404490
C       -1.302573       -0.575209        0.504786
H       -4.141719        1.198905       -0.110471
C       -2.826363        1.518746        1.573523
C       -0.906599        0.064122        1.685743
H       -0.002482       -0.273007        2.182009
C       -1.661332        1.100659        2.215150
H       -1.342336        1.581141        3.134809
Cl       -2.980206       -0.915692       -1.593693
N       -0.660712       -1.758318        0.055273
N        0.575101       -1.834499       -0.112681
C        1.434216       -0.734452       -0.112750
C        1.325486        0.550346       -0.657414
C        2.778005       -0.841009        0.337377
N        3.428805        0.292431        0.136198
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N        2.541558        1.108892       -0.474919
C        2.988065        2.403570       -0.926078
H        3.085292        2.433625       -2.016374
H        2.295855        3.185897       -0.604897
H        3.964638        2.574647       -0.475837
C        0.233789        1.230357       -1.399138
H        0.633512        1.933254       -2.135074
H       -0.374711        0.496747       -1.932830
H       -0.433878        1.777891       -0.723788
C        3.410244       -2.013358        0.998203
H        3.107167       -2.094294        2.047713
H        3.100774       -2.936298        0.500055
H        4.497345       -1.922325        0.962545
H       -3.419543        2.329098        1.984961
30
4pzMeCl1A-cis-n ; E = -1143.34158459 Hartree
C        2.617707       -0.232942        0.006436
C        3.427454        0.894665        0.067394
C        1.406370       -0.214660       -0.692132
H        4.350682        0.854617        0.635239
C        3.042868        2.054190       -0.597329
C        1.038825        0.956431       -1.364118
H        0.110101        0.964101       -1.925216
C        1.849867        2.081374       -1.317165
H        1.551203        2.981738       -1.844833
Cl        3.078495       -1.666860        0.865236
N        0.690451       -1.420757       -0.884228
N       -0.542164       -1.510411       -0.703557
C       -1.336075       -0.545360       -0.081052
C       -2.697308       -0.504012       -0.391653
C       -1.173069        0.376392        1.004516
N       -2.337404        0.937412        1.293616
N       -3.234455        0.416381        0.427250
C       -4.602764        0.864772        0.472755
H       -4.878777        1.381073       -0.451858
H       -5.283633        0.022937        0.628113
H       -4.683556        1.554703        1.311362
C       -3.451843       -1.272221       -1.410470
H       -3.718109       -0.655898       -2.276956
H       -2.821117       -2.093534       -1.757138
H       -4.378302       -1.684902       -0.998235
C        0.007539        0.681048        1.859183
H        0.553922       -0.229938        2.119728
H        0.710229        1.353894        1.358499
H       -0.338433        1.158911        2.777845
H        3.678955        2.932481       -0.555317
30
4pzMeCl1A-trans-m ; E = -1143.36111639 Hartree
C       -2.819880       -0.634036        0.000209
C       -4.173094       -0.311512        0.000291
C       -1.836812        0.366461       -0.000315
H       -4.908281       -1.108636        0.000732
C       -4.561785        1.022137       -0.000205
C       -2.253249        1.705165       -0.000819
H       -1.480154        2.466103       -0.001255
C       -3.598188        2.031636       -0.000764
H       -3.901943        3.073999       -0.001189
Cl       -2.364770       -2.310294        0.000845
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N       -0.493406       -0.043430       -0.000489
N        0.337694        0.907652        0.000204
C        1.654758        0.522053        0.000039
C        2.240045       -0.754548       -0.000440
C        2.740785        1.438906        0.000500
N        3.892786        0.792689        0.000332
N        3.565111       -0.526583       -0.000250
C        4.632346       -1.497432       -0.000367
H        5.564796       -0.935365       -0.000682
H        4.589761       -2.128989        0.891530
H        4.589270       -2.129196       -0.892081
C        1.622767       -2.102473       -0.000863
H        0.969988       -2.221084        0.868768
H        0.970770       -2.220955       -0.871096
H        2.374700       -2.895193       -0.000571
C        2.678640        2.924643        0.001020
H        2.145266        3.294150       -0.879919
H        2.142765        3.293404        0.880734
H        3.689192        3.336918        0.002549
H       -5.618339        1.271538       -0.000178
30
4pzMeCl1A-trans-n ; E = -1143.36175490 Hartree
C        2.939574       -0.442611        0.000708
C        4.240014        0.052216        0.000725
C        1.836128        0.424011       -0.000501
H        5.071326       -0.644083        0.001725
C        4.454904        1.424519       -0.000557
C        2.078279        1.804750       -0.001817
H        1.215352        2.461765       -0.002836
C        3.369924        2.302001       -0.001842
H        3.537198        3.374793       -0.002923
Cl        2.704950       -2.161781        0.002331
N        0.556664       -0.157037       -0.000642
N       -0.390947        0.676220        0.000172
C       -1.646587        0.121495       -0.000197
C       -2.800085        0.909768        0.000541
C       -2.108855       -1.232466       -0.001533
N       -3.429842       -1.255752       -0.001637
N       -3.826719        0.042259       -0.000577
C       -5.238466        0.324214        0.001639
H       -5.701854       -0.099108        0.896228
H       -5.391833        1.403454       -0.009006
H       -5.706738       -0.117448       -0.881290
C       -2.923621        2.388310        0.002280
H       -3.453330        2.753076        0.888903
H       -1.918978        2.814366        0.002498
H       -3.453727        2.755144       -0.883271
C       -1.318368       -2.489681       -0.002877
H       -0.659899       -2.534236       -0.875069
H       -0.659740       -2.535972        0.869095
H       -1.993884       -3.347709       -0.003703
H        5.470810        1.807246       -0.000599
30
4pzMeCl1B-cis-m ; E = -1143.33848826 Hartree
C       -2.607504        0.240785       -1.348653
C       -3.561580        0.904634       -0.593562
C       -1.590769       -0.507738       -0.743907
H       -4.325387        1.496962       -1.087416
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C       -3.544796        0.792933        0.795358
C       -1.615532       -0.650221        0.650944
Cl       -0.490446       -1.685155        1.471308
C       -2.582139        0.003069        1.411983
H       -2.573766       -0.125076        2.489179
H       -2.613372        0.292245       -2.433260
N       -0.730316       -1.231294       -1.613491
N        0.516599       -1.162587       -1.561818
C        1.234183       -0.281652       -0.758200
C        1.065873        1.058471       -0.387281
C        2.496751       -0.663403       -0.226537
N        3.040530        0.332377        0.449807
N        2.171525        1.360737        0.327561
C        2.535051        2.640897        0.882249
H        2.786156        3.360474        0.095763
H        1.723762        3.043885        1.493666
H        3.411530        2.474478        1.506509
C        0.044739        2.083445       -0.727220
H        0.486141        3.083429       -0.754010
H       -0.382944        1.879217       -1.709501
H       -0.782205        2.089711       -0.008151
C        3.133007       -2.002750       -0.319842
H        2.646097       -2.715585        0.354112
H        3.032736       -2.398387       -1.334200
H        4.188703       -1.936881       -0.050609
H       -4.291947        1.297724        1.399284
30
4pzMeCl1B-cis-n ; E = -1143.34017951 Hartree
C       -2.760390       -0.465524        1.251107
C       -3.748291       -0.910934        0.387205
C       -1.706331        0.334674        0.796429
H       -4.541097       -1.552806        0.758065
C       -3.726094       -0.521395       -0.950722
C       -1.721634        0.754869       -0.540692
Cl       -0.532140        1.866253       -1.146245
C       -2.722046        0.323418       -1.407792
H       -2.704688        0.661697       -2.438262
H       -2.766396       -0.738434        2.301824
N       -0.804491        0.830792        1.772124
N        0.433805        0.681863        1.699941
C        1.107531       -0.095861        0.762730
C        2.419110        0.266659        0.444660
C        0.880056       -1.324693        0.059530
N        1.961923       -1.649584       -0.631769
N        2.864479       -0.668791       -0.409184
C        4.129481       -0.707713       -1.097066
H        4.176006        0.054666       -1.881238
H        4.953719       -0.550693       -0.396558
H        4.218559       -1.695150       -1.547749
C        3.193344        1.450679        0.885235
H        3.256446        2.209413        0.096867
H        2.681756        1.895008        1.741377
H        4.214052        1.182417        1.175940
C       -0.259425       -2.284238        0.081973
H       -0.620186       -2.449762        1.100223
H       -1.106841       -1.930635       -0.511976
H        0.081801       -3.236025       -0.330047
H       -4.498643       -0.855610       -1.635677
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4pzMeCl1B-trans-m ; E = -1143.35362662 Hartree
C       -2.571403       -1.752212        0.546774
C       -3.952292       -1.769805        0.657787
C       -1.878952       -0.611985        0.120120
H       -4.458096       -2.662628        1.011271
C       -4.681589       -0.638932        0.300601
C       -2.632174        0.514278       -0.257907
Cl       -1.909189        1.942772       -0.931438
C       -4.021548        0.490522       -0.168186
H       -4.578306        1.369137       -0.475935
H       -1.971967       -2.620317        0.802900
N       -0.480747       -0.766121        0.052441
N        0.175741        0.278182        0.314895
C        1.541072        0.156093        0.216153
C        2.354319       -0.911820       -0.191727
C        2.433664        1.216358        0.529347
N        3.685620        0.841038        0.336663
N        3.612060       -0.444958       -0.096824
C        4.840271       -1.132734       -0.412260
H        5.651250       -0.445922       -0.175542
H        4.946911       -2.041031        0.187245
H        4.885821       -1.393445       -1.473803
C        2.005527       -2.278124       -0.651801
H        1.557897       -2.855136        0.163359
H        1.245438       -2.225128       -1.435348
H        2.878441       -2.816513       -1.028870
C        2.086436        2.578494        1.013912
H        1.344080        3.043514        0.359632
H        1.648538        2.537238        2.016066
H        2.982364        3.200935        1.046858
H       -5.764859       -0.635602        0.369527
30
4pzMeCl1B-trans-n ; E = -1143.35582843 Hartree
C       -2.780296        1.618789        0.469964
C       -4.147984        1.473054        0.635340
C       -1.962952        0.547578        0.086607
H       -4.750364        2.318438        0.952126
C       -4.740445        0.239606        0.378761
C       -2.581184       -0.685615       -0.189517
Cl       -1.709314       -2.059611       -0.801034
C       -3.958699       -0.828199       -0.045150
H       -4.409935       -1.787386       -0.275471
H       -2.286309        2.569311        0.645678
N       -0.599482        0.875053       -0.042694
N        0.195074       -0.064889        0.227142
C        1.528979        0.230528        0.084686
C        2.510265       -0.725059        0.356871
C        2.239082        1.403196       -0.319717
N        3.539940        1.173374       -0.291425
N        3.682684       -0.113095        0.117622
C        5.013732       -0.648003        0.239363
H        5.583649       -0.067376        0.968885
H        4.956559       -1.685803        0.568087
H        5.523463       -0.600687       -0.725976
C        2.341382       -2.128534        0.807156
H        2.814938       -2.305549        1.778837
H        1.272122       -2.328052        0.899914
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H        2.764564       -2.839638        0.089612
C        1.704733        2.727424       -0.729503
H        1.034600        2.626466       -1.587943
H        1.108363        3.170873        0.073075
H        2.531431        3.394081       -0.983797
H       -5.811933        0.107009        0.490879
30
4pzMeCl2-cis-m ; E = -1602.77490089 Hartree
C        2.468649       -0.367725       -0.280356
C        3.289523       -0.272139        0.833776
C        1.326722        0.431277       -0.440258
H        4.149636       -0.926525        0.919501
C        2.992098        0.663696        1.818075
C        1.072399        1.386680        0.557044
Cl       -0.244245        2.502176        0.393683
C        1.889308        1.496838        1.677488
H        1.656635        2.246757        2.425225
Cl        2.824184       -1.553451       -1.495137
N        0.648683        0.401961       -1.685457
N       -0.576347        0.187008       -1.796952
C       -1.408899       -0.215577       -0.761426
C       -1.258733       -1.084627        0.328483
C       -2.774444        0.183104       -0.741278
N       -3.401145       -0.351032        0.290782
N       -2.476579       -1.120266        0.909798
C       -2.890923       -1.928838        2.029759
H       -2.940862       -2.988850        1.759571
H       -2.207031       -1.803172        2.872710
H       -3.884502       -1.585753        2.313762
C       -0.142684       -1.952786        0.784226
H       -0.522236       -2.857292        1.266954
H        0.468616       -2.261959       -0.065807
H        0.514251       -1.435885        1.492772
C       -3.441076        1.125465       -1.676563
H       -3.150221        2.159763       -1.464531
H       -3.141544        0.910930       -2.705923
H       -4.525320        1.044166       -1.581744
H        3.629697        0.753610        2.691205
30
4pzMeCl2-cis-n ; E = -1602.77645797 Hartree
C        2.574859       -0.517274       -0.103579
C        3.461171        0.075271        0.783426
C        1.428398        0.144834       -0.564737
H        4.321740       -0.485031        1.130959
C        3.225471        1.376820        1.212912
C        1.234084        1.465828       -0.134142
Cl       -0.101367        2.396533       -0.735389
C        2.116973        2.075306        0.750936
H        1.928829        3.096199        1.063730
Cl        2.846606       -2.151225       -0.614551
N        0.667289       -0.447469       -1.600579
N       -0.554034       -0.686479       -1.505580
C       -1.320294       -0.572369       -0.353578
C       -2.693219       -0.358142       -0.514354
C       -1.129751       -0.725977        1.060784
N       -2.291175       -0.593680        1.681825
N       -3.211883       -0.347645        0.722443
C       -4.575180       -0.085074        1.107733
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H       -4.823122        0.973743        0.983099
H       -5.265546       -0.686882        0.511367
H       -4.669289       -0.357016        2.158066
C       -3.464747       -0.135410       -1.759473
H       -3.748509        0.916602       -1.876765
H       -2.835469       -0.413525       -2.607053
H       -4.380646       -0.734614       -1.779979
C        0.062870       -1.106823        1.867988
H        0.614228       -1.927433        1.401099
H        0.756363       -0.270891        1.996584
H       -0.276895       -1.428762        2.854294
H        3.914057        1.852355        1.903315
30
4pzMeCl2-trans-m ; E = -1602.78838145 Hartree
C       -2.546210       -1.155109        0.253382
C       -3.923756       -1.013403        0.331489
C       -1.697215       -0.080622       -0.057761
H       -4.533922       -1.869480        0.595569
C       -4.493305        0.226446        0.067156
C       -2.307900        1.156706       -0.329580
Cl       -1.376852        2.532604       -0.832726
C       -3.689460        1.306869       -0.271769
H       -4.122596        2.274406       -0.499079
Cl       -1.847371       -2.709113        0.590381
N       -0.327582       -0.356310       -0.180944
N        0.408322        0.501182        0.350529
C        1.750147        0.275098        0.214740
C        2.459952       -0.782787       -0.378865
C        2.735547        1.167022        0.715694
N        3.945506        0.711077        0.452885
N        3.754978       -0.465312       -0.203531
C        4.938205       -1.180818       -0.612140
H        5.541490       -1.420742        0.266256
H        4.661526       -2.100618       -1.124389
H        5.527609       -0.554971       -1.286015
C        1.945345       -2.001440       -1.050063
H        1.206160       -2.489502       -0.409872
H        1.412271       -1.731422       -1.966881
H        2.736215       -2.712381       -1.296424
C        2.515958        2.447881        1.437346
H        1.861940        3.109278        0.862553
H        2.027077        2.272409        2.400481
H        3.471848        2.944996        1.610751
H       -5.570243        0.349159        0.116569
30
4pzMeCl2-trans-n ; E = -1602.79095332 Hartree
C       -2.706732        0.966382        0.294741
C       -4.049104        0.651167        0.446229
C       -1.744124        0.002651       -0.048509
H       -4.749932        1.427444        0.731173
C       -4.467852       -0.655605        0.226987
C       -2.204113       -1.307312       -0.270607
Cl       -1.130742       -2.564576       -0.801225
C       -3.550381       -1.631459       -0.139149
H       -3.866889       -2.650411       -0.331443
Cl       -2.194970        2.600836        0.577733
N       -0.427025        0.449559       -0.250390
N        0.452774       -0.297581        0.254155
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C        1.749562        0.094302        0.037288
C        2.822339       -0.655632        0.525535
C        2.335523        1.211643       -0.635506
N        3.651846        1.140375       -0.558098
N        3.924751        0.008476        0.142536
C        5.303678       -0.330303        0.381135
H        5.789598        0.466859        0.948904
H        5.354073       -1.260657        0.947002
H        5.825438       -0.455223       -0.570683
C        2.797720       -1.922116        1.297621
H        3.269407       -1.809885        2.279675
H        1.755166       -2.210400        1.443888
H        3.308943       -2.732051        0.766501
C        1.664358        2.336034       -1.336253
H        1.054972        1.966503       -2.166120
H        0.976747        2.856223       -0.663536
H        2.414420        3.034025       -1.713732
H       -5.516517       -0.913158        0.333244
30
4pzMeF1A-cis-m ; E = -783.046043499 Hartree
C       -2.598813       -0.215390       -0.571423
C       -3.467670        0.613072        0.117358
C       -1.475726       -0.782233        0.031219
H       -4.314355        1.041235       -0.408326
C       -3.228643        0.867993        1.464920
C       -1.253837       -0.518219        1.386395
H       -0.396435       -0.971360        1.873251
C       -2.123530        0.300161        2.096666
H       -1.941714        0.489101        3.149860
F       -2.795763       -0.436377       -1.877610
N       -0.740314       -1.765684       -0.686112
N        0.508242       -1.755578       -0.740716
C        1.289505       -0.673936       -0.326286
C        1.149336        0.701813       -0.529629
C        2.575906       -0.841969        0.251588
N        3.160013        0.330705        0.436739
N        2.291720        1.242989       -0.052342
C        2.687576        2.628337       -0.094793
H        2.915122        2.946711       -1.117678
H        1.901159        3.267936        0.313851
H        3.584840        2.720024        0.515363
C        0.100252        1.504934       -1.207210
H        0.535577        2.351242       -1.746426
H       -0.441441        0.888794       -1.927952
H       -0.635478        1.891974       -0.492248
C        3.213124       -2.120424        0.664854
H        2.790942       -2.494788        1.603803
H        3.042788       -2.888011       -0.095304
H        4.285699       -1.975717        0.806327
H       -3.907337        1.508396        2.019033
30
4pzMeF1A-cis-n ; E = -783.046721669 Hartree
C       -2.772236        0.472286        0.383319
C       -3.672640       -0.534991        0.084504
C       -1.591707        0.649349       -0.339387
H       -4.562680       -0.642828        0.694951
C       -3.408506       -1.379488       -0.990692
C       -1.347739       -0.200771       -1.422084
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H       -0.445687       -0.054859       -2.007184
C       -2.249077       -1.208202       -1.744457
H       -2.047830       -1.858630       -2.589644
F       -3.001363        1.269986        1.432162
N       -0.804881        1.801848       -0.086796
N        0.437758        1.748556        0.033301
C        1.175288        0.570193        0.175964
C        2.508523        0.552093       -0.236261
C        0.978968       -0.672165        0.860108
N        2.097204       -1.381812        0.831961
N        2.995532       -0.642212        0.145510
C        4.316235       -1.169253       -0.084739
H        4.500360       -1.317227       -1.153344
H        5.079944       -0.498133        0.318959
H        4.369827       -2.128100        0.428619
C        3.281846        1.587928       -0.962111
H        3.440500        1.322791       -2.013855
H        2.718972        2.523210       -0.927959
H        4.264778        1.748819       -0.507637
C       -0.188082       -1.182013        1.631857
H       -0.665478       -0.381023        2.203254
H       -0.948843       -1.615121        0.974825
H        0.154633       -1.954147        2.323620
H       -4.110756       -2.169077       -1.238014
30
4pzMeF1A-trans-m ; E = -783.066407739 Hartree
C       -2.914792       -1.002776       -0.000028
C       -4.285877       -0.801279       -0.000015
C       -2.008510        0.063549       -0.000001
H       -4.944064       -1.663195       -0.000020
C       -4.775156        0.500133        0.000010
C       -2.524670        1.366091        0.000019
H       -1.815310        2.186675        0.000035
C       -3.893344        1.582919        0.000017
H       -4.280315        2.597146        0.000033
F       -2.446955       -2.255317       -0.000010
N       -0.645966       -0.274672        0.000009
N        0.132012        0.717616        0.000004
C        1.476896        0.419147        0.000003
C        2.178613       -0.796191        0.000004
C        2.476391        1.431285        0.000001
N        3.684510        0.896153       -0.000007
N        3.477999       -0.444815       -0.000010
C        4.615577       -1.328585        0.000019
H        5.505599       -0.701396        0.000073
H        4.616692       -1.964729        0.890390
H        4.616770       -1.964684       -0.890384
C        1.731634       -2.212968        0.000002
H        2.104236       -2.744613        0.883673
H        0.642929       -2.245398       -0.000060
H        2.104354       -2.744650       -0.883595
C        2.275996        2.905030       -0.000023
H        1.709432        3.223243       -0.880224
H        1.709365        3.223256        0.880130
H        3.244014        3.409264        0.000007
H       -5.847552        0.668834        0.000017
30
4pzMeF1A-trans-n ; E = -783.067189005 Hartree
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C        3.052979       -0.807998        0.000375
C        4.389003       -0.438302        0.000472
C        2.021638        0.138552       -0.000107
H        5.147648       -1.213289        0.000877
C        4.715571        0.912893        0.000041
C        2.375895        1.494244       -0.000555
H        1.572872        2.223153       -0.000975
C        3.707276        1.878726       -0.000482
H        3.966140        2.933009       -0.000852
F        2.745474       -2.107350        0.000795
N        0.709667       -0.364935       -0.000221
N       -0.182496        0.527672       -0.000044
C       -1.472156        0.052214       -0.000109
C       -2.573392        0.910661       -0.000110
C       -2.018607       -1.269294       -0.000369
N       -3.338877       -1.210323       -0.000519
N       -3.653538        0.109253       -0.000331
C       -5.044461        0.479972        0.000924
H       -5.535211        0.084938        0.893900
H       -5.129009        1.566831       -0.007013
H       -5.539231        0.071543       -0.883641
C       -2.603414        2.394134        0.000342
H       -3.109076        2.792848        0.886444
H       -1.573540        2.755100        0.000591
H       -3.108741        2.793419       -0.885712
C       -1.309358       -2.574605       -0.000600
H       -0.655748       -2.661942       -0.873084
H       -0.655644       -2.662208        0.871776
H       -2.038046       -3.388017       -0.000686
H        5.759179        1.211916        0.000097
30
4pzMeF1B-cis-m ; E = -783.046231322 Hartree
C       -2.722297       -0.149107       -1.111189
C       -3.626462        0.608964       -0.378490
C       -1.605889       -0.730481       -0.503564
H       -4.473743        1.069163       -0.876528
C       -3.452948        0.759338        0.995643
C       -1.478039       -0.597423        0.883434
F       -0.471700       -1.211630        1.516695
C       -2.378317        0.143271        1.630868
H       -2.226728        0.216560        2.702577
H       -2.849765       -0.299627       -2.178956
N       -0.786264       -1.584278       -1.292343
N        0.463690       -1.536237       -1.254552
C        1.176500       -0.533647       -0.599333
C        1.022375        0.854442       -0.573367
C        2.386580       -0.794122        0.095833
N        2.914373        0.330296        0.549515
N        2.087241        1.310012        0.124488
C        2.453583        2.682725        0.365136
H        2.800986        3.170940       -0.551837
H        1.608106        3.243192        0.772117
H        3.264614        2.670769        1.091747
C        0.040986        1.761744       -1.222013
H        0.514839        2.693905       -1.543081
H       -0.386874        1.280127       -2.102879
H       -0.791156        2.008631       -0.552343
C        2.983975       -2.125101        0.378176
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H        2.413673       -2.653106        1.149683
H        2.965710       -2.747532       -0.521023
H        4.012615       -2.010015        0.724477
H       -4.160543        1.339492        1.579225
30
4pzMeF1B-cis-n ; E = -783.047470797 Hartree
C       -2.900640        0.420999        0.999766
C       -3.838196       -0.413584        0.406496
C       -1.731185        0.785968        0.326949
H       -4.726073       -0.706364        0.957494
C       -3.644100       -0.859386       -0.899497
C       -1.579650        0.355978       -0.995492
F       -0.512601        0.753317       -1.700954
C       -2.514099       -0.462018       -1.608252
H       -2.342013       -0.771416       -2.633639
H       -3.039806        0.797718        2.008361
N       -0.869788        1.728173        0.945403
N        0.373012        1.586473        0.974856
C        1.049109        0.429595        0.594681
C        2.337319        0.537021        0.071557
C        0.821263       -0.975435        0.744512
N        1.881972       -1.648707        0.323108
N        2.769491       -0.724510       -0.103104
C        4.015650       -1.157130       -0.681408
H        4.056620       -0.923975       -1.750089
H        4.862466       -0.680714       -0.179628
H        4.073298       -2.235866       -0.543863
C        3.106899        1.753694       -0.280401
H        3.121222        1.928138       -1.362360
H        2.627136        2.612779        0.193402
H        4.144357        1.690414        0.063161
C       -0.304640       -1.720111        1.375245
H       -0.656373       -1.213017        2.277641
H       -1.161776       -1.817629        0.702162
H        0.041844       -2.720005        1.644314
H       -4.376694       -1.503478       -1.375125
30
4pzMeF1B-trans-m ; E = -783.061798528 Hartree
C       -2.760766       -1.559253        0.190117
C       -4.147296       -1.547412        0.201220
C       -2.008400       -0.387434        0.031639
H       -4.698570       -2.472673        0.333184
C       -4.823481       -0.340835        0.037777
C       -2.720119        0.814510       -0.137449
F       -2.085512        1.972071       -0.323260
C       -4.106056        0.838327       -0.135985
H       -4.601800        1.793413       -0.274142
H       -2.201471       -2.482003        0.309214
N       -0.617304       -0.578589        0.037222
N        0.078835        0.476055        0.064667
C        1.438513        0.273730        0.048449
C        2.209741       -0.894537       -0.045081
C        2.374238        1.341063        0.114502
N        3.611596        0.879453        0.066878
N        3.486635       -0.469785       -0.028342
C        4.687474       -1.264324       -0.112549
H        5.524399       -0.571420       -0.042488
H        4.742099       -1.983356        0.709709
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H        4.740982       -1.800647       -1.064636
C        1.809939       -2.319220       -0.152158
H        1.283653       -2.637973        0.752676
H        1.101294       -2.448960       -0.974175
H        2.670982       -2.973101       -0.310863
C        2.079970        2.793794        0.233313
H        1.317725        3.093389       -0.490563
H        1.688406        3.033045        1.227276
H        2.989674        3.373821        0.067839
H       -5.908631       -0.312572        0.040556
30
4pzMeF1B-trans-n ; E = -783.064215244 Hartree
C       -2.980525        1.394155       -0.001483
C       -4.353627        1.200900       -0.001937
C       -2.077918        0.321821       -0.000056
H       -5.023342        2.054640       -0.003132
C       -4.863201       -0.095140       -0.000777
C       -2.623877       -0.975269        0.001158
F       -1.841919       -2.057487        0.002903
C       -3.994332       -1.181721        0.000826
H       -4.358180       -2.203835        0.001858
H       -2.547669        2.389605       -0.002269
N       -0.725314        0.700449        0.000290
N        0.105273       -0.250609       -0.000534
C        1.426110        0.126120       -0.000165
C        2.442132       -0.831642       -0.001065
C        2.094114        1.389749        0.000716
N        3.403283        1.207482        0.000409
N        3.592861       -0.136216       -0.000809
C        4.942229       -0.637305        0.000022
H        5.467976       -0.294001        0.894497
H        4.921658       -1.727242       -0.011288
H        5.474438       -0.275535       -0.883121
C        2.318782       -2.310112       -0.001876
H        2.780668       -2.759382        0.883948
H        1.255349       -2.557911       -0.002098
H        2.780637       -2.758449       -0.888214
C        1.513661        2.757529        0.001801
H        0.874928        2.908820       -0.873091
H        0.874785        2.907355        0.876847
H        2.317207        3.497116        0.002521
H       -5.935188       -0.266049       -0.001065
30
4pzMeF2-cis-m ; E = -882.188736999 Hartree
C       -2.541735        0.170533       -0.675012
C       -3.394266        0.683829        0.287075
C       -1.432871       -0.618154       -0.364758
H       -4.224331        1.309305       -0.020743
C       -3.157247        0.371554        1.622772
C       -1.242345       -0.917471        0.988059
F       -0.223382       -1.711756        1.330354
C       -2.078155       -0.431735        1.979774
H       -1.877332       -0.699427        3.010892
F       -2.733768        0.484966       -1.961194
N       -0.724080       -1.271244       -1.412679
N        0.524606       -1.245289       -1.468682
C        1.295662       -0.400590       -0.673561
C        1.158042        0.960155       -0.392515
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C        2.538464       -0.784657       -0.105773
N        3.101418        0.240398        0.511782
N        2.264342        1.282346        0.314510
C        2.658811        2.591472        0.769091
H        2.983133        3.223303       -0.064875
H        1.833684        3.082342        1.291271
H        3.492243        2.452057        1.456047
C        0.155126        1.967725       -0.822108
H        0.635269        2.911226       -1.099251
H       -0.399712        1.604140       -1.689207
H       -0.575547        2.174825       -0.031140
C        3.133925       -2.146059       -0.096310
H        2.581491       -2.807664        0.579039
H        3.086485       -2.589329       -1.095228
H        4.172996       -2.099436        0.234192
H       -3.818507        0.756678        2.391633
30
4pzMeF2-cis-n ; E = -882.189401241 Hartree
C       -2.732279       -0.488626       -0.467928
C       -3.622972        0.549669       -0.260390
C       -1.549512       -0.630506        0.261359
H       -4.509285        0.617948       -0.880596
C       -3.347605        1.476176        0.741809
C       -1.323906        0.312012        1.269169
F       -0.232728        0.185977        2.032526
C       -2.195520        1.360608        1.513536
H       -1.963037        2.061108        2.307501
F       -2.963567       -1.368338       -1.446176
N       -0.785707       -1.817576        0.117034
N        0.456243       -1.789125       -0.026703
C        1.187672       -0.634762       -0.286118
C        2.504684       -0.535709        0.161752
C        0.978749        0.521580       -1.101833
N        2.077750        1.261324       -1.119521
N        2.972029        0.624081       -0.332922
C        4.259500        1.226752       -0.099532
H        4.347177        1.584034        0.931417
H        5.062390        0.512124       -0.299287
H        4.345999        2.070027       -0.783150
C        3.269297       -1.457110        1.035181
H        3.351085       -1.074213        2.058821
H        2.741949       -2.412650        1.073489
H        4.282847       -1.625548        0.657621
C       -0.175438        0.905912       -1.961875
H       -0.655491        0.025663       -2.398107
H       -0.938848        1.449574       -1.395976
H        0.179807        1.551627       -2.767578
H       -4.036158        2.294648        0.922703
30
4pzMeF2-trans-m ; E = -882.203494870 Hartree
C       -2.709970       -1.251482       -0.081650
C       -4.091564       -1.189299       -0.105679
C       -1.885841       -0.116776        0.013539
H       -4.660442       -2.107794       -0.190045
C       -4.702973        0.056973       -0.018554
C       -2.553970        1.119006        0.103809
F       -1.857830        2.246210        0.227987
C       -3.936628        1.212580        0.090185
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H       -4.388637        2.194930        0.168100
F       -2.122339       -2.447869       -0.163865
N       -0.513182       -0.375120        0.049836
N        0.240897        0.631123       -0.069813
C        1.589065        0.354421       -0.032598
C        2.312762       -0.845318        0.053948
C        2.569844        1.382864       -0.100267
N        3.787207        0.871673       -0.056131
N        3.605057       -0.470450        0.036325
C        4.759881       -1.330682        0.078887
H        5.634627       -0.685952        0.147649
H        4.720202       -1.989670        0.950824
H        4.829920       -1.942403       -0.826346
C        1.890669       -2.267148        0.139126
H        2.121822       -2.687170        1.125852
H        0.814140       -2.333129       -0.013149
H        2.406609       -2.880159       -0.608341
C        2.337485        2.848268       -0.198797
H        1.739569        3.088909       -1.082518
H        1.783455        3.215531        0.670142
H        3.293285        3.371789       -0.258984
H       -5.785448        0.129024       -0.033492
30
4pzMeF2-trans-n ; E = -882.205206512 Hartree
C       -2.892762        1.048922       -0.125147
C       -4.252092        0.791910       -0.154822
C       -1.919081        0.043902        0.008620
H       -4.942630        1.619103       -0.270268
C       -4.684636       -0.524075       -0.033007
C       -2.409770       -1.269727        0.132732
F       -1.565305       -2.287536        0.297215
C       -3.765199       -1.557214        0.115098
H       -4.075879       -2.590466        0.221355
F       -2.478545        2.310997       -0.240644
N       -0.593766        0.489986        0.046516
N        0.283732       -0.412952       -0.061471
C        1.578495        0.041567       -0.010062
C        2.657614       -0.838023       -0.110594
C        2.156919        1.342648        0.123053
N        3.475279        1.252587        0.102983
N        3.757050       -0.068580       -0.042618
C        5.132275       -0.494734       -0.045597
H        5.423641       -0.907217        0.926264
H        5.293524       -1.251515       -0.817226
H        5.743353        0.381038       -0.260359
C        2.656516       -2.313150       -0.258881
H        3.171723       -2.805373        0.573261
H        1.619766       -2.654413       -0.278397
H        3.145911       -2.628320       -1.187328
C        1.478896        2.657460        0.261768
H        0.790586        2.831047       -0.569956
H        0.866544        2.684271        1.167922
H        2.225250        3.453780        0.300158
H       -5.746256       -0.747279       -0.051406
34
4pzMeOMe1A-cis-m ; E = -798.306503177 Hartree
C       -2.391399       -0.208933       -0.124109
C       -3.153075        0.534140        0.775891
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C       -1.192972       -0.811408        0.301792
H       -4.072972        1.009562        0.455588
C       -2.730537        0.668783        2.097731
C       -0.786829       -0.665710        1.626866
C       -1.550411        0.071922        2.525797
H       -1.227563        0.169105        3.557312
N       -0.554009       -1.729436       -0.575761
N        0.676228       -1.702555       -0.793403
C        1.504076       -0.642028       -0.408140
C        1.335981        0.742008       -0.492353
C        2.855963       -0.835156       -0.020190
N        3.459523        0.328056        0.166598
N        2.531686        1.262266       -0.134825
C        2.913787        2.651487       -0.127857
H        2.991693        3.049547       -1.145330
H        2.192804        3.248765        0.436386
H        3.889052        2.709042        0.353234
C        0.199629        1.576513       -0.956900
H        0.551647        2.471890       -1.477804
H       -0.429053        1.006576       -1.645119
H       -0.437390        1.888710       -0.120632
C        3.544816       -2.132460        0.212693
H        3.254938       -2.575001        1.172033
H        3.272494       -2.847601       -0.568647
H        4.626717       -1.987292        0.216715
H       -3.335143        1.244690        2.791675
H        0.129224       -1.152164        1.946469
O       -2.679618       -0.361598       -1.438101
C       -3.900987        0.162681       -1.905264
H       -4.755411       -0.266958       -1.367929
H       -3.932838        1.256211       -1.814512
H       -3.963498       -0.111649       -2.958632
34
4pzMeOMe1A-cis-n ; E = -798.307030260 Hartree
C        2.538774       -0.227939       -0.116983
C        3.335706        0.902945        0.047987
C        1.305241       -0.121279       -0.786947
H        4.280795        0.836928        0.574399
C        2.914741        2.131119       -0.461257
C        0.903263        1.112680       -1.293387
C        1.702530        2.240152       -1.131958
H        1.381041        3.194784       -1.535615
N        0.611350       -1.314471       -1.111717
N       -0.614662       -1.451546       -0.914265
C       -1.396517       -0.580717       -0.145781
C       -2.760125       -0.471494       -0.416201
C       -1.198271        0.144560        1.071355
N       -2.347146        0.665154        1.478409
N       -3.268433        0.305884        0.558575
C       -4.625920        0.763910        0.702375
H       -4.895412        1.461126       -0.097444
H       -5.324187       -0.077947        0.690577
H       -4.689985        1.273413        1.662756
C       -3.545050       -1.049538       -1.533453
H       -3.813276       -0.296319       -2.283450
H       -2.934713       -1.812947       -2.020917
H       -4.472594       -1.511017       -1.179103
C        0.013782        0.289155        1.923655
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H        0.587389       -0.641662        1.954060
H        0.679952        1.070886        1.544759
H       -0.293472        0.552824        2.937886
H        3.546317        3.004186       -0.328443
H       -0.040294        1.173131       -1.826121
O        2.826041       -1.454000        0.376326
C        4.068718       -1.626090        1.016551
H        4.904457       -1.387362        0.346869
H        4.145839       -1.009063        1.921076
H        4.120812       -2.678885        1.295359
34
4pzMeOMe1A-trans-m ; E = -798.325364831 Hartree
C        2.779610        0.516603        0.000171
C        4.120126        0.124404        0.000148
C        1.766350       -0.468439       -0.000102
H        4.909762        0.866234        0.000372
C        4.451048       -1.227224       -0.000155
C        2.125348       -1.818876       -0.000419
C        3.457328       -2.203203       -0.000441
H        3.722582       -3.255708       -0.000697
N        0.443719        0.001839       -0.000129
N       -0.433580       -0.903733        0.000075
C       -1.740397       -0.460655        0.000042
C       -2.305972        0.822402       -0.000199
C       -2.843500       -1.357684        0.000262
N       -3.987686       -0.695217        0.000164
N       -3.637353        0.614640       -0.000109
C       -4.671448        1.616668       -0.000165
H       -5.624584        1.090164       -0.000590
H       -4.604341        2.249435        0.890298
H       -4.603789        2.249910       -0.890242
C       -1.706642        2.181925       -0.000489
H       -2.019085        2.751844        0.882874
H       -0.620624        2.091922       -0.000032
H       -2.018336        2.751133       -0.884585
C       -2.803532       -2.844622        0.000529
H       -2.274547       -3.222516       -0.879521
H       -2.274104       -3.222213        0.880433
H       -3.820338       -3.241660        0.000815
H        5.498415       -1.514602       -0.000176
H        1.320993       -2.546813       -0.000653
O        2.370938        1.805193        0.000434
C        3.360033        2.806849        0.000354
H        3.994669        2.751173        0.894094
H        3.994597        2.751114       -0.893431
H        2.825425        3.757446        0.000347
34
4pzMeOMe1A-trans-n ; E = -798.326208305 Hartree
C       -2.865808        0.346541        0.000134
C       -4.155442       -0.190649        0.000157
C       -1.750038       -0.521608       -0.000203
H       -5.021240        0.460739        0.000406
C       -4.336719       -1.570227       -0.000170
C       -1.960344       -1.902931       -0.000549
C       -3.242143       -2.431462       -0.000531
H       -3.390471       -3.506747       -0.000825
N       -0.488289        0.094162       -0.000292
N        0.486515       -0.707294        0.000020
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C         1.721142       -0.097852       -0.000052
C         2.908418       -0.830234        0.000077
C         2.120091        1.274623       -0.000524
N         3.439711        1.361365       -0.000676
N         3.896273        0.084853       -0.000464
C         5.318617       -0.133433        0.000903
H         5.764808        0.310515        0.894470
H         5.519749       -1.204940       -0.008293
H         5.767655        0.326419       -0.882995
C         3.099631       -2.301783        0.000829
H         3.645051       -2.644091        0.887088
H         2.114462       -2.771465        0.000953
H         3.645134       -2.645029       -0.885037
C         1.270652        2.493651       -0.000944
H         0.609510        2.506185       -0.872059
H         0.609329        2.506618        0.870020
H         1.905014        3.382915       -0.001118
H        -5.346352       -1.970570       -0.000160
H        -1.082577       -2.540225       -0.000840
O        -2.600236        1.670407        0.000417
C        -3.691707        2.559129        0.001072
H        -4.316921        2.435787       -0.892640
H        -4.316600        2.434855        0.894877
H        -3.262226        3.561578        0.001512
34
4pzMeOMe1B-cis-m ; E = -798.307178815 Hartree
C        -2.715505        0.322438       -1.236962
C        -3.600422        0.812581       -0.282965
C        -1.598196       -0.424795       -0.870970
H        -4.449080        1.417241       -0.585548
C        -3.389995        0.508044        1.056592
C        -1.426263       -0.785998        0.483150
C        -2.316856       -0.295608        1.438217
H        -2.184577       -0.548630        2.483930
N        -0.783886       -0.922766       -1.928585
N         0.464867       -0.845044       -1.909571
C         1.169424       -0.133532       -0.935001
C         0.993948        1.145565       -0.410494
C         2.363443       -0.624609       -0.348304
N         2.863783        0.257629        0.502645
N         2.033209        1.321104        0.440967
C         2.378132        2.518260        1.163641
H         2.756974        3.297425        0.493027
H         1.512105        2.905100        1.707110
H         3.160392        2.247932        1.871660
C         0.004795        2.214989       -0.702023
H         0.470687        3.204842       -0.680048
H        -0.423000        2.064847       -1.694415
H        -0.826814        2.205609        0.012270
C         2.971188       -1.965279       -0.553226
H         2.340917       -2.750907       -0.122668
H         3.064005       -2.182906       -1.621330
H         3.956648       -2.007699       -0.085677
H        -4.072355        0.876263        1.816693
O        -0.399102       -1.616980        0.761479
C        -0.069280       -1.838742        2.113270
H         0.133769       -0.894799        2.633420
H        -0.862841       -2.383104        2.640169
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H        0.838202       -2.442702        2.105508
H       -2.854504        0.530972       -2.293675
34
4pzMeOMe1B-cis-n ; E = -798.307416181 Hartree
C        2.881749       -1.113645       -0.636718
C        3.823360       -0.709401        0.302175
C        1.725134       -0.371292       -0.865541
H        4.701550       -1.318001        0.491190
C        3.630694        0.485493        0.985733
C        1.563522        0.869174       -0.212166
C        2.514920        1.278104        0.722436
H        2.392893        2.218289        1.247761
N        0.854763       -0.834235       -1.887634
N       -0.385030       -0.912343       -1.740596
C       -1.056719       -0.719148       -0.533144
C       -2.342906       -0.185029       -0.554302
C       -0.817466       -1.065217        0.833929
N       -1.871349       -0.740374        1.571273
N       -2.764863       -0.185539        0.724535
C       -4.023549        0.290599        1.236019
H       -4.152392        1.357794        1.030337
H       -4.861456       -0.259055        0.795991
H       -4.011926        0.127077        2.312651
C       -3.122559        0.335081       -1.702554
H       -3.143334        1.431155       -1.721459
H       -2.644805       -0.007277       -2.623013
H       -4.158484       -0.018806       -1.684101
C        0.315684       -1.791800        1.473283
H        0.660402       -2.615246        0.842454
H        1.175501       -1.139260        1.651760
H       -0.020448       -2.196690        2.430217
H        4.357124        0.821061        1.719555
O        0.480891        1.599722       -0.562191
C        0.194648        2.756475        0.186769
H        0.064623        2.520821        1.250375
H        0.976843        3.518075        0.075749
H       -0.741695        3.148268       -0.212442
H        3.004751       -2.034912       -1.198059
34
4pzMeOMe1B-trans-m ; E = -798.319731027 Hartree
C        2.407785       -2.004643        0.018154
C        3.785313       -2.161708        0.018812
C        1.794672       -0.746725        0.006732
H        4.226327       -3.152869        0.028386
C        4.586290       -1.026181        0.006648
C        2.625140        0.407981       -0.006015
C        4.013069        0.242026       -0.005951
H        4.659891        1.111071       -0.015704
N        0.393480       -0.815231        0.007689
N       -0.232122        0.280286        0.009113
C       -1.609384        0.184731        0.007073
C       -2.506210       -0.892137       -0.006585
C       -2.425222        1.349344        0.017065
N       -3.707634        1.028253        0.010392
N       -3.730380       -0.327330       -0.003491
C       -4.999602       -1.006968       -0.018970
H       -5.771464       -0.239282        0.005908
H       -5.113036       -1.608188       -0.926650
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H       -5.105761       -1.659428        0.853270
C       -2.306446       -2.363876       -0.023605
H       -2.775710       -2.819945       -0.903430
H       -1.237964       -2.572432       -0.042227
H       -2.744425       -2.835592        0.864253
C       -1.969249        2.764905        0.034875
H       -1.380912        2.972923        0.933694
H       -1.323862        2.975332       -0.822977
H       -2.831312        3.434114        0.009495
H        5.668575       -1.116566        0.006588
O        2.033507        1.617212       -0.018681
C        2.854407        2.761191       -0.034535
H        3.490969        2.817793        0.857661
H        3.487638        2.795554       -0.930242
H        2.173448        3.612946       -0.043736
H        1.742750       -2.862622        0.027056
34
4pzMeOMe1B-trans-n ; E = -798.321884117 Hartree
C        2.653475       -1.818791        0.003945
C        4.039814       -1.799378        0.005304
C        1.885220       -0.649021        0.001397
H        4.603373       -2.726412        0.007275
C        4.689525       -0.571172        0.004075
C        2.561616        0.601616        0.000142
C        3.959179        0.613874        0.001529
H        4.491021        1.557698        0.000618
N        0.505390       -0.902737        0.000353
N       -0.261926        0.099119       -0.001873
C       -1.605492       -0.206656       -0.001999
C       -2.568215        0.801769       -0.005230
C       -2.341254       -1.431725       -0.003110
N       -3.640120       -1.180171       -0.006553
N       -3.756966        0.171448       -0.011770
C       -5.067566        0.764952        0.021356
H       -5.277722        1.213050        0.998421
H       -5.161793        1.534338       -0.750070
H       -5.785706       -0.031254       -0.170101
C       -2.385072        2.272995       -0.002285
H       -2.834265        2.738143        0.882431
H       -1.312753        2.478754       -0.000833
H       -2.831416        2.740988       -0.887139
C       -1.838377       -2.830539       -0.005044
H       -1.208474       -3.016320       -0.879662
H       -1.210417       -3.019228        0.870307
H       -2.682818       -3.523417       -0.007196
H        5.774495       -0.522543        0.005082
O        1.821775        1.729155       -0.002356
C        2.496686        2.964879       -0.003921
H        3.120448        3.089706        0.890386
H        3.122207        3.086472       -0.897442
H        1.718107        3.728733       -0.006069
H        2.099637       -2.752384        0.004801
38
4pzMeOMe2-cis-m ; E = -912.710258974 Hartree
C        2.437917       -0.111961       -0.239164
C        3.134341        0.312706        0.893008
C        1.203535        0.461165       -0.581779
H        4.076662       -0.143076        1.170705
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C         2.597979        1.333232        1.669903
C         0.695202        1.510275        0.204786
C         1.389553        1.934750        1.340181
H         1.000614        2.736771        1.955281
N         0.636442        0.113888       -1.842272
N        -0.555901       -0.243830       -1.952850
C        -1.361257       -0.522741       -0.845348
C        -1.121037       -1.293025        0.290143
C        -2.721126       -0.131252       -0.759639
N        -3.268419       -0.585134        0.357371
N        -2.293834       -1.292894        0.968622
C        -2.608311       -2.027739        2.165976
H        -2.698357       -3.101494        1.966962
H        -1.840834       -1.869688        2.928323
H        -3.564107       -1.652302        2.529163
C         0.060814       -2.080687        0.723291
H        -0.237060       -3.049612        1.136820
H         0.722856       -2.259837       -0.126584
H         0.646045       -1.546590        1.481546
C        -3.465280        0.728241       -1.717069
H        -3.067625        1.748591       -1.718791
H        -3.359311        0.345279       -2.736520
H        -4.523087        0.761007       -1.449580
H         3.135021        1.669065        2.551649
O        -0.459772        2.064369       -0.224945
C        -1.072373        3.035816        0.590221
H        -1.295365        2.638418        1.587803
H        -0.450359        3.934399        0.686816
H        -2.007113        3.297599        0.093834
O         2.833132       -1.127301       -1.043988
C         4.093701       -1.705374       -0.796964
H         4.896355       -0.959611       -0.848698
H         4.126560       -2.201166        0.181870
H         4.242256       -2.448945       -1.580505
38
4pzMeOMe2-cis-n ; E = -912.709808065 Hartree
C         2.582856       -0.277796       -0.189697
C         3.346970        0.480296        0.697520
C         1.332573        0.181349       -0.634608
H         4.299983        0.117529        1.061980
C         2.861749        1.711666        1.123636
C         0.877347        1.442280       -0.212169
C         1.639148        2.200647        0.680293
H         1.290429        3.168023        1.019928
N         0.689101       -0.548557       -1.669062
N        -0.511036       -0.889546       -1.596828
C        -1.285731       -0.781155       -0.440757
C        -2.652181       -0.538036       -0.547353
C        -1.053162       -1.014924        0.949182
N        -2.190698       -0.901150        1.622672
N        -3.134498       -0.587307        0.709673
C        -4.488325       -0.359427        1.141965
H        -4.796208        0.673664        0.950530
H        -5.181537       -1.035812        0.632908
H        -4.517016       -0.552879        2.213338
C        -3.459163       -0.238505       -1.754114
H        -3.718655        0.824728       -1.821086
H        -2.865936       -0.495737       -2.634239
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H       -4.391958       -0.811624       -1.773069
C        0.181492       -1.444052        1.663524
H        0.783233       -2.111939        1.041035
H        0.812479       -0.588989        1.926967
H       -0.098421       -1.965175        2.581788
H        3.450319        2.304224        1.817229
O       -0.298806        1.852887       -0.739901
C       -0.835325        3.071530       -0.285998
H       -1.015765        3.053020        0.796096
H       -0.182567        3.919430       -0.529220
H       -1.785883        3.193205       -0.807000
O        2.923325       -1.510010       -0.632316
C        4.186516       -2.011471       -0.263266
H        4.996787       -1.351664       -0.597582
H        4.263448       -2.153296        0.822405
H        4.282445       -2.978219       -0.758407
38
4pzMeOMe2-trans-m ; E = -912.720681427 Hartree
C       -2.410458       -1.223497       -0.099919
C       -3.801750       -1.138858       -0.129733
C       -1.607427       -0.061987       -0.003211
H       -4.412961       -2.027521       -0.220938
C       -4.402844        0.110314       -0.042085
C       -2.252732        1.195806        0.090094
C       -3.649028        1.269558        0.074349
H       -4.148470        2.227242        0.148225
N       -0.236330       -0.310276        0.090047
N        0.538334        0.634314       -0.225057
C        1.882536        0.333207       -0.108516
C        2.566553       -0.859654        0.158894
C        2.893948        1.311765       -0.301107
N        4.096954        0.779870       -0.160797
N        3.873332       -0.528601        0.115016
C        5.000090       -1.408830        0.283959
H        5.891001       -0.783337        0.316331
H        4.914464       -1.973043        1.216928
H        5.083562       -2.113244       -0.550553
C        2.091896       -2.242742        0.420830
H        2.195523       -2.500325        1.482431
H        1.033259       -2.310016        0.168252
H        2.663953       -2.977912       -0.155963
C        2.703696        2.756468       -0.599598
H        2.030139        2.889237       -1.450682
H        2.249004        3.275048        0.250675
H        3.666099        3.221807       -0.821088
H       -5.486131        0.182015       -0.064607
O       -1.465924        2.280100        0.229873
C       -2.082801        3.523952        0.461284
H       -2.694741        3.838955       -0.393440
H       -2.707298        3.508274        1.363659
H       -1.268864        4.236894        0.597868
O       -1.734542       -2.392810       -0.181280
C       -2.485020       -3.581788       -0.243353
H       -3.127651       -3.703758        0.637854
H       -3.105345       -3.623891       -1.147746
H       -1.757802       -4.394181       -0.271736
38
4pzMeOMe2-trans-n ; E = -912.722044178 Hartree
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C        2.606426       -0.984225       -0.152405
C        3.967134       -0.684085       -0.210333
C        1.636707        0.037749       -0.014087
H        4.705380       -1.466106       -0.333373
C        4.370294        0.641002       -0.109044
C        2.082382        1.377685        0.092745
C        3.449498        1.667396        0.048669
H        3.797331        2.689204        0.132255
N        0.322349       -0.420905        0.106502
N       -0.591480        0.394013       -0.198658
C       -1.865330       -0.110217       -0.035874
C       -2.992164        0.664902       -0.300078
C       -2.366822       -1.387458        0.361333
N       -3.689970       -1.381894        0.337397
N       -4.048329       -0.136869       -0.065735
C       -5.444331        0.201903       -0.144181
H       -5.749682        0.838155        0.693784
H       -5.661057        0.721331       -1.081595
H       -6.005310       -0.731146       -0.107713
C       -3.077709        2.077368       -0.743276
H       -3.611704        2.701328       -0.017625
H       -2.060621        2.459447       -0.851619
H       -3.592379        2.172824       -1.706222
C       -1.611237       -2.607637        0.748172
H       -0.889629       -2.879215       -0.026978
H       -1.021335       -2.428077        1.651982
H       -2.307241       -3.431524        0.922461
H        5.428622        0.880121       -0.153455
O        1.141681        2.327512        0.275972
C        1.571265        3.639072        0.552091
H        2.214664        3.679512        1.440238
H        2.106705        4.079561       -0.298670
H        0.664302        4.215904        0.737898
O        2.116285       -2.240035       -0.242793
C        3.037436       -3.299943       -0.334634
H        3.637174       -3.239271       -1.251939
H        3.710396       -3.330341        0.531793
H        2.441383       -4.213005       -0.357788
42
4pzMePyr1A-cis-m ; E = -895.077124832 Hartree
C       -3.023194       -0.385740        1.187924
C       -3.919369       -0.493480        0.135698
C       -1.737604        0.132412        1.006605
H       -4.898228       -0.935581        0.289059
C       -3.531895       -0.032954       -1.121839
C       -1.389359        0.728769       -0.235037
C       -2.297321        0.575171       -1.301570
H       -2.038811        0.969438       -2.277823
N       -0.911583        0.063921        2.162313
N        0.282526       -0.329870        2.128181
C        0.901743       -0.865002        0.995377
C        0.477225       -1.785454        0.032260
C        2.276445       -0.638715        0.714218
N        2.653719       -1.309567       -0.363874
N        1.559526       -1.999952       -0.749686
C        1.675433       -2.928570       -1.845365
H        1.676129       -3.965579       -1.492600
H        0.855795       -2.793482       -2.555750
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H        2.623648       -2.719603       -2.338531
C       -0.788477       -2.544318       -0.139160
H       -0.596152       -3.548516       -0.528489
H       -1.295491       -2.644996        0.820980
H       -1.480801       -2.033198       -0.817264
C        3.221954        0.232714        1.464003
H        3.214250        1.264085        1.093037
H        2.941210        0.260430        2.520190
H        4.240658       -0.148410        1.365260
H       -4.208677       -0.115564       -1.967439
C        1.196255        3.292262       -0.130537
C        0.349041        2.281182        0.642019
N       -0.219626        1.429950       -0.400580
C        0.255188        1.812440       -1.717779
C        1.555429        2.539123       -1.410156
H        0.602017        4.179380       -0.376993
H       -0.447823        2.746742        1.234493
H        0.391823        0.926125       -2.347585
H        2.346286        1.805685       -1.219294
H       -0.449654        2.489210       -2.230940
H        1.876014        3.192649       -2.225208
H        2.067813        3.622063        0.441009
H        0.966597        1.706406        1.340526
H       -3.267493       -0.757706        2.178908
42
4pzMePyr1A-cis-n ; E = -895.077080682 Hartree
C       -3.143966       -0.778193        0.977660
C       -4.026806       -0.703564       -0.088083
C       -1.876122       -0.192423        0.919176
H       -4.989674       -1.201330       -0.041278
C       -3.646313        0.010667       -1.223421
C       -1.536343        0.643902       -0.176574
C       -2.431840        0.680801       -1.262348
H       -2.177390        1.262664       -2.140801
N       -1.056954       -0.446161        2.050472
N        0.148846       -0.788325        1.953538
C        0.790441       -1.093393        0.749791
C        2.143724       -0.796684        0.595934
C        0.435497       -1.831096       -0.423413
N        1.484803       -1.932252       -1.228052
N        2.494126       -1.280538       -0.612576
C        3.769894       -1.171826       -1.269710
H        3.994071       -0.132481       -1.532639
H        4.572206       -1.557571       -0.633938
H        3.711385       -1.769139       -2.178527
C        3.068795       -0.093813        1.518122
H        3.270326        0.937567        1.203504
H        2.608953       -0.062363        2.508658
H        4.031080       -0.610815        1.593462
C       -0.817603       -2.559548       -0.766057
H       -1.226888       -3.064647        0.112713
H       -1.593148       -1.889223       -1.146004
H       -0.594184       -3.306399       -1.530902
H       -4.312637        0.074086       -2.078779
C        0.940297        3.236516        0.444507
C        0.137658        2.062164        1.003618
N       -0.382268        1.394757       -0.186592
C        0.099824        2.020431       -1.403881
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C        1.356077        2.742215       -0.939553
H        0.302054        4.121412        0.342890
H       -0.682668        2.373503        1.661182
H        0.288895        1.262868       -2.172721
H        2.183323        2.027591       -0.858723
H       -0.622970        2.747917       -1.811857
H        1.658163        3.543702       -1.618231
H        1.783993        3.504791        1.085926
H        0.778500        1.395554        1.592289
H       -3.382557       -1.346979        1.871638
42
4pzMePyr1A-trans-m ; E = -895.088860267 Hartree
C        1.693101       -2.763648       -0.034912
C        2.962535       -3.198004        0.299470
C        1.342997       -1.405847       -0.045482
H        3.195698       -4.256861        0.333026
C        3.921986       -2.239648        0.624320
C        2.359712       -0.419156        0.143734
C        3.630916       -0.888101        0.542632
H        4.414912       -0.173763        0.762555
N       -0.040105       -1.213335       -0.178984
N       -0.514923       -0.185905        0.381077
C       -1.889029       -0.032966        0.289503
C       -2.902342       -0.786908       -0.314384
C       -2.552793        1.069394        0.892659
N       -3.858156        1.005934        0.685855
N       -4.044125       -0.119641       -0.042522
C       -5.378200       -0.484585       -0.442419
H       -5.477814       -0.483152       -1.532647
H       -5.642762       -1.476916       -0.064440
H       -6.051786        0.257695       -0.016865
C       -2.882746       -2.046945       -1.101129
H       -3.375876       -1.920249       -2.072018
H       -1.847826       -2.346848       -1.258849
H       -3.402094       -2.855087       -0.571670
C       -1.935045        2.185983        1.657886
H       -1.246629        1.803738        2.416112
H       -1.354331        2.842204        0.999557
H       -2.712504        2.781957        2.139720
H        4.921973       -2.544715        0.919724
C        1.838040        2.744692       -1.531826
C        1.203212        1.448582       -1.037702
N        2.170953        0.918948       -0.084979
C        3.233286        1.878812        0.171907
C        2.650894        3.195332       -0.322153
H        2.506957        2.545975       -2.377253
H        1.015845        0.724724       -1.839615
H        3.497397        1.894444        1.235580
H        1.990568        3.623829        0.440005
H        4.145482        1.628771       -0.395705
H        3.423867        3.930633       -0.558655
H        1.091439        3.474396       -1.855359
H        0.242117        1.632196       -0.541895
H        0.890710       -3.466896       -0.237062
42
4pzMePyr1A-trans-n ; E = -895.090304196 Hartree
C       -2.035689       -2.621733       -0.038764
C       -3.329323       -2.878979       -0.456222
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C       -1.510843       -1.323495        0.014034
H       -3.699011       -3.896763       -0.520826
C       -4.131063       -1.798613       -0.820532
C       -2.372258       -0.208547       -0.219803
C       -3.668172       -0.498150       -0.698331
H       -4.335617        0.316549       -0.951754
N       -0.124924       -1.316838        0.240616
N        0.515525       -0.370470       -0.296933
C        1.884049       -0.414909       -0.105124
C        2.723175        0.541961       -0.671986
C        2.746402       -1.295214        0.615849
N        4.003964       -0.899460        0.493023
N        3.969789        0.210161       -0.283370
C        5.203416        0.860088       -0.639062
H        5.452393        0.694318       -1.692750
H        5.140198        1.936174       -0.454214
H        5.984799        0.429686       -0.014125
C        2.385122        1.703949       -1.529688
H        2.888524        1.654223       -2.501654
H        1.306279        1.702492       -1.698716
H        2.664783        2.654167       -1.059816
C        2.403170       -2.496368        1.421873
H        1.690231       -2.245640        2.212485
H        1.917153       -3.255572        0.802598
H        3.311337       -2.911923        1.864270
H       -5.143024       -1.964488       -1.179345
C       -1.548395        2.821143        1.569979
C       -1.054767        1.465296        1.073913
N       -2.015200        1.091451        0.040772
C       -2.934410        2.183727       -0.237228
C       -2.222051        3.402567        0.330926
H       -2.288343        2.690068        2.367992
H       -1.020096        0.704128        1.862202
H       -3.136330        2.261715       -1.311809
H       -1.468098        3.762736       -0.378065
H       -3.900760        2.035934        0.274141
H       -2.909161        4.224432        0.546742
H       -0.737059        3.440619        1.960679
H       -0.045009        1.533014        0.651436
H       -1.347446       -3.426130        0.202757
42
4pzMePyr1B-cis-m ; E = -895.075168267 Hartree
C        1.805844        0.762185       -0.350033
C        2.143958        2.101401       -0.050625
C        0.532047        0.540136       -0.941075
H        3.090343        2.315701        0.430144
C        1.299730        3.156373       -0.357170
C       -0.295729        1.622880       -1.253513
C        0.071594        2.929069       -0.974663
H       -0.580527        3.752910       -1.244642
N        0.183710       -0.755040       -1.405012
N       -0.958888       -1.246283       -1.247633
C       -1.937042       -0.711119       -0.399656
C       -1.877315       -0.157188        0.883466
C       -3.321209       -0.874095       -0.671681
N       -4.055871       -0.422823        0.332843
N       -3.167659       -0.007676        1.261304
C       -3.661102        0.470725        2.527846
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H       -3.432208       -0.231073        3.336948
H       -3.233969        1.447784        2.769246
H       -4.741776        0.561673        2.429528
C       -0.739569        0.173953        1.779167
H       -1.030310        0.109769        2.831431
H        0.090128       -0.517671        1.617620
H       -0.355668        1.181757        1.581096
C       -3.928505       -1.426261       -1.911813
H       -3.906182       -0.696908       -2.728981
H       -3.365859       -2.302424       -2.246139
H       -4.968560       -1.703541       -1.729764
H        1.613442        4.168247       -0.117174
C        3.561686       -2.286820        0.687188
C        2.486431       -1.677832       -0.203171
N        2.673036       -0.242409       -0.008334
C        3.996298        0.057245        0.521271
C        4.709129       -1.292503        0.545392
H        3.213595       -2.318923        1.726117
H        2.625424       -1.964790       -1.252922
H        4.521873        0.786303       -0.108982
H        5.449698       -1.356441        1.346405
H        1.477476       -1.985703        0.077016
H        3.825835       -3.303303        0.385289
H        5.227585       -1.456502       -0.405604
H        3.921983        0.490834        1.530723
H       -1.240095        1.413023       -1.745119
42
4pzMePyr1B-cis-n ; E = -895.076317642 Hartree
C        1.964644        0.765167       -0.273478
C        2.409394        2.045058        0.124657
C        0.642571        0.675486       -0.788136
H        3.401056        2.156454        0.545546
C        1.611503        3.170197       -0.009407
C       -0.138743        1.827312       -0.923437
C        0.328495        3.075055       -0.544113
H       -0.289744        3.956816       -0.674666
N        0.202064       -0.534368       -1.377213
N       -0.959905       -0.979314       -1.227225
C       -1.875744       -0.514828       -0.273166
C       -3.240293       -0.675050       -0.509375
C       -1.784809       -0.071756        1.085828
N       -2.998966        0.042949        1.605794
N       -3.861403       -0.297493        0.625181
C       -5.277514       -0.252918        0.880132
H       -5.778336        0.437260        0.194224
H       -5.728072       -1.245165        0.777557
H       -5.405557        0.096562        1.903588
C       -3.931991       -1.143825       -1.734246
H       -4.411312       -0.321985       -2.279130
H       -3.188748       -1.599686       -2.392158
H       -4.704315       -1.885222       -1.504175
C       -0.600104        0.176631        1.953586
H        0.149807       -0.612159        1.842504
H       -0.110267        1.123701        1.706873
H       -0.925821        0.206141        2.995588
H        2.003674        4.133573        0.303650
C        3.514039       -2.451244        0.517237
C        2.426915       -1.725166       -0.267042
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N         2.787962       -0.317280       -0.116090
C         4.151707       -0.161186        0.365494
C         4.735611       -1.567591        0.286873
H         3.259210       -2.470603        1.583185
H         2.422643       -2.027592       -1.320449
H         4.709235        0.556972       -0.248926
H         5.537250       -1.725557        1.012571
H         1.424825       -1.915840        0.124102
H         3.650999       -3.482332        0.181910
H         5.144378       -1.747021       -0.713668
H         4.162641        0.214156        1.401647
H        -1.125897        1.722022       -1.361329
42
4pzMePyr1B-trans-m ; E = -895.094123380 Hartree
C        -2.448178       -0.489670       -0.150136
C        -3.631466       -1.237765       -0.348815
C        -1.219858       -1.211088       -0.153862
H        -4.586919       -0.728841       -0.373973
C        -3.606538       -2.612989       -0.495283
C        -1.227762       -2.606880       -0.288807
C        -2.400851       -3.316519       -0.453608
H        -2.382306       -4.394610       -0.575846
N        -0.021073       -0.484053       -0.115939
N         1.004705       -1.167598        0.162928
C         2.207576       -0.495944        0.085082
C         2.570297        0.714457       -0.517247
C         3.413166       -1.021757        0.623968
N         4.427559       -0.205281        0.390820
N         3.897520        0.832064       -0.299300
C         4.772545        1.875358       -0.768209
H         4.906936        1.826447       -1.854208
H         4.379222        2.860209       -0.501775
H         5.735337        1.724465       -0.282099
C         1.786409        1.699681       -1.302212
H         2.369944        2.112824       -2.131123
H         0.889920        1.214852       -1.691387
H         1.451858        2.537579       -0.677558
C         3.586320       -2.290693        1.380241
H         3.123885       -2.227551        2.370671
H         3.105688       -3.120659        0.854899
H         4.648809       -2.507489        1.505931
H        -4.543213       -3.142947       -0.644495
C        -2.315688        2.868381        1.245994
C        -1.515057        1.707741        0.663798
N        -2.531616        0.865957        0.035025
C        -3.813978        1.551097       -0.036366
C        -3.468909        3.004939        0.257614
H        -2.701852        2.601970        2.236576
H        -0.785404        2.061855       -0.072564
H        -4.279206        1.414356       -1.019930
H        -4.322681        3.563485        0.649128
H        -0.957259        1.144692        1.417017
H        -1.716871        3.777053        1.349691
H        -3.126552        3.502768       -0.656606
H        -4.515931        1.161377        0.719249
H        -0.261240       -3.099558       -0.289245
42
4pzMePyr1B-trans-n ; E = -895.095381617 Hartree
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C       -2.467063        0.634752        0.085312
C       -3.556728        1.533275        0.172619
C       -1.159145        1.199394        0.134088
H       -4.567773        1.146389        0.151487
C       -3.370958        2.899954        0.268276
C       -1.005048        2.591019        0.220101
C       -2.086476        3.447143        0.283838
H       -1.939206        4.518708        0.371628
N       -0.048310        0.340790        0.192268
N        1.050936        0.896193       -0.088882
C        2.181290        0.122334        0.068377
C        3.425583        0.578289       -0.368634
C        2.440183       -1.145429        0.673881
N        3.731721       -1.429377        0.603935
N        4.306731       -0.383139       -0.034215
C        5.724603       -0.398524       -0.280828
H        5.938694       -0.412115       -1.354375
H        6.209226        0.474655        0.166610
H        6.117864       -1.304885        0.177343
C        3.781134        1.838227       -1.064567
H        4.174185        1.652406       -2.070723
H        2.879880        2.447246       -1.154033
H        4.537157        2.408460       -0.513086
C        1.502275       -2.082590        1.345456
H        0.816919       -1.542027        2.003209
H        0.885025       -2.614157        0.613784
H        2.068709       -2.818195        1.920870
H       -4.241905        3.546187        0.334153
C       -2.663297       -2.817283       -1.068106
C       -1.771106       -1.718494       -0.500923
N       -2.718516       -0.703858       -0.049615
C       -4.079059       -1.220315       -0.025408
C       -3.903430       -2.725278       -0.185463
H       -2.925506       -2.591804       -2.108224
H       -1.167015       -2.089761        0.333808
H       -4.586794       -0.951223        0.908781
H       -4.787732       -3.202998       -0.614465
H       -1.075996       -1.301316       -1.234412
H       -2.181166       -3.798047       -1.045176
H       -3.707186       -3.185986        0.789138
H       -4.674574       -0.807671       -0.856271
H        0.012712        2.963040        0.267394
54
4pzMePyr2-cis-m ; E = -1106.24555520 Hartree
C        2.145084        0.570763        0.535724
C        2.312241        0.927915        1.891271
C        0.828141        0.642084       -0.011082
H        3.276466        0.814842        2.367362
C        1.242004        1.382498        2.643279
C       -0.222836        1.248798        0.732837
C       -0.014543        1.559038        2.087225
H       -0.814995        1.979231        2.681990
N        0.650669        0.159407       -1.329546
N       -0.296955       -0.605306       -1.660779
C       -1.189326       -1.182243       -0.754828
C       -1.003516       -1.783546        0.493590
C       -2.547427       -1.431629       -1.089479
N       -3.164428       -2.077902       -0.110967
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N       -2.214370       -2.287838        0.825053
C       -2.548051       -3.064690        1.991250
H       -2.090867       -4.059513        1.954464
H       -2.222490       -2.555685        2.902316
H       -3.631864       -3.171034        2.000707
C        0.209702       -2.012536        1.319699
H        0.134738       -2.949738        1.879388
H        1.093219       -2.070934        0.680856
H        0.378975       -1.193703        2.027332
C       -3.256115       -1.049153       -2.341341
H       -3.648876       -0.026974       -2.299542
H       -2.565300       -1.098573       -3.187547
H       -4.097219       -1.723769       -2.514986
H        1.401917        1.634932        3.687965
C       -2.842822        2.837161       -1.225488
C       -1.572210        1.990062       -1.239305
N       -1.433266        1.538759        0.142531
C       -2.573686        1.942871        0.946698
C       -3.652487        2.216759       -0.089138
H       -2.605809        3.879935       -0.985116
H       -0.679425        2.543711       -1.552874
H       -2.842822        1.152780        1.656626
H       -4.106352        1.272122       -0.407114
C        4.682171       -0.978991       -1.646630
C        3.313166       -0.319854       -1.550470
N        3.232980        0.077941       -0.145602
C        4.560868        0.144289        0.456401
C        5.523244       -0.140252       -0.693217
H        4.622884       -2.014086       -1.290705
H        3.238773        0.548616       -2.218945
H        4.744750        1.129820        0.902509
H        6.437491       -0.635383       -0.356153
H        2.497390       -0.989886       -1.818602
H        5.064789       -0.993698       -2.670317
H        5.809932        0.799157       -1.178783
H        4.660892       -0.601538        1.259832
H       -2.362111        2.859672        1.522747
H       -4.443133        2.868400        0.291178
H       -3.358751        2.823296       -2.189305
H       -1.676226        1.146511       -1.932077
54
4pzMePyr2-cis-n ; E = -1106.24541809 Hartree
C        2.293676        0.670493        0.301270
C        2.543017        1.523255        1.396950
C        0.951486        0.579833       -0.177960
H        3.529759        1.565293        1.837600
C        1.525322        2.279488        1.953970
C       -0.045382        1.465576        0.317131
C        0.243817        2.273633        1.428091
H       -0.515166        2.921418        1.846687
N        0.706796       -0.343833       -1.217809
N       -0.281772       -1.127389       -1.224193
C       -1.159174       -1.298483       -0.151704
C       -2.491916       -1.625192       -0.394791
C       -1.005369       -1.399141        1.267427
N       -2.162881       -1.726062        1.826454
N       -3.051204       -1.831190        0.815504
C       -4.426937       -2.129660        1.112105
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H       -5.079472       -1.285288        0.865049
H       -4.765122       -3.011650        0.559951
H       -4.485648       -2.329620        2.181151
C       -3.213809       -1.750300       -1.684666
H       -3.858456       -0.887601       -1.892523
H       -2.473738       -1.820089       -2.485381
H       -3.842801       -2.646435       -1.708287
C        0.217101       -1.318543        2.114289
H        1.062740       -1.814930        1.629515
H        0.515003       -0.283832        2.304645
H        0.020110       -1.810436        3.069511
H        1.746909        2.912603        2.808673
C       -2.745566        2.316618       -1.966180
C       -1.478015        1.496749       -1.733623
N       -1.283942        1.549428       -0.287985
C       -2.384815        2.231641        0.368385
C       -3.507059        2.142343       -0.654249
H       -2.497209        3.374401       -2.109668
H       -0.599505        1.894115       -2.255224
H       -2.619061        1.748207        1.323439
H       -3.972697        1.151122       -0.609873
C        4.648570       -1.815681       -1.054982
C        3.295057       -1.131309       -1.205982
N        3.333099       -0.080454       -0.189427
C        4.692641        0.154036        0.278846
C        5.565009       -0.661927       -0.667908
H        4.607797       -2.552668       -0.244492
H        3.168392       -0.712724       -2.211783
H        4.939903        1.222518        0.251503
H        6.501859       -0.977430       -0.201642
H        2.458162       -1.810258       -1.039904
H        4.955596       -2.332516       -1.967854
H        5.812024       -0.066488       -1.554009
H        4.814885       -0.184051        1.320413
H       -2.152234        3.290903        0.571736
H       -4.283670        2.894548       -0.494232
H       -3.301752        1.980090       -2.845326
H       -1.613196        0.466740       -2.085998
54
4pzMePyr2-trans-m ; E = -1106.25444011 Hartree
C        2.513760       -0.279460        0.176685
C        3.715586        0.381490        0.501299
C        1.312598        0.501078        0.102326
H        4.628718       -0.181722        0.633212
C        3.730638        1.746464        0.724200
C        1.382774        1.931781        0.186716
C        2.599370        2.526909        0.564868
H        2.670763        3.598905        0.688391
N        0.132073       -0.230809       -0.002706
N       -0.877947        0.236396        0.602891
C       -2.036464       -0.512186        0.458684
C       -2.432664       -1.464293       -0.484894
C       -3.151299       -0.359749        1.326068
N       -4.143180       -1.158836        0.964588
N       -3.690480       -1.813517       -0.128206
C       -4.573905       -2.716040       -0.818516
H       -4.923702       -2.290200       -1.765623
H       -4.074097       -3.667472       -1.020697
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H       -5.429625       -2.886268       -0.166537
C       -1.764620       -1.992599       -1.700739
H       -2.452330       -2.036583       -2.552252
H       -0.918732       -1.350069       -1.948099
H       -1.366456       -3.002476       -1.542358
C       -3.250443        0.531047        2.513446
H       -2.656378        0.145858        3.348897
H       -2.861871        1.526061        2.279114
H       -4.290282        0.611008        2.836511
H        4.665897        2.223023        1.005495
C       -1.125249        3.703388       -1.733698
C       -0.732406        2.382486       -1.080898
N        0.328953        2.745390       -0.153203
C        0.441309        4.190506       -0.029914
C       -0.865225        4.706728       -0.615219
H       -0.472107        3.918374       -2.587641
H       -0.378842        1.632583       -1.798649
H        0.591984        4.484078        1.015424
H       -1.662779        4.652564        0.134138
C        2.111343       -3.944291        0.126026
C        1.454065       -2.588860       -0.108405
N        2.560189       -1.643306        0.008388
C        3.844814       -2.330735       -0.030551
C        3.500790       -3.749142       -0.465797
H        2.184833       -4.143800        1.201279
H        0.995662       -2.542230       -1.104723
H        4.532337       -1.836551       -0.727393
H        4.236740       -4.479830       -0.120696
H        0.664128       -2.366349        0.610636
H        1.549043       -4.762739       -0.331729
H        3.455244       -3.804292       -1.559399
H        4.325637       -2.330612        0.961094
H        1.296706        4.574879       -0.610475
H       -0.787502        5.741435       -0.958255
H       -2.158917        3.698954       -2.089069
H       -1.579963        1.939106       -0.542981
54
4pzMePyr2-trans-n ; E = -1106.25528133 Hartree
C        2.565660        0.089490        0.316870
C        3.577814        0.938185        0.812192
C        1.250884        0.635427        0.149341
H        4.560772        0.542728        1.026786
C        3.311010        2.264717        1.094624
C        1.042262        2.047586        0.295482
C        2.076406        2.833184        0.832875
H        1.929799        3.890702        1.005385
N        0.231322       -0.286729       -0.102177
N       -0.879564       -0.030275        0.447241
C       -1.895299       -0.935076        0.183599
C       -3.074961       -0.912388        0.925954
C       -2.091150       -1.952930       -0.797385
N       -3.288638       -2.504011       -0.651774
N       -3.861995       -1.870102        0.395493
C       -5.167088       -2.281006        0.840458
H       -5.113204       -2.818978        1.793044
H       -5.824746       -1.415292        0.959481
H       -5.573115       -2.943035        0.076675
C       -3.447762       -0.045060        2.069740
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H       -3.562923       -0.615429        2.998623
H       -2.650884        0.687777        2.212492
H       -4.388341        0.487665        1.888924
C       -1.199779       -2.384989       -1.907506
H       -0.697564       -1.525062       -2.357860
H       -0.414392       -3.059174       -1.552395
H       -1.786296       -2.910327       -2.664740
H        4.103090        2.885417        1.504861
C       -1.514492        3.424796       -1.861177
C       -0.969174        2.167343       -1.192875
N       -0.105685        2.672090       -0.134089
C       -0.268689        4.107970        0.029562
C       -1.569843        4.411099       -0.699480
H       -0.815437        3.786339       -2.624368
H       -0.405663        1.522520       -1.877282
H       -0.294876        4.382213        1.090792
H       -2.426474        4.187433       -0.053682
C        2.888440       -3.563309       -0.087821
C        2.013189       -2.329332       -0.272263
N        2.894196       -1.224428        0.087095
C        4.286064       -1.653907        0.138501
C        4.272420       -3.052639       -0.465966
H        2.876299       -3.876571        0.962484
H        1.666966       -2.238228       -1.310192
H        4.929218       -0.966897       -0.424483
H        5.091162       -3.674209       -0.094447
H        1.120263       -2.341153        0.354619
H        2.549661       -4.406544       -0.695673
H        4.363927       -2.988510       -1.556111
H        4.656851       -1.675087        1.175929
H        0.565443        4.659970       -0.435447
H       -1.639285        5.456798       -1.009509
H       -2.481797        3.254024       -2.340768
H       -1.781386        1.560137       -0.774019
24
4pzH-ts-B-m ; E = -605.300223945 Hartree
C        2.390899       -0.143536        1.220656
C        3.618130        0.498183        1.196611
C        1.750942       -0.476895       -0.000158
H        4.089995        0.740516        2.145318
C        4.250194        0.831889        0.000228
C        2.390527       -0.142103       -1.220777
H        1.909954       -0.400013       -2.157877
C        3.617788        0.499549       -1.196352
H        4.089381        0.742963       -2.144918
H        1.910608       -0.402538        2.157599
N        0.575894       -1.086562       -0.000342
N       -0.498176       -1.674443       -0.000559
C       -1.649061       -0.862675       -0.000260
C       -1.782827        0.522263        0.000099
C       -2.971933       -1.352168       -0.000275
N       -3.849337       -0.361358        0.000029
N       -3.102836        0.761409        0.000237
C       -3.770329        2.041267        0.000603
H       -4.397111        2.129634        0.890389
H       -3.020447        2.832522        0.000422
H       -4.397716        2.129793       -0.888739
H       -1.042115        1.308389        0.000142
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H       -3.298792       -2.382696       -0.000525
H        5.211445        1.333457        0.000376
24
4pzH-ts-B-n ; E = -605.300668029 Hartree
C       -2.516767        0.155681        1.220780
C       -3.799091       -0.367249        1.195836
C       -1.849111        0.430174        0.000692
H       -4.290691       -0.568202        2.144162
C       -4.460287       -0.635912       -0.001059
C       -2.516889        0.159990       -1.220290
H       -2.012746        0.370094       -2.156874
C       -3.799195       -0.363061       -1.197065
H       -4.290876       -0.560696       -2.146046
H       -2.012535        0.362486        2.158051
N       -0.623589        0.931895        0.001518
N        0.499207        1.419897        0.002314
C        1.569863        0.505144        0.000858
C        2.899920        0.897383        0.001412
C        1.610302       -0.910189       -0.001304
N        2.858129       -1.345945       -0.002013
N        3.622651       -0.234249       -0.000331
C        5.058583       -0.373910       -0.000825
H        5.377404       -0.918781       -0.891939
H        5.511028        0.618058        0.001867
H        5.377407       -0.923614        0.887301
H        3.344921        1.881304        0.002891
H        0.781565       -1.604705       -0.002301
H       -5.464226       -1.045436       -0.001732
24
4pzH-ts-H-m ; E = -605.295863534 Hartree
C       -1.735526        0.776478        0.307693
C       -2.815404        1.646350        0.362547
C       -1.940202       -0.563044       -0.029499
H       -2.661089        2.687383        0.632954
C       -4.101847        1.186964        0.075818
C       -3.227512       -1.026727       -0.296718
H       -3.350180       -2.078172       -0.539509
C       -4.305991       -0.150908       -0.254078
H       -5.307107       -0.510448       -0.473145
H       -0.729072        1.110461        0.541461
N       -0.902438       -1.558031       -0.092092
N        0.260899       -1.128732       -0.009742
C        1.500285       -0.690266        0.044029
C        1.987462        0.615574       -0.194905
C        2.700215       -1.428581        0.327613
N        3.771579       -0.667225        0.276258
N        3.316533        0.561439       -0.075747
C        4.280007        1.604179       -0.329024
H        4.810876        1.413218       -1.265743
H        3.763549        2.562688       -0.390443
H        5.000394        1.626851        0.490062
H        1.466139        1.516674       -0.484362
H        2.775197       -2.472836        0.600526
H       -4.943635        1.871907        0.116599
24
4pzH-ts-H-n ; E = -605.296293711 Hartree
C       -1.904227        0.807698        0.214257
C       -3.077175        1.547823        0.258873
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C       -1.962837       -0.571796        0.007569
H       -3.035435        2.620657        0.425631
C       -4.311771        0.917907        0.093466
C       -3.196545       -1.204219       -0.140218
H       -3.203134       -2.280610       -0.284988
C       -4.369592       -0.459404       -0.106404
H       -5.329760       -0.951253       -0.231740
H       -0.935110        1.277464        0.351877
N       -0.818990       -1.444049       -0.034718
N        0.290231       -0.882596       -0.042646
C        1.470908       -0.302289       -0.085302
C        2.726437       -0.900081        0.164768
C        1.825088        1.057181       -0.393994
N        3.125440        1.251663       -0.344350
N        3.647538        0.055123        0.026451
C        5.067695       -0.030289        0.263016
H        5.597014        0.403570       -0.586852
H        5.334998        0.520587        1.168723
H        5.349164       -1.077696        0.375368
H        2.968303       -1.911868        0.455966
H        1.163421        1.861129       -0.689638
H       -5.226874        1.501846        0.126308
52
4pzHAmid2-ts-B-m ; E = -1478.12028087 Hartree
C        2.121389        1.655123        0.009619
C        2.352425        3.013553        0.212479
C        0.781794        1.166699       -0.127203
H        3.366387        3.363133        0.348452
C        1.269998        3.888679        0.205075
C       -0.299713        2.109606       -0.128905
C       -0.045267        3.469082        0.020113
H       -0.869750        4.168466        0.002771
N        0.541107       -0.131374       -0.248895
N        0.344139       -1.358220       -0.419171
C       -0.887749       -1.837137        0.064147
C       -1.616309       -1.462921        1.196153
C       -1.623393       -2.892471       -0.531823
N       -2.734230       -3.126000        0.153263
N       -2.696741       -2.274376        1.202663
C       -3.798388       -2.255055        2.130008
H       -3.432286       -2.175989        3.156228
H       -4.473229       -1.416881        1.922938
H       -4.340842       -3.192148        2.010621
C       -1.332269       -0.488012        2.281867
H       -1.371976       -0.968516        3.265607
H       -0.338336       -0.059706        2.151253
H       -2.049863        0.339442        2.284358
C       -1.294617       -3.639046       -1.775590
H       -1.428936       -3.010233       -2.661989
H       -0.249966       -3.962013       -1.765211
H       -1.942397       -4.512672       -1.869267
H        1.461143        4.949255        0.339302
N        3.105351        0.686976       -0.044781
H        2.760260       -0.241518       -0.266016
N       -1.554233        1.559947       -0.326280
H       -1.559771        0.548928       -0.416676
C        4.456258        0.841672        0.128004
O        5.018435        1.890814        0.404718
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C       -2.771418        2.191388       -0.358904
O       -2.951012        3.393756       -0.240548
C        6.558667       -0.640894        0.045468
C        6.732189       -2.028963       -0.217475
C        5.486396       -2.528536       -0.448564
O        4.557355       -1.553262       -0.347864
C        5.219370       -0.401103       -0.045801
H        7.309668        0.100256        0.273517
H        7.658110       -2.584877       -0.233923
H        5.112571       -3.512315       -0.687114
C       -5.246285        1.484859       -0.571797
C       -5.851466        0.210578       -0.770009
C       -4.830181       -0.688413       -0.856254
O       -3.641882       -0.059147       -0.723303
C       -3.899779        1.267188       -0.548595
H       -5.724880        2.445913       -0.458163
H       -6.906248       -0.010789       -0.842829
H       -4.770499       -1.758956       -0.987559
52
4pzHAmid2-ts-B-n ; E = -1478.11684741 Hartree
C       -2.104529       -1.713990        0.005353
C       -2.359900       -3.070608        0.174920
C       -0.757504       -1.241081       -0.131842
H       -3.379882       -3.402138        0.311346
C       -1.296734       -3.967700        0.119665
C        0.305261       -2.200997       -0.157457
C        0.019968       -3.561016       -0.068222
H        0.830190       -4.273980       -0.135805
N       -0.530477        0.057242       -0.281020
N       -0.286594        1.262931       -0.503547
C        0.886813        1.798395        0.046152
C        1.512238        2.909942       -0.514471
C        1.602617        1.520531        1.247012
N        2.600296        2.384321        1.387435
N        2.536370        3.201030        0.310467
C        3.547446        4.211519        0.135195
H        4.304598        3.896138       -0.591166
H        3.096189        5.145603       -0.207205
H        4.019601        4.371102        1.104055
C        1.188468        3.644960       -1.761357
H        1.940820        3.481054       -2.541020
H        0.227343        3.285270       -2.133671
H        1.115201        4.724029       -1.589013
C        1.307006        0.518872        2.309498
H        1.811663        0.812322        3.232054
H        0.231006        0.458472        2.496322
H        1.647396       -0.485161        2.040742
H       -1.504767       -5.028833        0.217730
N       -3.076734       -0.729736       -0.024306
H       -2.722570        0.194338       -0.247943
N        1.584692       -1.687671       -0.302396
H        1.653170       -0.679193       -0.221083
C       -4.426541       -0.866474        0.158191
O       -5.004344       -1.908186        0.432492
C        2.760733       -2.376477       -0.467270
O        2.855810       -3.575170       -0.682888
C       -6.509186        0.644791        0.106975
C       -6.668059        2.037399       -0.142220
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C       -5.418631        2.523518       -0.380692
O       -4.500523        1.535709       -0.297340
C       -5.174167        0.389060        0.001001
H       -7.266857       -0.089192        0.335984
H       -7.587165        2.604794       -0.144762
H       -5.035110        3.504842       -0.613839
C        5.280209       -1.801982       -0.509085
C        5.975830       -0.603025       -0.180711
C        5.022890        0.306832        0.167715
O        3.793981       -0.241002        0.068558
C        3.954306       -1.529108       -0.341487
H        5.687880       -2.751403       -0.822002
H        7.043720       -0.440585       -0.190407
H        5.044113        1.324726        0.525489
52
4pzHAmid2-ts-H-m ; E = -1478.11838419 Hartree
C        0.111351       -1.954017       -0.168188
C       -0.132107       -3.312097        0.053369
C       -0.963961       -1.037001       -0.132526
H        0.698627       -4.003579        0.039375
C       -1.433574       -3.742904        0.277383
C       -2.284646       -1.517903        0.027968
C       -2.518062       -2.874568        0.254565
H       -3.531171       -3.217231        0.410604
N       -0.879995        0.368494       -0.352176
N        0.155484        0.956245        0.021250
C        1.263350        1.587897        0.328491
C        2.251356        1.192288        1.272432
C        1.802199        2.785568       -0.267436
N        2.989109        3.060543        0.230278
N        3.212421        2.117255        1.192442
C        4.450717        2.162466        1.928384
H        4.272151        1.923534        2.979029
H        5.173138        1.452438        1.512063
H        4.846372        3.173931        1.843319
C        2.240586        0.073523        2.241812
H        2.160305        0.432665        3.274545
H        1.378228       -0.565161        2.039409
H        3.148922       -0.533394        2.166046
C        1.187915        3.575726       -1.362963
H        1.290827        3.062888       -2.325657
H        0.116956        3.701960       -1.179915
H        1.665179        4.554111       -1.440880
H       -1.611058       -4.799366        0.454867
N        1.384709       -1.478455       -0.497393
H        1.434282       -0.517889       -0.801008
N       -3.288902       -0.557479       -0.027381
H       -2.946325        0.371546       -0.256331
C        2.589932       -2.109207       -0.355315
O        2.766919       -3.238922        0.076579
C       -4.633231       -0.733103        0.137371
O       -5.191621       -1.789280        0.400822
C        5.078228       -1.472461       -0.567146
C        5.722374       -0.282717       -1.016801
C        4.728544        0.556764       -1.422574
O        3.522302       -0.029482       -1.258944
C        3.740112       -1.266932       -0.730824
H        5.525375       -2.369899       -0.166873
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H        6.782853       -0.078365       -1.042417
H        4.711008        1.561894       -1.814976
C       -6.759133        0.715190        0.065361
C       -6.959576        2.102398       -0.184579
C       -5.723541        2.627763       -0.408702
O       -4.775598        1.669402       -0.315703
C       -5.415685        0.501888       -0.025632
H       -7.495269       -0.043065        0.285227
H       -7.896038        2.640574       -0.197135
H       -5.369049        3.621082       -0.637179
52
4pzHAmid2-ts-H-n ; E = -1478.11386239 Hartree
C        0.108413       -2.035276       -0.112141
C       -0.173008       -3.389137        0.089609
C       -0.946051       -1.094237       -0.100881
H        0.642563       -4.098589        0.097454
C       -1.490322       -3.791574        0.268158
C       -2.281942       -1.545681        0.013316
C       -2.553656       -2.898389        0.218516
H       -3.578721       -3.218981        0.339010
N       -0.824189        0.311334       -0.295388
N        0.215289        0.870633        0.110830
C        1.297690        1.492237        0.514659
C        1.812278        2.714574        0.009755
C        2.266714        1.081357        1.508980
N        3.246591        1.956412        1.584377
N        2.971474        2.907704        0.646369
C        3.968680        3.917432        0.402525
H        3.508529        4.788262       -0.066052
H        4.407815        4.202813        1.358833
H        4.760545        3.530303       -0.247503
C        1.250794        3.570223       -1.058595
H        0.242074        3.213690       -1.281591
H        1.190621        4.618795       -0.749124
H        1.838276        3.525951       -1.982870
C        2.170109       -0.082925        2.428270
H        1.961502        0.245446        3.451325
H        1.361860       -0.745957        2.113454
H        3.107382       -0.645123        2.442899
H       -1.697316       -4.844927        0.431662
N        1.398190       -1.586407       -0.404190
H        1.477477       -0.620623       -0.683357
N       -3.262483       -0.561646       -0.062505
H       -2.891124        0.362494       -0.263811
C        2.584748       -2.250007       -0.255031
O        2.726877       -3.386699        0.170613
C       -4.614851       -0.708235        0.053341
O       -5.207163       -1.754451        0.279844
C        5.088371       -1.697681       -0.503185
C        5.767035       -0.551177       -1.006896
C        4.796928        0.313025       -1.412475
O        3.571114       -0.213697       -1.198194
C        3.756121       -1.443158       -0.638537
H        5.509923       -2.600466       -0.087851
H        6.833605       -0.389696       -1.061262
H        4.816071        1.291797       -1.866581
C       -6.704217        0.788735       -0.065152
C       -6.866571        2.183845       -0.298631
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C       -5.612941        2.685250       -0.473766
O       -4.689118        1.704825       -0.365893
C       -5.363530        0.547224       -0.115886
H       -7.463125        0.043438        0.118557
H       -7.790369        2.742622       -0.332447
H       -5.230134        3.674164       -0.673874
24
4pzHCl1A-ts-B-m ; E = -1064.73982498 Hartree
C        2.077083        0.652267        0.249680
C        3.315610        0.968978       -0.279365
C        1.561451       -0.669734        0.182132
H        3.673643        1.989007       -0.183294
C        4.069370        0.004097       -0.942047
C        2.352669       -1.644473       -0.479406
H        1.975957       -2.659184       -0.538808
C        3.565342       -1.292339       -1.044221
H        4.139933       -2.058345       -1.557021
Cl        1.103963        1.864869        1.029464
N        0.389677       -0.966612        0.706228
N       -0.691045       -1.260044        1.206871
C       -1.829279       -0.758283        0.560916
C       -1.949391        0.119926       -0.513104
C       -3.157983       -1.057639        0.932122
N       -4.024447       -0.428380        0.156216
N       -3.265645        0.280199       -0.706560
C       -3.920850        1.100600       -1.697114
H       -4.511442        0.472115       -2.367273
H       -4.581535        1.814206       -1.201127
H       -3.164209        1.637580       -2.269343
H       -1.200605        0.628560       -1.101403
H       -3.495128       -1.706252        1.728295
H        5.032105        0.263006       -1.367754
24
4pzHCl1A-ts-B-n ; E = -1064.73984731 Hartree
C       -2.244315       -0.671891        0.055940
C       -3.532503       -0.725637       -0.445874
C       -1.620116        0.569513        0.348132
H       -3.971104       -1.699721       -0.637243
C       -4.236555        0.443775       -0.719764
C       -2.357861        1.751077        0.080500
H       -1.896889        2.707542        0.298935
C       -3.628454        1.671520       -0.461310
H       -4.161481        2.595097       -0.668228
Cl       -1.343402       -2.128437        0.357781
N       -0.399638        0.612562        0.844336
N        0.726692        0.661575        1.324990
C        1.784656        0.381233        0.448873
C        3.117862        0.444964        0.829045
C        1.814223       -0.015163       -0.911086
N        3.057475       -0.177677       -1.326100
N        3.830661        0.108733       -0.256383
C        5.264702        0.023586       -0.389556
H        5.724825        0.269706        0.567713
H        5.548066       -0.989523       -0.682178
H        5.608577        0.725482       -1.152330
H        3.569278        0.701531        1.775836
H        0.980450       -0.193844       -1.575534
H       -5.240046        0.392950       -1.126547
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24
4pzHCl1A-ts-H-m ; E = -1064.72983880 Hartree
C       -1.891053       -0.614856       -0.271214
C       -3.035343       -1.329496        0.073311
C       -1.822624        0.768114       -0.070010
H       -3.063530       -2.398923       -0.108450
C       -4.126485       -0.671598        0.627686
C       -2.950488        1.413443        0.445890
H       -2.885321        2.492320        0.554810
C       -4.085597        0.708953        0.813781
H       -4.939246        1.231542        1.233842
Cl       -0.590654       -1.497186       -1.024440
N       -0.746037        1.668232       -0.401537
N        0.409914        1.229926       -0.298388
C        1.645562        0.813550       -0.143325
C        2.103079       -0.348880        0.521330
C        2.866270        1.431966       -0.582681
N        3.923855        0.734997       -0.234217
N        3.433242       -0.328901        0.458617
C        4.371532       -1.256305        1.041290
H        3.823054       -2.092409        1.475779
H        5.046343       -1.622837        0.265464
H        4.958017       -0.757848        1.817081
H        1.551157       -1.122882        1.033286
H        2.967868        2.342102       -1.158935
H       -5.013153       -1.238028        0.894922
24
4pzHCl1A-ts-H-n ; E = -1064.72919826 Hartree
C       -2.010750       -0.612014       -0.191691
C       -3.242156       -1.157988        0.161228
C       -1.820011        0.774524       -0.194871
H       -3.364924       -2.235927        0.141482
C       -4.296658       -0.326963        0.519713
C       -2.909001        1.591010        0.122865
H       -2.744347        2.663602        0.072729
C       -4.131030        1.056460        0.499087
H       -4.954360        1.711970        0.765002
Cl       -0.759407       -1.710815       -0.693487
N       -0.638376        1.508029       -0.573826
N        0.456426        0.990925       -0.303706
C        1.630349        0.499004        0.021383
C        2.896639        0.920625       -0.443300
C        1.960624       -0.573375        0.921676
N        3.259015       -0.764288        1.000011
N        3.802719        0.136525        0.138136
C        5.231219        0.118512       -0.059001
H        5.521176        0.984706       -0.654354
H        5.726995        0.156685        0.912488
H        5.528459       -0.798139       -0.574878
H        3.155148        1.687710       -1.158565
H        1.279048       -1.160088        1.521824
H       -5.251091       -0.763774        0.796709
24
4pzHCl1B-ts-B-m ; E = -1064.73982867 Hartree
C       -2.356218       -1.641744       -0.485171
C       -3.569369       -1.285477       -1.046344
C       -1.562365       -0.670948        0.179012
H       -4.146058       -2.048540       -1.561173
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C       -4.071213        0.011330       -0.938156
C       -2.075510        0.651741        0.251834
Cl       -1.098255        1.860533        1.034212
C       -3.314615        0.972501       -0.273316
H       -3.670707        1.992784       -0.172841
H       -1.981272       -2.656826       -0.549182
N       -0.390395       -0.971750        0.700366
N        0.690220       -1.267917        1.199667
C        1.828575       -0.763372        0.556086
C        1.948750        0.123361       -0.510903
C        3.157225       -1.069591        0.921733
N        4.023739       -0.436522        0.148969
N        3.265020        0.280860       -0.706572
C        3.920264        1.118455       -1.682581
H        3.163192        1.603804       -2.298668
H        4.521582        1.875771       -1.175162
H        4.570711        0.507768       -2.311904
H        1.199862        0.639724       -1.092824
H        3.494123       -1.727146        1.711037
H       -5.034329        0.273379       -1.361061
24
4pzHCl1B-ts-B-n ; E = -1064.73984738 Hartree
C        2.359092        1.750926        0.078785
C        3.629879        1.669944       -0.462351
C        1.620481        0.570147        0.347471
H        4.163620        2.592940       -0.670014
C        4.237276        0.441514       -0.719202
C        2.243907       -0.671993        0.056725
Cl        1.341607       -2.127560        0.358893
C        3.532266       -0.727130       -0.444512
H        3.970240       -1.701709       -0.634797
H        1.898648        2.707932        0.295957
N        0.399853        0.614491        0.843196
N       -0.726435        0.663931        1.323916
C       -1.784450        0.382133        0.448346
C       -3.117617        0.446577        0.828550
C       -1.814187       -0.016324       -0.911011
N       -3.057499       -0.179407       -1.325628
N       -3.830551        0.108658       -0.256260
C       -5.264598        0.023081       -0.389103
H       -5.607668        0.719584       -1.157120
H       -5.548621       -0.991971       -0.674367
H       -5.724874        0.276553        0.566174
H       -3.568889        0.704676        1.774960
H       -0.980589       -0.196028       -1.575338
H        5.240948        0.389577       -1.125401
24
4pzHCl1B-ts-H-m ; E = -1064.73075532 Hartree
C        1.029105        1.336958       -0.406494
C        1.920393        2.396555       -0.342166
C        1.450899        0.024445       -0.186160
H        1.578525        3.410245       -0.528835
C        3.260870        2.152808       -0.045326
C        2.801806       -0.205323        0.093121
Cl        3.378911       -1.817677        0.370923
C        3.701885        0.852752        0.174339
H        4.741027        0.647687        0.408104
H       -0.017385        1.492748       -0.653321
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N        0.580366       -1.115573       -0.302692
N       -0.634564       -0.860223       -0.265196
C       -1.924405       -0.615138       -0.181770
C       -2.575287        0.564634        0.250486
C       -3.023325       -1.493374       -0.476274
N       -4.185152       -0.919461       -0.257605
N       -3.884953        0.322560        0.206194
C       -4.970581        1.183496        0.607821
H       -4.572005        2.165922        0.862186
H       -5.681162        1.276338       -0.215558
H       -5.482931        0.758950        1.474601
H       -2.167159        1.499790        0.606552
H       -2.966970       -2.503372       -0.860139
H        3.968544        2.974202        0.010344
24
4pzHCl1B-ts-H-n ; E = -1064.73140827 Hartree
C        1.237515        1.403490        0.275485
C        2.258989        2.338255        0.215536
C        1.500631        0.038361        0.149418
H        2.037882        3.395713        0.325050
C        3.572677        1.913052        0.020647
C        2.825194       -0.373181       -0.029812
Cl        3.208265       -2.058511       -0.188870
C        3.856576        0.557830       -0.103893
H        4.872981        0.211870       -0.257910
H        0.206649        1.703289        0.440827
N        0.488746       -0.978618        0.260513
N       -0.682854       -0.577936        0.158426
C       -1.927295       -0.177181        0.008939
C       -3.099849       -0.925019        0.262769
C       -2.449438        1.083034       -0.447938
N       -3.763750        1.092577       -0.471296
N       -4.133984       -0.133738       -0.015691
C       -5.542026       -0.413785        0.127360
H       -5.670165       -1.456134        0.419899
H       -5.976229        0.238252        0.889005
H       -6.044998       -0.233924       -0.824601
H       -3.212817       -1.933111        0.634556
H       -1.890078        1.947921       -0.780756
H        4.381299        2.635686       -0.030010
24
4pzHCl2-ts-B-m ; E = -1524.17686965 Hartree
C        2.245300       -1.029455        0.194695
C        3.442381       -0.693576        0.799670
C        1.360763       -0.034458       -0.302741
H        4.075067       -1.493972        1.168322
C        3.831048        0.638471        0.917700
C        1.771618        1.315889       -0.133102
Cl        0.686173        2.557176       -0.682134
C        2.986608        1.638151        0.443031
H        3.255816        2.685501        0.529584
Cl        1.757154       -2.687988        0.046076
N        0.221609       -0.338628       -0.879988
N       -0.830743       -0.583503       -1.457251
C       -2.004110       -0.402913       -0.721534
C       -2.203771        0.091650        0.565893
C       -3.299859       -0.694875       -1.201424
N       -4.218802       -0.411331       -0.295206
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N       -3.527347        0.065038        0.763246
C       -4.256510        0.485918        1.936139
H       -3.548007        0.826426        2.691282
H       -4.935271        1.300207        1.674464
H       -4.836518       -0.352557        2.326620
H       -1.504867        0.454031        1.304963
H       -3.575009       -1.099667       -2.165322
H        4.778394        0.893994        1.377493
24
4pzHCl2-ts-B-n ; E = -1524.17720122 Hartree
C        2.121249       -1.204834        0.007557
C        3.398293       -1.191845        0.537721
C        1.428846       -0.000794       -0.289102
H        3.879525       -2.142192        0.742965
C        4.045886        0.011713        0.802011
C        2.111370        1.209869        0.003642
Cl        1.278958        2.700365       -0.315862
C        3.388827        1.209065        0.532994
H        3.862535        2.163986        0.734493
Cl        1.301039       -2.703274       -0.307122
N        0.220887       -0.006440       -0.805623
N       -0.895189       -0.010129       -1.306677
C       -1.976562       -0.005269       -0.422396
C       -3.297688       -0.009762       -0.850509
C       -2.053299        0.004781        0.992900
N       -3.310613        0.006302        1.393447
N       -4.047195       -0.002690        0.259808
C       -5.486522       -0.003194        0.364638
H       -5.815673       -0.888660        0.912233
H       -5.817594        0.890839        0.896970
H       -5.914925       -0.012265       -0.637790
H       -3.714815       -0.017402       -1.846502
H       -1.244130        0.010982        1.709725
H        5.047506        0.016477        1.215241
24
4pzHCl2-ts-H-m ; E = -1524.16381404 Hartree
C        1.360627        1.294392       -0.271748
C        2.369061        2.129535        0.198354
C        1.493856       -0.098047       -0.263990
H        2.230452        3.204414        0.158183
C        3.538758        1.574881        0.700359
C        2.696984       -0.619729        0.228840
Cl        2.919413       -2.341098        0.265973
C        3.707103        0.194677        0.721254
H        4.611831       -0.255776        1.113797
Cl       -0.063385        2.051283       -0.933628
N        0.560869       -1.041281       -0.836513
N       -0.635452       -0.851804       -0.579013
C       -1.909529       -0.708231       -0.296397
C       -2.507282        0.223033        0.585654
C       -3.035767       -1.452155       -0.789563
N       -4.166559       -1.029363       -0.273755
N       -3.814869       -0.015029        0.566527
C       -4.860141        0.650756        1.305162
H       -4.418021        1.435952        1.918711
H       -5.578697        1.087929        0.608752
H       -5.375690       -0.070140        1.943374
H       -2.058236        0.995799        1.192063
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H       -3.021761       -2.265479       -1.503010
H        4.327687        2.221813        1.070011
24
4pzHCl2-ts-H-n ; E = -1524.16349670 Hartree
C        1.547114        1.274034       -0.193188
C        2.678267        1.957106        0.241694
C        1.515931       -0.122729       -0.266405
H        2.665530        3.041145        0.269460
C        3.805667        1.242528        0.624626
C        2.679071       -0.808087        0.104980
Cl        2.696645       -2.543189        0.034700
C        3.810730       -0.146478        0.560960
H        4.680471       -0.720471        0.860261
Cl        0.181048        2.225258       -0.705829
N        0.437895       -0.911973       -0.815640
N       -0.703605       -0.606578       -0.444968
C       -1.927026       -0.340400       -0.047915
C       -3.129147       -0.919702       -0.514806
C       -2.384270        0.587010        0.951485
N       -3.691365        0.565670        1.077203
N       -4.120135       -0.352863        0.166181
C       -5.538975       -0.587033        0.050824
H       -5.713241       -1.359549       -0.698375
H       -5.934856       -0.912402        1.015038
H       -6.041126        0.335881       -0.247449
H       -3.290273       -1.669816       -1.275564
H       -1.779890        1.241373        1.565014
H        4.688891        1.771382        0.967861
24
4pzHF1A-ts-B-m ; E = -704.442254488 Hartree
C        1.965486        0.713724        0.545500
C        3.179529        1.320925        0.325947
C        1.666938       -0.590126        0.075339
H        3.346598        2.311584        0.736463
C        4.142437        0.671658       -0.450596
C        2.666238       -1.236603       -0.691706
H        2.458578       -2.229501       -1.074297
C        3.862178       -0.590628       -0.969239
H        4.601507       -1.100286       -1.579871
F        0.997796        1.345961        1.239007
N        0.490305       -1.127305        0.337869
N       -0.588415       -1.640119        0.636188
C       -1.729592       -0.913896        0.255815
C       -1.849761        0.398486       -0.190802
C       -3.053152       -1.401781        0.299144
N       -3.916542       -0.480443       -0.097420
N       -3.162069        0.601024       -0.381544
C       -3.817484        1.816765       -0.799299
H       -4.436606        2.206686        0.012066
H       -3.060311        2.553489       -1.068497
H       -4.450957        1.609017       -1.663646
H       -1.104633        1.167739       -0.326446
H       -3.389596       -2.386847        0.591273
H        5.095396        1.151235       -0.644383
24
4pzHF1A-ts-B-n ; E = -704.442262177 Hartree
C        2.166784        0.802933        0.375208
C        3.438577        1.223664        0.064565
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C        1.740406       -0.535499        0.183665
H        3.703208        2.258149        0.258413
C        4.335052        0.330957       -0.528259
C        2.672569       -1.428758       -0.396189
H        2.366745       -2.455306       -0.563532
C        3.930866       -0.979544       -0.770886
H        4.617542       -1.679870       -1.237055
F        1.268459        1.657367        0.897548
N        0.513008       -0.884724        0.522452
N       -0.613694       -1.201946        0.901138
C       -1.672515       -0.497179        0.304483
C       -3.008125       -0.824752        0.486066
C       -1.691604        0.643267       -0.535295
N       -2.931293        0.982606       -0.842570
N       -3.712408        0.076248       -0.218374
C       -5.143175        0.156855       -0.381321
H       -5.415866       -0.041252       -1.420746
H       -5.616299       -0.581491        0.266676
H       -5.485069        1.156574       -0.107016
H       -3.469183       -1.620471        1.051884
H       -0.852197        1.228685       -0.882577
H        5.332676        0.661742       -0.794721
24
4pzHF1A-ts-H-m ; E = -704.438089288 Hartree
C        1.808935       -0.719833       -0.258335
C        2.927251       -1.531346       -0.163935
C        1.872305        0.658711       -0.026086
H        2.819842       -2.592634       -0.363276
C        4.155405       -0.968212        0.171003
C        3.122940        1.199126        0.283487
H        3.159923        2.273539        0.439492
C        4.254452        0.403245        0.395029
H        5.210980        0.848317        0.649633
F        0.647928       -1.300701       -0.612583
N        0.810183        1.626320       -0.108280
N       -0.351413        1.183520       -0.092022
C       -1.595765        0.767118       -0.054021
C       -2.071020       -0.542479        0.195321
C       -2.809575        1.517662       -0.230499
N       -3.878039        0.763193       -0.108089
N       -3.400179       -0.482350        0.165729
C       -4.351138       -1.541857        0.395660
H       -4.955300       -1.314043        1.277032
H       -5.008481       -1.636474       -0.471079
H       -3.812007       -2.476570        0.551505
H       -1.525593       -1.452703        0.391873
H       -2.900076        2.572273       -0.455348
H        5.032753       -1.602998        0.246309
24
4pzHF1A-ts-H-n ; E = -704.437401756 Hartree
C        1.973090       -0.713538        0.211449
C        3.184811       -1.377297        0.111185
C        1.877717        0.675285        0.064434
H        3.200472       -2.454550        0.240621
C        4.344992       -0.651187       -0.142146
C        3.062005        1.380580       -0.163307
H        2.973434        2.459589       -0.252567
C        4.284518        0.733994       -0.279204
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H        5.187546        1.305007       -0.469876
F        0.882100       -1.446511        0.485220
N        0.704111        1.499728        0.166996
N       -0.394506        0.923808        0.079943
C       -1.577950        0.365803       -0.033292
C       -2.839825        0.965780        0.184535
C       -1.926291       -0.977925       -0.412826
N       -3.227578       -1.162154       -0.428576
N       -3.759116        0.030027       -0.042858
C       -5.192035        0.129486        0.084092
H       -5.458017        1.157012        0.333442
H       -5.661108       -0.153112       -0.860475
H       -5.543593       -0.542509        0.870691
H       -3.088155        1.969375        0.498381
H       -1.250719       -1.777079       -0.682629
H        5.294671       -1.170873       -0.222621
24
4pzHF1B-ts-B-m ; E = -704.442254493 Hartree
C       -2.666346       -1.236625       -0.691575
C       -3.862252       -0.590583       -0.969095
C       -1.666953       -0.590160        0.075356
H       -4.601651       -1.100231       -1.579651
C       -4.142389        0.671763       -0.450536
C       -1.965385        0.713747        0.545441
F       -0.997647        1.345940        1.238813
C       -3.179399        1.321016        0.325919
H       -3.346375        2.311710        0.736386
H       -2.458786       -2.229575       -1.074084
N       -0.490343       -1.127410        0.337845
N        0.588405       -1.640184        0.636132
C        1.729563       -0.913952        0.255712
C        1.849727        0.398483       -0.190750
C        3.053127       -1.401836        0.298998
N        3.916512       -0.480451       -0.097463
N        3.162036        0.601049       -0.381458
C        3.817435        1.816822       -0.799146
H        4.451826        1.608809       -1.662747
H        3.060274        2.553140       -1.069490
H        4.435625        2.207411        0.012615
H        1.104613        1.167725       -0.326379
H        3.389583       -2.386924        0.591001
H       -5.095322        1.151399       -0.644313
24
4pzHF1B-ts-B-n ; E = -704.442262211 Hartree
C       -2.673023       -1.428719       -0.395950
C       -3.931219       -0.979209       -0.770633
C       -1.740495       -0.535616        0.183557
H       -4.618152       -1.679398       -1.236627
C       -4.334997        0.331442       -0.528118
C       -2.166548        0.802917        0.375179
F       -1.268081        1.657105        0.897772
C       -3.438273        1.223944        0.064636
H       -3.702667        2.258484        0.258511
H       -2.367503       -2.455386       -0.563122
N       -0.513067       -0.885058        0.522031
N        0.613698       -1.202572        0.900354
C        1.672474       -0.497474        0.304047
C        3.008086       -0.825014        0.485695
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C        1.691594        0.643338       -0.535236
N        2.931305        0.982922       -0.842159
N        3.712407        0.076385       -0.218195
C        5.143187        0.157048       -0.381017
H        5.484850        1.156995       -0.107273
H        5.616361       -0.580822        0.267494
H        5.416045       -0.041640       -1.420290
H        3.469065       -1.621026        1.051255
H        0.852160        1.228689       -0.882527
H       -5.332546        0.662484       -0.794546
24
4pzHF1B-ts-H-m ; E = -704.436550574 Hartree
C        1.396485        1.051566       -0.361079
C        2.389513        2.020321       -0.368594
C        1.694861       -0.282927       -0.079183
H        2.143649        3.052253       -0.599951
C        3.708372        1.662754       -0.086382
C        3.025742       -0.617498        0.182817
F        3.343632       -1.886035        0.446866
C        4.030271        0.338571        0.192075
H        5.045916        0.030016        0.415219
H        0.364885        1.298494       -0.594975
N        0.738956       -1.357562       -0.099898
N       -0.451471       -1.000991       -0.124241
C       -1.717959       -0.645321       -0.114403
C       -2.283891        0.603926        0.232597
C       -2.874185       -1.442177       -0.420885
N       -3.991486       -0.762486       -0.285394
N       -3.608102        0.468113        0.141530
C       -4.631910        1.426577        0.478431
H       -4.169690        2.399607        0.647403
H       -5.342297        1.495303       -0.347096
H       -5.162889        1.110933        1.380336
H       -1.814640        1.516654        0.570978
H       -2.887557       -2.468468       -0.763101
H        4.490862        2.415254       -0.086961
24
4pzHF1B-ts-H-n ; E = -704.437144932 Hartree
C       -1.581293        1.098071        0.240951
C       -2.684409        1.939119        0.242372
C       -1.728076       -0.280428        0.076504
H       -2.554428        3.008274        0.379176
C       -3.962898        1.405990        0.074290
C       -3.019984       -0.790592       -0.074139
F       -3.193370       -2.105340       -0.225106
C       -4.134113        0.035018       -0.085890
H       -5.114751       -0.409015       -0.218990
H       -0.576662        1.484905        0.384338
N       -0.649200       -1.231141        0.107247
N        0.490899       -0.737920        0.051557
C        1.703703       -0.235906       -0.042599
C        2.924412       -0.898644        0.218746
C        2.136572        1.079605       -0.432027
N        3.446726        1.193216       -0.414208
N        3.900153       -0.015019        0.009463
C        5.318925       -0.182940        0.208658
H        5.656463        0.431641        1.047062
H        5.528459       -1.232602        0.415985
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H        5.847099        0.126238       -0.694959
H        3.107405       -1.907997        0.557625
H        1.520641        1.908967       -0.755300
H       -4.830976        2.057939        0.071402
24
4pzHF2-ts-B-m ; E = -803.582855184 Hartree
C       -2.610755        0.943882        0.357243
C       -3.788500        0.301340        0.677541
C       -1.505973        0.266089       -0.220757
H       -4.582973        0.877433        1.139123
C       -3.947297       -1.049113        0.366007
C       -1.705363       -1.116540       -0.463235
F       -0.664446       -1.790089       -0.983781
C       -2.900629       -1.759034       -0.221812
H       -2.988258       -2.811994       -0.466337
F       -2.448305        2.238896        0.640213
N       -0.372672        0.866293       -0.510919
N        0.672943        1.446981       -0.814345
C        1.855875        0.838672       -0.368160
C        2.070672       -0.414851        0.198170
C        3.139055        1.423003       -0.442901
N        4.064831        0.611572        0.042063
N        3.391445       -0.495701        0.417436
C        4.131693       -1.610663        0.956645
H        4.715971       -1.278084        1.816770
H        3.430161       -2.385080        1.267561
H        4.808540       -2.011611        0.198616
H        1.385437       -1.223904        0.400675
H        3.401970        2.401338       -0.820456
H       -4.884609       -1.548093        0.584070
24
4pzHF2-ts-B-n ; E = -803.583037222 Hartree
C       -2.611874       -1.096190       -0.202830
C       -3.861115       -0.640600       -0.569404
C       -1.582427       -0.224985        0.236930
H       -4.591608       -1.360495       -0.921910
C       -4.167863        0.714081       -0.441627
C       -1.933680        1.147216        0.297036
F       -0.971541        1.995416        0.691608
C       -3.199650        1.610819        0.009350
H       -3.402833        2.671380        0.109612
F       -2.306164       -2.392815       -0.309768
N       -0.382755       -0.650263        0.568536
N        0.727049       -1.059863        0.917185
C        1.823101       -0.408319        0.331595
C        3.134272       -0.835037        0.487919
C        1.915938        0.749045       -0.480759
N        3.173533        1.006629       -0.794341
N        3.894100        0.030929       -0.202076
C        5.324652        0.010552       -0.383885
H        5.740666        0.979461       -0.101709
H        5.751797       -0.768503        0.248202
H        5.569311       -0.192474       -1.429388
H        3.542006       -1.677353        1.026683
H        1.117602        1.402262       -0.802378
H       -5.159214        1.070815       -0.696742
24
4pzHF2-ts-H-m ; E = -803.577850517 Hartree
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C        1.508363        1.013490        0.313157
C        2.546685        1.918377        0.165897
C        1.667046       -0.364268        0.123769
H        2.355163        2.971444        0.339789
C        3.806946        1.446147       -0.186767
C        2.959693       -0.788217       -0.209297
F        3.168951       -2.091788       -0.391700
C        4.021407        0.085378       -0.378855
H        4.991649       -0.311652       -0.654474
F        0.310077        1.495692        0.683310
N        0.684819       -1.399089        0.319238
N       -0.501894       -1.041633        0.223794
C       -1.770522       -0.723692        0.118429
C       -2.327633        0.526382       -0.243655
C       -2.934104       -1.544067        0.321154
N       -4.047446       -0.880351        0.109846
N       -3.648940        0.375469       -0.238313
C       -4.665474        1.350347       -0.549149
H       -5.324793        1.479859        0.311758
H       -4.186498        2.299281       -0.791343
H       -5.256530        1.007815       -1.401470
H       -1.841087        1.458738       -0.486701
H       -2.957916       -2.584938        0.616231
H        4.628544        2.144284       -0.308329
24
4pzHF2-ts-H-n ; E = -803.577403869 Hartree
C        1.700008        1.020389       -0.248435
C        2.851501        1.772585       -0.082370
C        1.684559       -0.375674       -0.143709
H        2.794171        2.850308       -0.187125
C        4.047430        1.121199        0.202027
C        2.918181       -0.982751        0.121195
F        2.959458       -2.312019        0.219749
C        4.088320       -0.265261        0.307445
H        5.005152       -0.799576        0.528551
F        0.567520        1.670660       -0.552687
N        0.571065       -1.257840       -0.372500
N       -0.555742       -0.760386       -0.203099
C       -1.768853       -0.292293       -0.022926
C       -2.996114       -0.956271       -0.254878
C       -2.190563        0.994703        0.463611
N       -3.499363        1.093066        0.522004
N       -3.964996       -0.105606        0.072197
C       -5.392428       -0.300624        0.005330
H       -5.826999       -0.169651        0.998618
H       -5.832895        0.431623       -0.675012
H       -5.598303       -1.308419       -0.355990
H       -3.188689       -1.951753       -0.628261
H       -1.559594        1.819721        0.762909
H        4.955353        1.699321        0.338792
28
4pzHOMe1A-ts-B-m ; E = -719.702897244 Hartree
C        1.912059       -0.545617       -0.248393
C        3.152519       -0.982275        0.181542
C        1.553983        0.833529       -0.135408
H        3.424408       -2.027313        0.078309
C        4.045122       -0.092719        0.790984
C        2.483028        1.718799        0.452137
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C         3.693493         1.242987         0.939944
H         4.379847         1.937775         1.414627
N         0.363054         1.221627        -0.554874
N        -0.725798         1.572946        -1.007679
C        -1.848158         0.929647        -0.455181
C        -1.928392        -0.162195         0.402452
C        -3.189665         1.286739        -0.708155
N        -4.028857         0.493216        -0.060761
N        -3.238710        -0.377005         0.600686
C        -3.854884        -1.416706         1.387908
H        -4.540599        -0.969294         2.110041
H        -4.413347        -2.097471         0.740821
H        -3.077492        -1.969331         1.916186
H        -1.152351        -0.781551         0.825808
H        -3.557054         2.093037        -1.327745
H         5.006537        -0.454017         1.139905
H         2.210866         2.764685         0.538942
O         0.942800        -1.322252        -0.807201
C         1.253299        -2.676585        -1.029586
H         2.110616        -2.784513        -1.705776
H         1.473026        -3.203480        -0.091278
H         0.370919        -3.119612        -1.493301
28
4pzHOMe1A-ts-B-n ; E = -719.703154772 Hartree
C         2.070680         0.551147         0.163915
C         3.361526         0.825374        -0.252485
C         1.611751        -0.800148         0.241383
H         3.709032         1.851897        -0.297059
C         4.209830        -0.210468        -0.661272
C         2.496317        -1.830925        -0.140143
C         3.763313        -1.525176        -0.621391
H         4.415465        -2.332724        -0.940266
N         0.372569        -1.031335         0.638160
N        -0.762024        -1.221581         1.074306
C        -1.797316        -0.592560         0.358642
C        -3.142719        -0.793124         0.627293
C        -1.778420         0.340371        -0.706477
N        -3.006278         0.682244        -1.058942
N        -3.817651        -0.018769        -0.239904
C        -5.245530         0.105081        -0.395863
H        -5.523037         1.160533        -0.373275
H        -5.562462        -0.326646        -1.348701
H        -5.739214        -0.419301         0.422960
H        -3.630647        -1.420897         1.357998
H        -0.916465         0.778074        -1.188836
H         5.211959         0.022907        -1.004809
H         2.146394        -2.855476        -0.081512
O         1.141658         1.469370         0.541216
C         1.522771         2.823521         0.506139
H         2.353750         3.024093         1.194385
H         1.814463         3.136294        -0.505125
H         0.647982         3.393816         0.820712
28
4pzHOMe1A-ts-H-m ; E = -719.695229731 Hartree
C         2.737636        -0.215014         0.064599
C         3.624139         0.865362         0.087282
C         1.365787         0.022866        -0.164122
H         4.679529         0.704997         0.273388
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C        3.157359        2.159044       -0.129065
C        0.925005        1.325743       -0.381458
C        1.807114        2.397486       -0.368576
H        1.450875        3.406777       -0.550075
N        0.506893       -1.127128       -0.223635
N       -0.710807       -0.878388       -0.212969
C       -2.004646       -0.644397       -0.169009
C       -2.677748        0.493910        0.330717
C       -3.086281       -1.495119       -0.583479
N       -4.260138       -0.939629       -0.370305
N       -3.987742        0.250860        0.217908
C       -5.087824        1.047618        0.701242
H       -4.741432        2.065087        0.886908
H       -5.871274        1.059318       -0.057653
H       -5.492502        0.624757        1.625398
H       -2.289153        1.392052        0.788842
H       -3.009987       -2.461985       -1.062834
H        3.862872        2.984668       -0.112856
H       -0.133175        1.468920       -0.582105
O        3.105201       -1.497066        0.265015
C        4.470683       -1.764071        0.476943
H        5.083829       -1.448347       -0.377004
H        4.844132       -1.275024        1.386040
H        4.549882       -2.845279        0.594392
28
4pzHOMe1A-ts-H-n ; E = -719.695612043 Hartree
C        2.758146       -0.339807        0.001912
C        3.757695        0.636965        0.013290
C        1.409125        0.054559       -0.122673
H        4.798696        0.355632        0.119962
C        3.422947        1.982585       -0.111611
C        1.101167        1.406395       -0.250145
C        2.094670        2.375663       -0.247598
H        1.839909        3.425274       -0.356154
N        0.428863       -0.994308       -0.172740
N       -0.753584       -0.620791       -0.080580
C       -2.009453       -0.251229        0.054358
C       -3.162922       -0.984109       -0.302550
C       -2.561448        0.962007        0.595114
N       -3.877731        0.957157        0.575398
N       -4.217704       -0.220829       -0.003896
C       -5.610317       -0.476403       -0.276581
H       -5.742824       -1.534075       -0.506995
H       -6.195341       -0.216809        0.606862
H       -5.952541        0.127948       -1.121459
H       -3.253318       -1.953671       -0.770122
H       -2.022681        1.793104        1.031743
H        4.214354        2.726453       -0.105395
H        0.054637        1.672784       -0.368480
O        2.995217       -1.663009        0.118632
C        4.333563       -2.082783        0.231164
H        4.926399       -1.791251       -0.645525
H        4.810863       -1.682078        1.134898
H        4.302151       -3.170911        0.296240
28
4pzHOMe1B-ts-B-m ; E = -719.702897244 Hartree
C        2.482993       -1.718833        0.452121
C        3.693476       -1.243083        0.939937
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C         1.553977       -0.833516       -0.135407
H         4.379801       -1.937908        1.414608
C         4.045162        0.092611        0.790996
C         1.912111        0.545619       -0.248367
C         3.152595        0.982211        0.181567
H         3.424534        2.027236        0.078342
N         0.363041       -1.221571       -0.554884
N        -0.725811       -1.572851       -1.007716
C        -1.848189       -0.929583       -0.455211
C        -1.928470        0.162240        0.402437
C        -3.189682       -1.286726       -0.708198
N        -4.028908       -0.493244       -0.060799
N        -3.238799        0.376997        0.600668
C        -3.855007        1.416654        1.387925
H        -3.077672        1.969191        1.916386
H        -4.413338        2.097509        0.740823
H        -4.540849        0.969189        2.109904
H        -1.152447        0.781608        0.825803
H        -3.557027       -2.093022       -1.327815
H         5.006594        0.453864        1.139917
O         0.942903        1.322316       -0.807173
C         1.253469        2.676642       -1.029513
H         1.473240        3.203490       -0.091190
H         2.110779        2.784550       -1.705715
H         0.371104        3.119732       -1.493197
H         2.210788       -2.764709        0.538908
28
4pzHOMe1B-ts-B-n ; E = -719.703154772 Hartree
C         2.496242       -1.830944        0.140081
C         3.763239       -1.525271        0.621376
C         1.611727       -0.800112       -0.241418
H         4.415342       -2.332862        0.940244
C         4.209816       -0.210586        0.661315
C         2.070723        0.551157       -0.163907
C         3.361571        0.825307        0.252536
H         3.709124        1.851813        0.297150
N         0.372555       -1.031261       -0.638253
N        -0.762053       -1.221470       -1.074373
C        -1.797338       -0.592494       -0.358660
C        -3.142735       -0.792986       -0.627393
C        -1.778465        0.340235        0.706634
N        -3.006330        0.682072        1.059114
N        -3.817685       -0.018769        0.239911
C        -5.245567        0.105135        0.395797
H        -5.562494       -0.326283        1.348773
H        -5.523109        1.160573        0.372853
H        -5.739227       -0.419535       -0.422856
H        -3.630623       -1.420628       -1.358242
H        -0.916516        0.777815        1.189109
H         5.211944        0.022733        1.004895
O         1.141765        1.469436       -0.541224
C         1.522950        2.823565       -0.506107
H         1.814611        3.136306        0.505176
H         2.353973        3.024103       -1.194311
H         0.648207        3.393913       -0.820713
H         2.146274       -2.855477        0.081406
28
4pzHOMe1B-ts-H-m ; E = -719.696239438 Hartree
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C        3.044218       -1.489500        0.281477
C        4.218738       -0.767574        0.440543
C        1.824996       -0.865213        0.020941
H        5.153166       -1.275540        0.655520
C        4.177821        0.616089        0.311442
C        1.795501        0.541827       -0.122485
C        2.979710        1.266736        0.025844
H        2.976779        2.345333       -0.081409
N        0.736681       -1.787081       -0.129571
N       -0.412390       -1.320156       -0.122208
C       -1.652755       -0.896466       -0.108113
C       -2.152851        0.281842        0.489026
C       -2.832870       -1.499478       -0.664618
N       -3.907706       -0.772601       -0.440923
N       -3.477674        0.280405        0.296078
C       -4.458327        1.182045        0.845545
H       -5.226384        1.359722        0.091853
H       -4.926007        0.752358        1.736798
H       -3.976417        2.125213        1.107629
H       -1.639979        1.039626        1.061163
H       -2.890907       -2.403694       -1.255809
H        5.083748        1.204475        0.423689
O        0.606310        1.118373       -0.420375
C        0.600783        2.486626       -0.754996
H        0.877689        3.117993        0.099324
H        1.277771        2.700059       -1.591292
H       -0.423746        2.714824       -1.052503
H        3.021653       -2.572928        0.356778
28
4pzHOMe1B-ts-H-n ; E = -719.696350169 Hartree
C        2.982965       -1.647358        0.057911
C        4.232623       -1.047704        0.126214
C        1.810190       -0.898844       -0.034286
H        5.130323       -1.651472        0.209663
C        4.313034        0.339482        0.079450
C        1.902522        0.512203       -0.094801
C        3.161275        1.114347       -0.035902
H        3.252170        2.193418       -0.080424
N        0.629391       -1.708565       -0.109904
N       -0.466216       -1.139645        0.008958
C       -1.653822       -0.600622        0.144925
C       -2.886534       -1.059539       -0.366717
C       -2.023462        0.604453        0.836868
N       -3.318630        0.836238        0.761857
N       -3.813021       -0.160238       -0.009485
C       -5.196026       -0.103760       -0.410198
H       -5.784759        0.256714        0.434014
H       -5.329503        0.578034       -1.255935
H       -5.533301       -1.102340       -0.692038
H       -3.110093       -1.914854       -0.987154
H       -1.377972        1.242331        1.423939
H        5.278732        0.834395        0.125126
O        0.752021        1.210020       -0.226454
C        0.835676        2.604743       -0.408503
H        1.268413        3.104130        0.467683
H        1.427360        2.860817       -1.296192
H       -0.191069        2.946454       -0.544963
H        2.862212       -2.726734        0.078160
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32
4pzHOMe2-ts-B-m ; E = -834.104218701 Hartree
C 2.459090 -0.733016 0.127710
C 3.568621 -0.018317 0.563238
C 1.270513 -0.052180 -0.270493
H 4.463810 -0.539314 0.881869
C 3.547982 1.375200 0.551185
C 1.270740 1.371988 -0.220342
C 2.411815 2.073382 0.148460
H 2.415351 3.157180 0.152754
N 0.206996 -0.713830 -0.676045
N -0.770610 -1.348672 -1.081453
C -2.006848 -0.987923 -0.512836
C -2.339528 0.039536 0.363052
C -3.223054 -1.665368 -0.745561
N -4.221664 -1.111791 -0.074144
N -3.659115 -0.080444 0.587513
C -4.497917 0.768606 1.396131
H -3.868065 1.463799 1.952131
H -5.192154 1.329077 0.764556
H -5.069883 0.155036 2.094795
H -1.731830 0.826205 0.783469
H -3.389628 -2.532794 -1.369188
H 4.430710 1.924750 0.860814
O 0.093590 1.935832 -0.601243
C 0.044496 3.340519 -0.677961
H 0.231813 3.809408 0.297150
H 0.770822 3.726732 -1.403670
H -0.963854 3.591063 -1.010333
O 2.363490 -2.080638 0.084137
C 3.495362 -2.822868 0.468257
H 4.364655 -2.590517 -0.160545
H 3.757039 -2.644437 1.519298
H 3.227693 -3.871932 0.337599
32
4pzHOMe2-ts-B-n ; E = -834.104481023 Hartree
C 1.515693 -1.336015 -0.138122
C 2.753201 -1.872702 0.195324
C 1.335822 0.073452 -0.248405
H 2.891580 -2.946262 0.248523
C 3.812427 -1.020815 0.500159
C 2.449771 0.913871 0.045101
C 3.661199 0.363519 0.447396
H 4.499987 1.005005 0.690732
N 0.176008 0.577406 -0.616268
N -0.895542 1.057316 -0.996329
C -2.043494 0.566003 -0.345091
C -3.318485 1.055145 -0.584703
C -2.226585 -0.443282 0.631676
N -3.503110 -0.564340 0.958568
N -4.147644 0.353740 0.209589
C -5.570849 0.513908 0.369007
H -6.051007 -0.464865 0.318498
H -5.800276 0.973738 1.334294
H -5.950175 1.147492 -0.433651
H -3.661381 1.832506 -1.251198
H -1.474577 -1.084696 1.067242
H 4.771098 -1.441970 0.784467

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O        2.185805        2.236502       -0.052901
C        3.234475        3.128326        0.236515
H        3.567944        3.034657        1.278172
H        4.094033        2.973097       -0.428525
H        2.833143        4.129710        0.076448
O        0.402548       -2.054660       -0.430020
C        0.502802       -3.457892       -0.376562
H        1.225028       -3.835877       -1.111018
H        0.793756       -3.806391        0.622893
H       -0.489834       -3.840830       -0.616202
32
4pzHOMe2-ts-H-m ; E = -834.094683432 Hartree
C        2.769949       -0.535318        0.118666
C        3.749239        0.434845        0.337763
C        1.427206       -0.167790       -0.123758
H        4.775263        0.154147        0.539070
C        3.394158        1.777451        0.299676
C        1.101455        1.205634       -0.155867
C        2.087338        2.174406        0.052054
H        1.842340        3.228901        0.023507
N        0.549882       -1.252917       -0.435312
N       -0.667486       -1.042752       -0.314924
C       -1.965594       -0.895120       -0.217105
C       -2.664807        0.023681        0.596766
C       -3.025487       -1.604938       -0.880130
N       -4.213179       -1.166859       -0.517432
N       -3.970307       -0.206346        0.408038
C       -5.086842        0.360407        1.120704
H       -4.794760        1.321490        1.546960
H       -5.908179        0.505457        0.417901
H       -5.417589       -0.307332        1.922389
H       -2.289729        0.751815        1.299861
H       -2.927760       -2.374425       -1.634423
H        4.155574        2.533463        0.466888
O       -0.188886        1.520748       -0.420183
C       -0.502523        2.868436       -0.681645
H       -0.372045        3.498397        0.207821
H        0.106021        3.274100       -1.499146
H       -1.553580        2.875547       -0.973780
O        3.017635       -1.861069        0.140168
C        4.347306       -2.279040        0.332325
H        5.012914       -1.890749       -0.449253
H        4.732022       -1.973949        1.314173
H        4.328765       -3.368104        0.278866
32
4pzHOMe2-ts-H-n ; E = -834.094714688 Hartree
C        2.765649       -0.668167        0.015691
C        3.840820        0.215278        0.125221
C        1.441168       -0.187912       -0.095508
H        4.854444       -0.151256        0.225951
C        3.598344        1.582954        0.108764
C        1.230963        1.209136       -0.111100
C        2.311835        2.089893       -0.012035
H        2.155697        3.161299       -0.027100
N        0.450238       -1.198657       -0.293779
N       -0.731106       -0.880036       -0.084094
C       -1.998382       -0.612445        0.115567
C       -3.129005       -1.228893       -0.462992
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C       -2.582307        0.394402        0.960279
N       -3.899136        0.378751        0.908173
N       -4.205515       -0.586081        0.008283
C       -5.581448       -0.751172       -0.385899
H       -5.721939       -1.749162       -0.803847
H       -6.209942       -0.632538        0.497453
H       -5.866984       -0.001269       -1.130347
H       -3.194702       -2.021971       -1.193278
H       -2.061320        1.067713        1.626792
H        4.433900        2.271634        0.191828
O       -0.045888        1.631123       -0.250480
C       -0.279927        3.009942       -0.417168
H        0.011429        3.582231        0.472655
H        0.252190        3.408180       -1.290073
H       -1.355465        3.109104       -0.568673
O        2.902377       -2.010381        0.026952
C        4.204285       -2.538289        0.101670
H        4.824446       -2.214195       -0.743999
H        4.703460       -2.259636        1.038812
H        4.089548       -3.622271        0.067021
36
4pzHPyr1A-ts-B-m ; E = -816.469106927 Hartree
C       -2.012417        0.740450        0.043542
C       -2.882837        1.836244       -0.096311
C       -0.609531        1.015670        0.253267
H       -3.944992        1.660531       -0.222657
C       -2.420083        3.143636       -0.036770
C       -0.171249        2.365715        0.213098
C       -1.061181        3.419836        0.124924
H       -0.706266        4.444668        0.166396
N        0.236348        0.059582        0.602798
N        1.029178       -0.816968        0.993231
C        2.359998       -0.671608        0.553570
C        2.942045        0.250641       -0.309200
C        3.416700       -1.541218        0.900692
N        4.552067       -1.187993        0.314482
N        4.237265       -0.104221       -0.417835
C        5.278198        0.572407       -1.150386
H        5.897191        1.174242       -0.478500
H        5.906136       -0.173147       -1.639999
H        4.824879        1.219613       -1.902510
H        2.521358        1.090950       -0.841084
H        3.376556       -2.404040        1.551089
H       -3.133060        3.957840       -0.128759
C       -2.660224       -2.751795       -0.776665
C       -1.656680       -1.726003       -0.254064
N       -2.475485       -0.538834       -0.016314
C       -3.895813       -0.828523       -0.128040
C       -3.956352       -2.349909       -0.079117
H       -2.774474       -2.649987       -1.861975
H       -1.155625       -2.075374        0.657563
H       -4.456522       -0.353152        0.685627
H       -4.854633       -2.746870       -0.558305
H       -0.870537       -1.502688       -0.982764
H       -2.350790       -3.778154       -0.564855
H       -3.946664       -2.690093        0.962198
H       -4.303208       -0.448391       -1.079030
H        0.891594        2.539839        0.351803
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36
4pzHPyr1A-ts-B-n ; E = -816.469678615 Hartree
C       -2.140690        0.623652        0.051621
C       -3.140871        1.607563       -0.048365
C       -0.768603        1.064058        0.154976
H       -4.181536        1.307943       -0.095989
C       -2.829763        2.960141       -0.050324
C       -0.493861        2.453425        0.056253
C       -1.504290        3.395168        0.007705
H       -1.269002        4.454610       -0.000372
N        0.204893        0.220986        0.463098
N        1.118235       -0.545033        0.822235
C        2.396594       -0.239231        0.312776
C        3.540371       -0.955232        0.630991
C        2.841917        0.741179       -0.607604
N        4.144143        0.638726       -0.828720
N        4.547322       -0.397425       -0.070466
C        5.947945       -0.733627       -0.027944
H        6.061722       -1.750517        0.350604
H        6.354138       -0.672989       -1.038417
H        6.496209       -0.042341        0.619112
H        3.684218       -1.796749        1.292210
H        2.256281        1.492287       -1.119217
H       -3.637186        3.684357       -0.109153
C       -2.430982       -2.939809       -0.655577
C       -1.521295       -1.792148       -0.221805
N       -2.455157       -0.701493        0.050722
C       -3.836328       -1.154881        0.040683
C       -3.716563       -2.671409        0.121146
H       -2.627266       -2.880039       -1.732227
H       -0.923412       -2.057574        0.659325
H       -4.394444       -0.726256        0.881667
H       -4.592137       -3.180972       -0.288584
H       -0.816692       -1.498613       -1.006720
H       -1.991324       -3.918237       -0.446808
H       -3.599351       -2.981273        1.165425
H       -4.346311       -0.848687       -0.887230
H        0.548558        2.751625        0.111108
36
4pzHPyr1A-ts-H-m ; E = -816.463134887 Hartree
C        3.003385       -1.885121       -0.247781
C        4.050747       -1.490135        0.570338
C        1.852264       -1.109967       -0.389538
H        4.925032       -2.120809        0.694434
C        3.938403       -0.283265        1.256056
C        1.790338        0.181631        0.200113
C        2.835384        0.540622        1.070035
H        2.803011        1.493143        1.586384
N        0.789369       -1.816213       -1.055784
N       -0.358017       -1.500331       -0.691248
C       -1.596636       -1.252086       -0.328983
C       -2.011867       -0.421494        0.736422
C       -2.841684       -1.707672       -0.884064
N       -3.876866       -1.210948       -0.241137
N       -3.346875       -0.448730        0.751363
C       -4.244329        0.163524        1.698792
H       -5.047549        0.664929        1.156230
H       -4.678867       -0.593079        2.358014
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H       -3.692752        0.892013        2.294317
H       -1.417237        0.128649        1.450298
H       -2.983264       -2.352665       -1.741368
H        4.730372        0.040544        1.925544
C       -0.083666        2.682452       -1.607706
C        0.279824        1.203381       -1.471024
N        0.762743        1.067484       -0.087791
C        0.709856        2.356086        0.586189
C       -0.380814        3.097425       -0.169298
H        0.771410        3.254608       -1.985009
H        1.055306        0.888023       -2.178761
H        0.501100        2.227310        1.654732
H       -1.367718        2.731715        0.136736
H        1.661452        2.908363        0.498053
H       -0.345656        4.177596       -0.007135
H       -0.921310        2.841234       -2.291349
H       -0.596804        0.572520       -1.639726
H        3.003765       -2.845221       -0.756525
36
4pzHPyr1A-ts-H-n ; E = -816.462052174 Hartree
C       -3.087697       -1.928716        0.259092
C       -4.292935       -1.409103       -0.186231
C       -1.917131       -1.167501        0.276034
H       -5.185062       -2.026256       -0.214901
C       -4.325840       -0.086762       -0.619074
C       -1.966186        0.210738       -0.070497
C       -3.187514        0.708034       -0.552719
H       -3.256668        1.746186       -0.856817
N       -0.767180       -1.972688        0.575494
N        0.336585       -1.518685        0.231543
C        1.530228       -1.113684       -0.132627
C        2.787960       -1.469980        0.400493
C        1.871093       -0.160818       -1.153302
N        3.173899        0.029765       -1.231394
N        3.703472       -0.739547       -0.251901
C        5.113686       -0.632469        0.025251
H        5.644928       -0.540587       -0.922621
H        5.324580        0.248491        0.639631
H        5.449947       -1.529020        0.548115
H        3.041075       -2.132004        1.215445
H        1.191397        0.319904       -1.842214
H       -5.251176        0.345262       -0.989605
C        0.858258        2.218509        1.189205
C       -0.229361        1.155369        1.379762
N       -0.856631        1.044425        0.062712
C       -0.915279        2.400407       -0.454679
C        0.459175        2.964722       -0.101163
H        0.905923        2.884066        2.055250
H       -0.976634        1.486279        2.120184
H       -1.120708        2.394083       -1.529635
H        1.173054        2.742942       -0.898443
H       -1.708151        2.993240        0.037873
H        0.428095        4.049822        0.025836
H        1.839668        1.752844        1.073198
H        0.166046        0.196589        1.714295
H       -2.988080       -2.967212        0.561973
36
4pzHPyr1B-ts-B-m ; E = -816.470599862 Hartree
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C       -2.423743       -2.274327       -0.191243
C       -3.570452       -2.114826        0.570824
C       -1.510280       -1.204952       -0.351824
H       -4.226751       -2.963497        0.737988
C       -3.885549       -0.865845        1.098491
C       -1.858295        0.091316        0.153005
C       -3.048218        0.225813        0.868487
H       -3.314742        1.190597        1.285692
N       -0.314796       -1.421659       -0.879893
N        0.794847       -1.707261       -1.348134
C        1.885783       -1.234866       -0.589523
C        1.901072       -0.459203        0.566383
C        3.247018       -1.466829       -0.882757
N        4.037687       -0.886845        0.008083
N        3.197878       -0.279070        0.870025
C        3.748750        0.434203        1.995614
H        4.203007       -0.264033        2.703473
H        4.511792        1.131211        1.644384
H        2.948900        0.985231        2.491531
H        1.085556       -0.023350        1.125953
H        3.663208       -2.030368       -1.706335
H       -4.791914       -0.728464        1.679732
C       -0.237252        2.893082       -1.489949
C       -0.366241        1.372240       -1.381046
N       -0.971195        1.143710       -0.053432
C       -1.229767        2.422038        0.594000
C       -0.195315        3.342758       -0.031629
H        0.640561        3.193577       -2.067380
H        0.617895        0.898202       -1.445814
H       -2.242145        2.800416        0.370743
H       -0.432173        4.400446        0.107741
H       -1.143826        2.326067        1.682079
H        0.792970        3.149617        0.401328
H       -1.121448        3.317659       -1.978205
H       -0.995825        0.947292       -2.170992
H       -2.151094       -3.236335       -0.611457
36
4pzHPyr1B-ts-B-n ; E = -816.470394752 Hartree
C        2.277891       -2.414936        0.373558
C        3.474585       -2.429051       -0.325418
C        1.473659       -1.250455        0.408377
H        4.044248       -3.350264       -0.400284
C        3.947171       -1.257177       -0.909660
C        1.988139       -0.030788       -0.145047
C        3.222643       -0.071393       -0.796726
H        3.613173        0.829965       -1.255649
N        0.231189       -1.320719        0.865307
N       -0.932021       -1.474055        1.260674
C       -1.916971       -0.934161        0.405524
C       -3.280246       -1.032025        0.639234
C       -1.813590       -0.219550       -0.814368
N       -3.010619        0.098772       -1.282007
N       -3.884400       -0.402946       -0.386351
C       -5.297712       -0.279505       -0.641438
H       -5.516887        0.745562       -0.944188
H       -5.606879       -0.960668       -1.439269
H       -5.847346       -0.516068        0.270517
H       -3.827196       -1.495347        1.446870
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H       -0.910388        0.082617       -1.327008
H        4.891711       -1.253572       -1.444738
C        0.567276        3.002382        1.243715
C        0.512876        1.475016        1.192897
N        1.227725        1.123659       -0.046190
C        1.665351        2.330622       -0.732023
C        0.697258        3.388439       -0.227408
H       -0.309961        3.431643        1.734326
H       -0.526058        1.131647        1.157239
H        2.697037        2.607475       -0.454641
H        1.066786        4.405086       -0.382840
H        1.638934        2.187071       -1.817814
H       -0.267842        3.288245       -0.736353
H        1.456319        3.334786        1.791493
H        0.991516        1.006784        2.060502
H        1.879723       -3.312458        0.834502
36
4pzHPyr1B-ts-H-m ; E = -816.466937787 Hartree
C        2.042122        0.742056       -0.051898
C        2.640288        2.025790       -0.015252
C        0.620730        0.701785       -0.136771
H        3.717882        2.108705        0.054133
C        1.886275        3.183969       -0.045767
C       -0.114372        1.891483       -0.158252
C        0.491554        3.131600       -0.114159
H       -0.098372        4.042022       -0.145526
N       -0.007717       -0.570350       -0.291373
N       -1.250750       -0.582407       -0.268222
C       -2.564972       -0.627536       -0.236049
C       -3.459659        0.247303        0.419378
C       -3.446295       -1.594093       -0.831267
N       -4.711852       -1.330819       -0.576093
N       -4.694385       -0.235123        0.215678
C       -5.930625        0.213763        0.804689
H       -6.727984        0.074111        0.074180
H       -6.166351       -0.361322        1.705724
H       -5.849023        1.271536        1.060137
H       -3.267653        1.109214        1.041835
H       -3.171990       -2.422608       -1.470517
H        2.395211        4.143344       -0.011944
C        3.709075       -2.425821        0.704462
C        2.417107       -1.734926        0.278964
N        2.841204       -0.365676       -0.010114
C        4.291148       -0.252300       -0.057210
C        4.768385       -1.697780       -0.115864
H        3.888648       -2.265321        1.773890
H        1.974024       -2.204377       -0.606110
H        4.610902        0.333014       -0.927748
H        5.784238       -1.816317        0.269320
H        1.646665       -1.744915        1.053959
H        3.681445       -3.503545        0.524896
H        4.753525       -2.053925       -1.151920
H        4.681808        0.251818        0.842121
H       -1.193046        1.797428       -0.245584
36
4pzHPyr1B-ts-H-n ; E = -816.466985713 Hartree
C        2.110047        0.678006       -0.084349
C        2.823574        1.901304       -0.111129
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C         0.688588        0.767348       -0.068852
H         3.906427        1.885837       -0.121134
C         2.177281        3.123345       -0.104242
C         0.064429        2.018749       -0.053934
C         0.782360        3.198149       -0.070249
H         0.276308        4.158164       -0.069994
N        -0.060246       -0.444144       -0.163005
N        -1.295568       -0.345192       -0.061275
C        -2.602609       -0.268412        0.069757
C        -3.576580       -1.145421       -0.453512
C        -3.396686        0.702656        0.773188
N        -4.685564        0.437192        0.693243
N        -4.772490       -0.663068       -0.087062
C        -6.076357       -1.118924       -0.498278
H        -6.433942       -0.551739       -1.363408
H        -6.027333       -2.178608       -0.753850
H        -6.766905       -0.974092        0.333016
H        -3.464949       -2.015820       -1.083057
H        -3.043469        1.532270        1.371791
H         2.772113        4.032443       -0.121668
C         3.533081       -2.614645        0.629962
C         2.282044       -1.816904        0.274296
N         2.806012       -0.498778       -0.080303
C         4.253811       -0.518693       -0.223303
C         4.594443       -2.002398       -0.277703
H         3.799700       -2.450222        1.680449
H         1.737642       -2.262517       -0.565475
H         4.566553        0.019525       -1.126190
H         5.619659       -2.205772        0.041625
H         1.570099       -1.739881        1.099972
H         3.396730       -3.688764        0.480614
H         4.476385       -2.375405       -1.301173
H         4.747167       -0.036555        0.636804
H        -1.021746        2.024106       -0.059411
48
4pzHPyr2-ts-B-m ; E = -1027.64402182 Hartree
C         0.018016        1.708155        0.246514
C         0.472456        2.822309        0.950309
C         0.875322        0.554440        0.080208
H        -0.170515        3.676593        1.124471
C         1.782491        2.829122        1.425175
C         2.283638        0.678900        0.413052
C         2.678986        1.807496        1.162749
H         3.690269        1.887673        1.540309
N         0.369671       -0.613993       -0.247295
N        -0.086001       -1.773806       -0.395378
C        -1.430972       -1.950656       -0.013360
C        -2.263786       -1.151158        0.763717
C        -2.206642       -3.101404       -0.283264
N        -3.415538       -3.015171        0.254925
N        -3.427930       -1.824119        0.881093
C        -4.578842       -1.454727        1.664390
H        -5.475830       -1.793276        1.144481
H        -4.546532       -1.916050        2.656605
H        -4.607313       -0.368888        1.773454
H        -2.092151       -0.180084        1.202800
H        -1.923633       -3.969337       -0.862971
H         2.128904        3.689445        1.991947
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C         5.317409       -1.172559       -0.405431
C         4.593368       -0.141076        0.457836
N         3.183141       -0.295650        0.115887
C         2.981042       -1.393315       -0.836118
C         4.246560       -2.223677       -0.671083
H         5.628599       -0.711505       -1.349420
H         4.943731        0.876115        0.242632
H         2.076359       -1.961780       -0.627572
H         4.140173       -2.886637        0.194961
C        -2.653651        1.828858       -2.192626
C        -1.481359        1.032713       -1.616396
N        -1.243885        1.644357       -0.294524
C        -2.200188        2.713672       -0.050664
C        -3.371202        2.342163       -0.946651
H        -2.289063        2.677792       -2.782007
H        -1.737978       -0.024560       -1.518990
H        -2.454734        2.767518        1.013787
H        -4.038159        3.186022       -1.139866
H        -0.576873        1.104706       -2.230459
H        -3.287485        1.217912       -2.839951
H        -3.955953        1.536982       -0.486931
H        -1.794943        3.695899       -0.346699
H         2.897918       -0.999360       -1.861285
H         4.452965       -2.843464       -1.547229
H         6.211779       -1.566767        0.083591
H         4.748371       -0.321804        1.531251
48
4pzHPyr2-ts-B-n ; E = -1027.64570221 Hartree
C        -2.388032        0.534910        0.365765
C        -2.968947        1.605319        1.071082
C        -0.963671        0.580266        0.092335
H        -4.012152        1.567669        1.361439
C        -2.216660        2.731492        1.363547
C        -0.264436        1.832292        0.280721
C        -0.891959        2.880231        0.956622
H        -0.367951        3.807596        1.154800
N        -0.321587       -0.535912       -0.174845
N         0.265391       -1.640693       -0.269657
C         1.613651       -1.646326        0.154018
C         2.490274       -2.699390       -0.060972
C         2.353987       -0.737728        0.953613
N         3.580494       -1.186071        1.189189
N         3.641578       -2.376807        0.567061
C         4.881732       -3.108593        0.566452
H         5.557956       -2.741303       -0.212384
H         5.358725       -2.982423        1.539026
H         4.677486       -4.167032        0.395721
H         2.363816       -3.623234       -0.605707
H         2.019141        0.207687        1.356004
H        -2.693909        3.552597        1.892286
C         2.525310        2.230244       -1.995418
C         1.416192        1.314529       -1.475373
N         1.013283        1.932282       -0.201091
C         1.833125        3.097652        0.090963
C         3.095808        2.840040       -0.717102
H         3.265898        1.685000       -2.585802
H         1.790479        0.299669       -1.322558
H         1.346706        4.029066       -0.244800
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H        3.679444        3.748331       -0.886542
C       -4.081733       -2.175196       -1.365137
C       -2.751781       -1.501506       -1.026344
N       -3.111908       -0.566720        0.045936
C       -4.482292       -0.746246        0.488860
C       -4.845898       -2.125856       -0.044757
H       -4.618738       -1.595521       -2.125046
H       -1.996976       -2.220194       -0.692997
H       -4.548832       -0.676366        1.580627
H       -5.924717       -2.260688       -0.156319
H       -2.328127       -0.960867       -1.879476
H       -3.945047       -3.188619       -1.750741
H       -4.473190       -2.897787        0.637480
H       -5.147549        0.024955        0.065002
H        2.009541        3.182485        1.168790
H        3.727357        2.110498       -0.198144
H        2.105470        3.021241       -2.627436
H        0.556397        1.257867       -2.152619
48
4pzHPyr2-ts-H-m ; E = -1027.62970419 Hartree
C       -2.414245        0.478540       -0.466572
C       -2.796661        1.597562       -1.241128
C       -1.030468        0.365777       -0.112861
H       -3.805290        1.670529       -1.625085
C       -1.880366        2.577237       -1.574941
C       -0.157273        1.483032       -0.301714
C       -0.576690        2.555769       -1.097739
H        0.086886        3.384433       -1.308959
N       -0.598401       -0.939683        0.238016
N        0.610337       -1.196802        0.077661
C        1.857210       -1.565482       -0.100381
C        2.835718       -0.892330       -0.865038
C        2.580999       -2.692767        0.421699
N        3.838678       -2.696433        0.027415
N        3.962924       -1.614425       -0.777539
C        5.197330       -1.425719       -1.495558
H        6.020177       -1.736400       -0.850797
H        5.215373       -2.025696       -2.411083
H        5.311150       -0.370990       -1.752247
H        2.746078       -0.005354       -1.473726
H        2.215468       -3.452012        1.100658
H       -2.204216        3.409057       -2.194749
C        2.291451        1.964399        2.301818
C        1.234281        1.040911        1.697237
N        1.081283        1.511519        0.314434
C        1.994994        2.614060        0.056922
C        3.097241        2.400920        1.081302
H        1.820029        2.839646        2.763402
H        0.271934        1.086685        2.220261
H        2.344081        2.594987       -0.982112
H        3.762006        1.592373        0.756794
C       -4.583289       -2.317276        0.598152
C       -3.201407       -1.674099        0.628717
N       -3.372476       -0.447155       -0.148462
C       -4.783472       -0.152241       -0.372122
C       -5.523006       -1.120573        0.543697
H       -4.691247       -2.921857       -0.309755
H       -2.881044       -1.441468        1.655019
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H       -5.007207        0.891559       -0.123726
H       -6.524013       -1.359953        0.175553
H       -2.424171       -2.302865        0.198574
H       -4.754577       -2.969969        1.458012
H       -5.626652       -0.678775        1.541160
H       -5.059870       -0.306606       -1.426968
H        1.514057        3.592572        0.226984
H        3.695831        3.300089        1.247901
H        2.890938        1.462656        3.065511
H        1.573766        0.001906        1.719754
48
4pzHPyr2-ts-H-n ; E = -1027.62897678 Hartree
C        2.486232        0.398153        0.397684
C        3.007886        1.530468        1.062935
C        1.075779        0.380219        0.137061
H        4.041752        1.543711        1.380643
C        2.196654        2.605702        1.376693
C        0.313595        1.583777        0.284202
C        0.868573        2.666331        0.977191
H        0.288629        3.560950        1.164502
N        0.518244       -0.909231       -0.033635
N       -0.706806       -1.045226        0.141520
C       -1.971197       -1.282277        0.407523
C       -2.797223       -2.332523       -0.044079
C       -2.869484       -0.488555        1.201168
N       -4.085937       -1.002996        1.233485
N       -4.028129       -2.095357        0.443231
C       -5.248015       -2.796930        0.137124
H       -5.746660       -2.361531       -0.735390
H       -5.028188       -3.847983       -0.059755
H       -5.908332       -2.717818        1.000978
H       -2.581375       -3.161501       -0.701754
H       -2.620058        0.389590        1.780590
H        2.626504        3.446388        1.914738
C       -2.289458        2.074914       -2.169937
C       -1.233803        1.132093       -1.592441
N       -0.949720        1.674844       -0.260283
C       -1.785645        2.836046        0.003556
C       -2.973795        2.623389       -0.920349
H       -1.813293        2.894375       -2.720673
H       -0.314672        1.095005       -2.189266
H       -2.053918        2.885698        1.064622
H       -3.648325        1.873067       -0.493684
C        4.341690       -2.622532       -0.644212
C        3.016833       -1.868895       -0.610204
N        3.341168       -0.625105        0.087280
C        4.783897       -0.440523        0.201603
C        5.376419       -1.507742       -0.711388
H        4.465806       -3.195518        0.281902
H        2.640695       -1.655977       -1.622385
H        5.073182        0.567839       -0.115106
H        6.377981       -1.814261       -0.398743
H        2.227215       -2.410324       -0.093348
H        4.397709       -3.322909       -1.481535
H        5.445662       -1.120610       -1.734227
H        5.119852       -0.568832        1.242334
H       -1.271584        3.777094       -0.257113
H       -3.537704        3.542780       -1.097110
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H       -2.971817        1.562485       -2.852962
H       -1.624433        0.113084       -1.523226
30
4pzMe-ts-B-m ; E = -683.860614377 Hartree
C        2.672850       -0.314893        1.220558
C        3.954308        0.210544        1.196392
C        2.002065       -0.590815        0.000003
H        4.446029        0.410590        2.145001
C        4.615327        0.483596       -0.000010
C        2.672881       -0.315002       -1.220559
H        2.171426       -0.530261       -2.157817
C        3.954329        0.210456       -1.196406
H        4.446067        0.410434       -2.145020
H        2.171377       -0.530084        2.157822
N        0.771054       -1.067709        0.000007
N       -0.365194       -1.532473       -0.000019
C       -1.427397       -0.625285        0.000031
C       -1.436927        0.775155        0.000033
C       -2.788025       -1.024691        0.000018
N       -3.575635        0.037093        0.000004
N       -2.739538        1.107395        0.000023
C       -3.318809        2.429867       -0.000105
H       -4.399219        2.295844       -0.000507
H       -3.022908        2.988372        0.892224
H       -3.022262        2.988493       -0.892138
C       -0.322276        1.756128        0.000043
H        0.321357        1.617087        0.874547
H        0.321122        1.617383       -0.874678
H       -0.690305        2.784312        0.000278
C       -3.338767       -2.406129        0.000023
H       -3.001941       -2.961785       -0.879876
H       -3.002005       -2.961755        0.879965
H       -4.429404       -2.367288       -0.000013
H        5.618486        0.894927       -0.000017
30
4pzMe-ts-B-n ; E = -683.862607625 Hartree
C        2.788975        0.321153       -1.219554
C        4.106642       -0.105153       -1.194326
C        2.099504        0.545905        0.000084
H        4.612325       -0.269190       -2.142469
C        4.785632       -0.325464        0.002737
C        2.786817        0.321941        1.221089
H        2.268016        0.494025        2.157692
C        4.104526       -0.104396        1.198455
H        4.608533       -0.267827        2.147594
H        2.271827        0.492641       -2.157181
N        0.838072        0.938277       -0.001138
N       -0.325123        1.326916       -0.001704
C       -1.326175        0.352198       -0.001515
C       -2.675187        0.699685       -0.003147
C       -1.289533       -1.073187       -0.002008
N       -2.522237       -1.550265       -0.003647
N       -3.341466       -0.467441       -0.006407
C       -4.768938       -0.664399        0.011443
H       -5.202177       -0.322641        0.956647
H       -5.243994       -0.127679       -0.814474
H       -4.944696       -1.733145       -0.100710
C       -3.316405        2.036588       -0.001330
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H       -3.947377        2.179936        0.882606
H       -2.535831        2.799054        0.000800
H       -3.944834        2.183368       -0.886641
C       -0.111818       -1.981124       -0.003121
H        0.522406       -1.811691       -0.879139
H        0.522488       -1.813562        0.873192
H       -0.452634       -3.018203       -0.004233
H        5.816989       -0.659973        0.003755
30
4pzMe-ts-H-m ; E = -683.857597679 Hartree
C       -2.116417       -0.470672       -0.755591
C       -3.253437       -1.240696       -0.968823
C       -2.173989        0.632458        0.099757
H       -3.213980       -2.088850       -1.646883
C       -4.447886       -0.919513       -0.325277
C       -3.379683        0.979213        0.709039
H       -3.400580        1.862874        1.340114
C       -4.508115        0.192312        0.513635
H       -5.440156        0.449057        1.008736
H       -1.183891       -0.688775       -1.268535
N       -1.068699        1.519729        0.325970
N        0.064098        1.027337        0.177041
C        1.264786        0.507899        0.060772
C        1.662788       -0.850196        0.189820
C        2.500770        1.210925       -0.188162
N        3.518684        0.378797       -0.222084
N        2.993106       -0.852630        0.044311
C        3.892235       -1.967922        0.195193
H        3.605829       -2.791605       -0.464917
H        4.886019       -1.614123       -0.075950
H        3.902700       -2.326660        1.229474
C        0.863540       -2.046591        0.536003
H        1.048940       -2.375719        1.565425
H       -0.198659       -1.805662        0.451942
H        1.090516       -2.889276       -0.125887
C        2.641936        2.665753       -0.443406
H        3.665309        2.991398       -0.248470
H        2.395494        2.911280       -1.482149
H        1.946939        3.220760        0.193178
H       -5.333967       -1.525152       -0.490502
30
4pzMe-ts-H-n ; E = -683.857916569 Hartree
C       -2.222214        0.454656        0.754332
C       -3.426176        1.108382        0.985660
C       -2.191963       -0.676977       -0.063388
H       -3.453101        1.980703        1.632866
C       -4.601257        0.640485        0.398897
C       -3.374044       -1.170748       -0.615032
H       -3.322624       -2.072610       -1.218029
C       -4.572327       -0.500683       -0.401409
H       -5.488385       -0.871284       -0.852238
H       -1.300237        0.786800        1.222706
N       -1.006819       -1.448565       -0.304354
N        0.069786       -0.830843       -0.211155
C        1.214237       -0.188034       -0.172587
C        2.485718       -0.769287        0.067589
C        1.502424        1.217585       -0.355931
N        2.792938        1.447951       -0.232179
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N        3.359722        0.242070        0.060734
C        4.764238        0.200076        0.377330
H        5.246532       -0.636914       -0.133658
H        5.200182        1.137519        0.033996
H        4.923245        0.100377        1.456171
C        2.809684       -2.184676        0.346537
H        3.091461       -2.349370        1.393070
H        1.919506       -2.782640        0.135143
H        3.633576       -2.541626       -0.280418
C        0.555307        2.290567       -0.750739
H        0.313677        2.223289       -1.817066
H       -0.390066        2.196967       -0.209210
H        0.995494        3.271158       -0.560762
H       -5.540414        1.155256        0.578547
52
4pzMeAmid2-ts-B-m ; E = -1478.12028087 Hartree
C        2.121389        1.655123        0.009619
C        2.352425        3.013553        0.212479
C        0.781794        1.166699       -0.127203
H        3.366387        3.363133        0.348452
C        1.269998        3.888679        0.205075
C       -0.299713        2.109606       -0.128905
C       -0.045267        3.469082        0.020113
H       -0.869750        4.168466        0.002771
N        0.541107       -0.131374       -0.248895
N        0.344139       -1.358220       -0.419171
C       -0.887749       -1.837137        0.064147
C       -1.616309       -1.462921        1.196153
C       -1.623393       -2.892471       -0.531823
N       -2.734230       -3.126000        0.153263
N       -2.696741       -2.274376        1.202663
C       -3.798388       -2.255055        2.130008
H       -3.432286       -2.175989        3.156228
H       -4.473229       -1.416881        1.922938
H       -4.340842       -3.192148        2.010621
C       -1.332269       -0.488012        2.281867
H       -1.371976       -0.968516        3.265607
H       -0.338336       -0.059706        2.151253
H       -2.049863        0.339442        2.284358
C       -1.294617       -3.639046       -1.775590
H       -1.428936       -3.010233       -2.661989
H       -0.249966       -3.962013       -1.765211
H       -1.942397       -4.512672       -1.869267
H        1.461143        4.949255        0.339302
N        3.105351        0.686976       -0.044781
H        2.760260       -0.241518       -0.266016
N       -1.554233        1.559947       -0.326280
H       -1.559771        0.548928       -0.416676
C        4.456258        0.841672        0.128004
O        5.018435        1.890814        0.404718
C       -2.771418        2.191388       -0.358904
O       -2.951012        3.393756       -0.240548
C        6.558667       -0.640894        0.045468
C        6.732189       -2.028963       -0.217475
C        5.486396       -2.528536       -0.448564
O        4.557355       -1.553262       -0.347864
C        5.219370       -0.401103       -0.045801
H        7.309668        0.100256        0.273517
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H        7.658110       -2.584877       -0.233923
H        5.112571       -3.512315       -0.687114
C       -5.246285        1.484859       -0.571797
C       -5.851466        0.210578       -0.770009
C       -4.830181       -0.688413       -0.856254
O       -3.641882       -0.059147       -0.723303
C       -3.899779        1.267188       -0.548595
H       -5.724880        2.445913       -0.458163
H       -6.906248       -0.010789       -0.842829
H       -4.770499       -1.758956       -0.987559
52
4pzMeAmid2-ts-B-n ; E = -1478.11684741 Hartree
C       -2.104529       -1.713990        0.005353
C       -2.359900       -3.070608        0.174920
C       -0.757504       -1.241081       -0.131842
H       -3.379882       -3.402138        0.311346
C       -1.296734       -3.967700        0.119665
C        0.305261       -2.200997       -0.157457
C        0.019968       -3.561016       -0.068222
H        0.830190       -4.273980       -0.135805
N       -0.530477        0.057242       -0.281020
N       -0.286594        1.262931       -0.503547
C        0.886813        1.798395        0.046152
C        1.512238        2.909942       -0.514471
C        1.602617        1.520531        1.247012
N        2.600296        2.384321        1.387435
N        2.536370        3.201030        0.310467
C        3.547446        4.211519        0.135195
H        4.304598        3.896138       -0.591166
H        3.096189        5.145603       -0.207205
H        4.019601        4.371102        1.104055
C        1.188468        3.644960       -1.761357
H        1.940820        3.481054       -2.541020
H        0.227343        3.285270       -2.133671
H        1.115201        4.724029       -1.589013
C        1.307006        0.518872        2.309498
H        1.811663        0.812322        3.232054
H        0.231006        0.458472        2.496322
H        1.647396       -0.485161        2.040742
H       -1.504767       -5.028833        0.217730
N       -3.076734       -0.729736       -0.024306
H       -2.722570        0.194338       -0.247943
N        1.584692       -1.687671       -0.302396
H        1.653170       -0.679193       -0.221083
C       -4.426541       -0.866474        0.158191
O       -5.004344       -1.908186        0.432492
C        2.760733       -2.376477       -0.467270
O        2.855810       -3.575170       -0.682888
C       -6.509186        0.644791        0.106975
C       -6.668059        2.037399       -0.142220
C       -5.418631        2.523518       -0.380692
O       -4.500523        1.535709       -0.297340
C       -5.174167        0.389060        0.001001
H       -7.266857       -0.089192        0.335984
H       -7.587165        2.604794       -0.144762
H       -5.035110        3.504842       -0.613839
C        5.280209       -1.801982       -0.509085
C        5.975830       -0.603025       -0.180711
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C         5.022890        0.306832        0.167715
O         3.793981       -0.241002        0.068558
C         3.954306       -1.529108       -0.341487
H         5.687880       -2.751403       -0.822002
H         7.043720       -0.440585       -0.190407
H         5.044113        1.324726        0.525489
52
4pzMeAmid2-ts-H-m ; E = -1478.11838419 Hartree
C         0.111351       -1.954017       -0.168188
C        -0.132107       -3.312097        0.053369
C        -0.963961       -1.037001       -0.132526
H         0.698627       -4.003579        0.039375
C        -1.433574       -3.742904        0.277383
C        -2.284646       -1.517903        0.027968
C        -2.518062       -2.874568        0.254565
H        -3.531171       -3.217231        0.410604
N        -0.879995        0.368494       -0.352176
N         0.155484        0.956245        0.021250
C         1.263350        1.587897        0.328491
C         2.251356        1.192288        1.272432
C         1.802199        2.785568       -0.267436
N         2.989109        3.060543        0.230278
N         3.212421        2.117255        1.192442
C         4.450717        2.162466        1.928384
H         4.272151        1.923534        2.979029
H         5.173138        1.452438        1.512063
H         4.846372        3.173931        1.843319
C         2.240586        0.073523        2.241812
H         2.160305        0.432665        3.274545
H         1.378228       -0.565161        2.039409
H         3.148922       -0.533394        2.166046
C         1.187915        3.575726       -1.362963
H         1.290827        3.062888       -2.325657
H         0.116956        3.701960       -1.179915
H         1.665179        4.554111       -1.440880
H        -1.611058       -4.799366        0.454867
N         1.384709       -1.478455       -0.497393
H         1.434282       -0.517889       -0.801008
N        -3.288902       -0.557479       -0.027381
H        -2.946325        0.371546       -0.256331
C         2.589932       -2.109207       -0.355315
O         2.766919       -3.238922        0.076579
C        -4.633231       -0.733103        0.137371
O        -5.191621       -1.789280        0.400822
C         5.078228       -1.472461       -0.567146
C         5.722374       -0.282717       -1.016801
C         4.728544        0.556764       -1.422574
O         3.522302       -0.029482       -1.258944
C         3.740112       -1.266932       -0.730824
H         5.525375       -2.369899       -0.166873
H         6.782853       -0.078365       -1.042417
H         4.711008        1.561894       -1.814976
C        -6.759133        0.715190        0.065361
C        -6.959576        2.102398       -0.184579
C        -5.723541        2.627763       -0.408702
O        -4.775598        1.669402       -0.315703
C        -5.415685        0.501888       -0.025632
H        -7.495269       -0.043065        0.285227
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H       -7.896038        2.640574       -0.197135
H       -5.369049        3.621082       -0.637179
52
4pzMeAmid2-ts-H-n ; E = -1478.11386239 Hartree
C        0.108413       -2.035276       -0.112141
C       -0.173008       -3.389137        0.089609
C       -0.946051       -1.094237       -0.100881
H        0.642563       -4.098589        0.097454
C       -1.490322       -3.791574        0.268158
C       -2.281942       -1.545681        0.013316
C       -2.553656       -2.898389        0.218516
H       -3.578721       -3.218981        0.339010
N       -0.824189        0.311334       -0.295388
N        0.215289        0.870633        0.110830
C        1.297690        1.492237        0.514659
C        1.812278        2.714574        0.009755
C        2.266714        1.081357        1.508980
N        3.246591        1.956412        1.584377
N        2.971474        2.907704        0.646369
C        3.968680        3.917432        0.402525
H        3.508529        4.788262       -0.066052
H        4.407815        4.202813        1.358833
H        4.760545        3.530303       -0.247503
C        1.250794        3.570223       -1.058595
H        0.242074        3.213690       -1.281591
H        1.190621        4.618795       -0.749124
H        1.838276        3.525951       -1.982870
C        2.170109       -0.082925        2.428270
H        1.961502        0.245446        3.451325
H        1.361860       -0.745957        2.113454
H        3.107382       -0.645123        2.442899
H       -1.697316       -4.844927        0.431662
N        1.398190       -1.586407       -0.404190
H        1.477477       -0.620623       -0.683357
N       -3.262483       -0.561646       -0.062505
H       -2.891124        0.362494       -0.263811
C        2.584748       -2.250007       -0.255031
O        2.726877       -3.386699        0.170613
C       -4.614851       -0.708235        0.053341
O       -5.207163       -1.754451        0.279844
C        5.088371       -1.697681       -0.503185
C        5.767035       -0.551177       -1.006896
C        4.796928        0.313025       -1.412475
O        3.571114       -0.213697       -1.198194
C        3.756121       -1.443158       -0.638537
H        5.509923       -2.600466       -0.087851
H        6.833605       -0.389696       -1.061262
H        4.816071        1.291797       -1.866581
C       -6.704217        0.788735       -0.065152
C       -6.866571        2.183845       -0.298631
C       -5.612941        2.685250       -0.473766
O       -4.689118        1.704825       -0.365893
C       -5.363530        0.547224       -0.115886
H       -7.463125        0.043438        0.118557
H       -7.790369        2.742622       -0.332447
H       -5.230134        3.674164       -0.673874
30
4pzMeCl1A-ts-B-m ; E = -1143.30051289 Hartree
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C       -2.526970       -0.089443       -0.648197
C       -3.797384        0.425153       -0.462605
C       -1.742581       -0.537425        0.447543
H       -4.355732        0.745415       -1.336528
C       -4.339646        0.538265        0.814883
C       -2.309782       -0.413168        1.744361
H       -1.728308       -0.749458        2.595449
C       -3.577606        0.118036        1.904165
H       -3.979622        0.198316        2.910310
Cl       -1.835371       -0.201767       -2.243638
N       -0.534542       -1.024791        0.267597
N        0.598767       -1.494430        0.214264
C        1.666600       -0.605121        0.172861
C        1.698994        0.796715        0.149872
C        3.020981       -1.027669        0.127683
N        3.823980        0.020079        0.085565
N        3.004612        1.105225        0.098538
C        3.605634        2.417093        0.040521
H        3.312918        2.942778       -0.872561
H        3.323163        3.015646        0.910613
H        4.683637        2.265293        0.040216
C        0.601811        1.796546        0.152644
H       -0.054613        1.644000       -0.710159
H       -0.023597        1.690886        1.044241
H        0.987382        2.817576        0.118598
C        3.547107       -2.418249        0.129149
H        4.634638       -2.400386        0.040994
H        3.274366       -2.939631        1.051399
H        3.128961       -2.993152       -0.701843
H       -5.334557        0.945770        0.952080
30
4pzMeCl1A-ts-B-n ; E = -1143.30224341 Hartree
C       -2.620841       -0.672404       -0.024855
C       -3.929345       -0.427053       -0.400267
C       -1.827235        0.333750        0.586138
H       -4.492970       -1.233827       -0.857916
C       -4.502942        0.826516       -0.204894
C       -2.426376        1.606757        0.777853
H       -1.836671        2.389723        1.241143
C       -3.733099        1.830267        0.380883
H       -4.158874        2.816948        0.540567
Cl       -1.894246       -2.232179       -0.294794
N       -0.583393        0.096199        0.942484
N        0.576911       -0.055799        1.309933
C        1.581715        0.111598        0.363591
C        2.925786       -0.043286        0.704960
C        1.564631        0.433081       -1.026571
N        2.801419        0.472662       -1.487431
N        3.604857        0.183476       -0.431020
C        5.029843        0.163452       -0.643281
H        5.528281       -0.132876        0.279681
H        5.272892       -0.550083       -1.433520
H        5.377401        1.155548       -0.941711
C        3.526215       -0.384764        2.018130
H        4.185091        0.410275        2.382722
H        2.718886       -0.522466        2.739400
H        4.107393       -1.311465        1.968550
C        0.401001        0.686834       -1.916025
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H       -0.260341       -0.184739       -1.952659
H       -0.202184        1.526150       -1.556202
H        0.756180        0.908214       -2.924140
H       -5.527573        1.011379       -0.506150
30
4pzMeCl1A-ts-H-m ; E = -1143.29239648 Hartree
C        2.197202       -0.299728        0.598727
C        3.371216       -1.045137        0.524926
C        1.998588        0.808848       -0.231926
H        3.503715       -1.890084        1.192704
C        4.359903       -0.692932       -0.386027
C        3.026491        1.174442       -1.103433
H        2.869344        2.063128       -1.708045
C        4.188337        0.423547       -1.202369
H        4.963162        0.711208       -1.906268
Cl        1.023026       -0.742043        1.809828
N        0.860991        1.692105       -0.202819
N       -0.251290        1.138254       -0.173391
C       -1.438921        0.586814       -0.167914
C       -1.773473       -0.762168       -0.468087
C       -2.708394        1.204342        0.134059
N       -3.688698        0.335121        0.036990
N       -3.099914       -0.839145       -0.351494
C       -3.947683       -1.966595       -0.645100
H       -4.036003       -2.122469       -1.725314
H       -3.550386       -2.873984       -0.183677
H       -4.930872       -1.745881       -0.231420
C       -0.904154       -1.870898       -0.919173
H        0.134905       -1.537011       -0.892464
H       -1.002176       -2.748395       -0.271630
H       -1.140963       -2.180143       -1.943681
C       -2.922136        2.609548        0.559364
H       -2.652319        2.743238        1.612369
H       -2.281896        3.277498       -0.023611
H       -3.968096        2.893753        0.432023
H        5.270674       -1.280963       -0.441333
30
4pzMeCl1A-ts-H-n ; E = -1143.29188391 Hartree
C        2.282253       -0.316769        0.601080
C        3.522443       -0.939973        0.492330
C        2.009424        0.861538       -0.101449
H        3.710455       -1.845929        1.059054
C        4.503606       -0.392868       -0.326058
C        3.026033        1.421917       -0.876502
H        2.806991        2.359223       -1.379979
C        4.256050        0.794939       -1.011291
H        5.023545        1.233685       -1.641401
Cl        1.114825       -1.002693        1.700199
N        0.790550        1.624145       -0.014854
N       -0.258426        0.966199       -0.123737
C       -1.389922        0.323384       -0.271192
C       -2.680851        0.789230        0.090866
C       -1.630304       -0.995096       -0.812762
N       -2.912610       -1.284282       -0.780084
N       -3.522022       -0.203287       -0.203013
C       -4.931157       -0.287935        0.084052
H       -5.103931       -0.609353        1.116445
H       -5.406986        0.682137       -0.074221
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H       -5.360533       -1.022805       -0.596250
C       -3.046888        2.073184        0.726305
H       -2.161260        2.713369        0.729335
H       -3.848818        2.581394        0.180484
H       -3.378112        1.941130        1.762487
C       -0.631773       -1.902795       -1.430782
H       -0.384493       -1.574140       -2.446048
H        0.295007       -1.898898       -0.851864
H       -1.026184       -2.918919       -1.486349
H        5.466367       -0.887076       -0.410843
30
4pzMeCl1B-ts-B-m ; E = -1143.30051303 Hartree
C        2.306295       -0.414338        1.744410
C        3.574124        0.115934        1.907305
C        1.741938       -0.537531        0.446250
H        3.974078        0.195119        2.914359
C        4.338553        0.536908        0.820001
C        2.528697       -0.088869       -0.647507
Cl        1.840409       -0.199074       -2.243903
C        3.798808        0.425346       -0.458690
H        4.359040        0.746361       -1.331133
H        1.722826       -0.750959        2.594000
N        0.534171       -1.024536        0.263391
N       -0.599006       -1.494446        0.209543
C       -1.667104       -0.605334        0.170937
C       -1.699689        0.796515        0.148857
C       -3.021476       -1.028027        0.126845
N       -3.824646        0.019656        0.086340
N       -3.005390        1.104893        0.098969
C       -3.606629        2.416745        0.042790
H       -4.684577        2.264616        0.038872
H       -3.326939        3.013070        0.915333
H       -3.311347        2.944949       -0.867986
C       -0.602593        1.796409        0.150512
H       -0.988287        2.817429        0.117496
H        0.024144        1.690425        1.041134
H        0.052588        1.644244       -0.713318
C       -3.547411       -2.418663        0.128481
H       -3.123809       -2.995582       -0.698296
H       -3.280607       -2.937640        1.053858
H       -4.634381       -2.401215        0.033557
H        5.333337        0.943895        0.959627
30
4pzMeCl1B-ts-B-n ; E = -1143.30233100 Hartree
C        2.441702       -1.613524       -0.756322
C        3.749323       -1.820289       -0.353369
C        1.831195       -0.343342       -0.583286
H        4.183797       -2.805488       -0.497987
C        4.509498       -0.801556        0.219047
C        2.614945        0.678448        0.014385
Cl        1.874901        2.235792        0.260190
C        3.925032        0.449832        0.394962
H        4.481047        1.268031        0.841500
H        1.859642       -2.407975       -1.209593
N        0.585892       -0.121756       -0.945009
N       -0.574817        0.023109       -1.313577
C       -1.578435       -0.126884       -0.362190
C       -2.922660        0.019668       -0.704128
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C       -1.559629       -0.427578        1.032796
N       -2.796047       -0.462498        1.495563
N       -3.601464       -0.196293        0.433616
C       -5.025644       -0.115065        0.639299
H       -5.358632        0.926380        0.694312
H       -5.555196       -0.618699       -0.172800
H       -5.245731       -0.612501        1.582824
C       -3.541153        0.344834       -2.011751
H       -2.748732        0.472649       -2.750884
H       -4.209129       -0.454181       -2.351735
H       -4.124773        1.270188       -1.961617
C       -0.395550       -0.672883        1.924400
H        0.207584       -1.515707        1.572878
H        0.265657        0.199048        1.953325
H       -0.750645       -0.884826        2.934602
H        5.535101       -0.973271        0.524742
30
4pzMeCl1B-ts-H-m ; E = -1143.29336567 Hartree
C        1.485018       -1.149017        0.951699
C        2.463617       -2.126387        1.071157
C        1.753437        0.065136        0.314805
H        2.242950       -3.057848        1.583939
C        3.732987       -1.900168        0.543552
C        3.039940        0.286178       -0.185827
Cl        3.417376        1.782849       -0.979889
C        4.021156       -0.694084       -0.088053
H        5.003250       -0.504888       -0.508082
H        0.494651       -1.287831        1.377194
N        0.801239        1.136736        0.274240
N       -0.392925        0.795213        0.223308
C       -1.654449        0.446948        0.124597
C       -2.204121       -0.780094       -0.339059
C       -2.811838        1.255766        0.427414
N       -3.922960        0.595356        0.190199
N       -3.529492       -0.619405       -0.299761
C       -4.541982       -1.538776       -0.753970
H       -4.436666       -2.508766       -0.259928
H       -5.506083       -1.102420       -0.496541
H       -4.483555       -1.681179       -1.837621
C       -1.526815       -1.983139       -0.870792
H       -0.458149       -1.918982       -0.653470
H       -1.925980       -2.901180       -0.426515
H       -1.641425       -2.064470       -1.958089
C       -2.795821        2.630081        0.985907
H       -2.625027        2.613120        2.067717
H       -1.977269        3.201183        0.538980
H       -3.746269        3.131939        0.796538
H        4.506361       -2.657069        0.629501
30
4pzMeCl1B-ts-H-n ; E = -1143.29395053 Hartree
C       -1.624649        1.206748        0.852069
C       -2.696446        2.082053        0.958113
C       -1.789574       -0.071625        0.314630
H       -2.553411        3.067586        1.391028
C       -3.957629        1.685235        0.518928
C       -3.066985       -0.463660       -0.096224
Cl       -3.317368       -2.047498       -0.763752
C       -4.143446        0.411969       -0.011052
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H       -5.118256        0.089850       -0.361297
H       -0.635627        1.478435        1.210649
N       -0.728907       -1.035789        0.289894
N        0.415968       -0.568176        0.156648
C        1.628556       -0.106340       -0.038347
C        2.836180       -0.787246        0.268560
C        2.069756        1.152051       -0.599607
N        3.383459        1.217093       -0.618898
N        3.822307        0.048355       -0.062132
C        5.236816       -0.116458        0.156923
H        5.753220        0.560940       -0.522377
H        5.507380        0.131610        1.188511
H        5.534167       -1.145934       -0.054026
C        3.003171       -2.121561        0.882906
H        3.685960       -2.750920        0.302476
H        3.391926       -2.061006        1.905748
H        2.022409       -2.602587        0.916251
C        1.228639        2.223171       -1.190029
H        0.826299        1.909864       -2.159265
H        0.368617        2.443639       -0.551466
H        1.819998        3.128397       -1.337913
H       -4.803576        2.361189        0.595659
30
4pzMeCl2-ts-B-m ; E = -1602.73869229 Hartree
C       -2.291672        1.206109       -0.094275
C       -3.567756        1.202224        0.437661
C       -1.605234       -0.001300       -0.401671
H       -4.042379        2.155729        0.644143
C       -4.222397        0.002979        0.706169
C       -2.292744       -1.206329       -0.087474
Cl       -1.458158       -2.703585       -0.380894
C       -3.568805       -1.198345        0.444421
H       -4.044258       -2.150256        0.656277
Cl       -1.455880        2.700819       -0.396067
N       -0.400834       -0.003298       -0.915574
N        0.722051       -0.004560       -1.411185
C        1.810514       -0.002207       -0.555422
C        1.880873        0.003440        0.846240
C        3.154729       -0.004588       -1.014524
N        3.984794       -0.000895        0.011630
N        3.193634        0.003849        1.119330
C        3.831541        0.009434        2.415281
H        3.558718        0.903964        2.981494
H        3.560309       -0.881142        2.988465
H        4.904806        0.009684        2.233274
C        0.808978        0.007800        1.872243
H        0.165810        0.885388        1.752645
H        0.168331       -0.872988        1.762781
H        1.219270        0.014229        2.884060
C        3.642351       -0.010883       -2.418610
H        3.283092       -0.895687       -2.951838
H        3.275852        0.864519       -2.962242
H        4.733449       -0.006679       -2.429398
H       -5.224122        0.004579        1.119051
30
4pzMeCl2-ts-B-n ; E = -1602.74057169 Hartree
C       -2.373117        1.214048       -0.126854
C       -3.685897        1.219032        0.306855
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C       -1.674505        0.001646       -0.378864
H       -4.167771        2.175840        0.478075
C       -4.367709        0.024479        0.522661
C       -2.393792       -1.198646       -0.127531
Cl       -1.555257       -2.701471       -0.370961
C       -3.706384       -1.181476        0.306295
H       -4.204522       -2.129989        0.477115
Cl       -1.509199        2.703032       -0.369418
N       -0.433279       -0.008982       -0.797940
N        0.721674       -0.009470       -1.209471
C        1.743025       -0.009834       -0.273781
C        3.082237       -0.012772       -0.668440
C        1.754452       -0.013081        1.154051
N        3.001136       -0.017318        1.586325
N        3.784457       -0.022354        0.473948
C        5.216521        0.025943        0.631050
H        5.448864       -0.345442        1.628274
H        5.697986       -0.606925       -0.117405
H        5.590235        1.050072        0.531800
C        3.670213       -0.005427       -2.029255
H        4.292389        0.880542       -2.193995
H        4.292608       -0.889953       -2.202809
H        2.859992       -0.003116       -2.760017
C        0.607511       -0.018167        2.099081
H       -0.025902        0.862721        1.954049
H       -0.025695       -0.897703        1.945037
H        0.981567       -0.023385        3.124461
H       -5.397248        0.033203        0.860235
30
4pzMeCl2-ts-H-m ; E = -1602.72751287 Hartree
C        1.745773       -1.145446        0.661189
C        2.818605       -1.973711        0.346842
C        1.729282        0.206013        0.299789
H        2.798516       -3.012215        0.658700
C        3.901373       -1.454015       -0.350962
C        2.846064        0.699126       -0.382484
Cl        2.871643        2.370215       -0.855058
C        3.919119       -0.113815       -0.722296
H        4.754118        0.306127       -1.271990
Cl        0.428387       -1.826730        1.577433
N        0.711024        1.142817        0.710205
N       -0.454034        0.824315        0.427086
C       -1.693733        0.526368        0.131381
C       -2.155163       -0.514971       -0.720473
C       -2.902871        1.170180        0.587740
N       -3.963950        0.587481        0.079546
N       -3.483412       -0.420752       -0.717275
C       -4.428104       -1.190227       -1.487106
H       -5.402885       -1.075136       -1.014529
H       -4.482568       -0.827802       -2.518813
H       -4.142715       -2.244425       -1.490918
C       -1.376564       -1.487140       -1.518169
H       -0.314395       -1.334057       -1.316993
H       -1.631579       -2.519361       -1.256017
H       -1.547992       -1.358809       -2.592578
C       -2.991386        2.308942        1.534345
H       -2.755308        1.983841        2.552968
H       -2.261772        3.078476        1.267173
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H       -3.996135        2.734448        1.527652
H        4.740452       -2.095189       -0.600726
30
4pzMeCl2-ts-H-n ; E = -1602.72737419 Hartree
C       -1.901144       -1.168221       -0.542617
C       -3.068908       -1.830365       -0.179288
C       -1.749152        0.208584       -0.355638
H       -3.151921       -2.897797       -0.351745
C       -4.112115       -1.111592        0.391146
C       -2.827145        0.903271        0.198763
Cl       -2.683006        2.616747        0.450373
C       -3.995863        0.260397        0.585252
H       -4.798835        0.835042        1.033297
Cl       -0.633504       -2.095184       -1.300058
N       -0.610911        0.962956       -0.826949
N        0.487159        0.579059       -0.394494
C        1.669343        0.234536        0.050250
C        2.923269        0.709769       -0.418329
C        2.013921       -0.687331        1.108489
N        3.316884       -0.756479        1.258581
N        3.844184        0.086770        0.313859
C        5.277968        0.143082        0.182464
H        5.711451       -0.033107        1.166845
H        5.637321       -0.625282       -0.509474
H        5.579173        1.126409       -0.182537
C        3.185281        1.669537       -1.512165
H        2.223588        2.051454       -1.863149
H        3.795946        2.513452       -1.174121
H        3.700055        1.197996       -2.356234
C        1.077273       -1.438181        1.981034
H        0.473064       -0.750215        2.580873
H        0.385994       -2.032253        1.376702
H        1.632069       -2.096650        2.651241
H       -5.024799       -1.622683        0.679823
30
4pzMeF1A-ts-B-m ; E = -783.003123547 Hartree
C        2.518209        0.196039        0.877011
C        3.793923        0.676288        0.703130
C        1.874555       -0.625054       -0.080112
H        4.219029        1.294560        1.487499
C        4.498445        0.377701       -0.465927
C        2.604042       -0.920975       -1.257798
H        2.137992       -1.544102       -2.012554
C        3.882716       -0.409767       -1.434288
H        4.410861       -0.649920       -2.352647
F        1.807078        0.511872        1.983369
N        0.651503       -1.067023        0.138857
N       -0.489148       -1.502347        0.277909
C       -1.550432       -0.626898        0.059997
C       -1.573666        0.755337       -0.169487
C       -2.907320       -1.042540        0.071758
N       -3.703131       -0.009915       -0.142753
N       -2.877118        1.060408       -0.281115
C       -3.469449        2.360438       -0.490320
H       -3.288286        3.018297        0.364650
H       -3.075476        2.827015       -1.396778
H       -4.540644        2.200489       -0.600824
C       -0.471836        1.748048       -0.233139
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H        0.169683        1.649065        0.647008
H        0.163415        1.579007       -1.108267
H       -0.852546        2.770786       -0.274534
C       -3.441932       -2.415911        0.269248
H       -3.033566       -2.863909        1.179128
H       -4.530333       -2.381260        0.340930
H       -3.165212       -3.068843       -0.564194
H        5.503110        0.757857       -0.610463
30
4pzMeF1A-ts-B-n ; E = -783.004922900 Hartree
C       -2.608376       -0.276088        0.854214
C       -3.919580       -0.658509        0.701972
C       -1.964776        0.608898       -0.044528
H       -4.343998       -1.333706        1.438257
C       -4.659193       -0.196480       -0.389706
C       -2.730970        1.074662       -1.140021
H       -2.263977        1.748861       -1.848923
C       -4.044569        0.655424       -1.302381
H       -4.600527        1.021482       -2.160752
F       -1.868303       -0.745308        1.881462
N       -0.706751        0.952975        0.153335
N        0.460266        1.287846        0.336668
C        1.456562        0.360753        0.037518
C        2.805867        0.694611        0.147305
C        1.424751       -1.002812       -0.380785
N        2.658282       -1.456061       -0.515182
N        3.474874       -0.419078       -0.193231
C        4.901576       -0.594077       -0.294851
H        5.094353       -1.665464       -0.328265
H        5.294541       -0.128006       -1.204282
H        5.400398       -0.159526        0.574731
C        3.438993        1.975897        0.542277
H        4.047092        2.393206       -0.267638
H        2.653049        2.690744        0.791196
H        4.086917        1.851668        1.416766
C        0.249341       -1.883087       -0.612520
H       -0.376998       -1.931701        0.283003
H       -0.381195       -1.504163       -1.422681
H        0.591502       -2.887724       -0.867845
H       -5.690893       -0.502822       -0.518826
30
4pzMeF1A-ts-H-m ; E = -782.998860638 Hartree
C        2.142306       -0.435787        0.641703
C        3.296198       -1.196140        0.742203
C        2.084148        0.720483       -0.143211
H        3.288574       -2.077875        1.374712
C        4.434115       -0.802452        0.043916
C        3.251218        1.116848       -0.798516
H        3.206081        2.037855       -1.372703
C        4.411784        0.357587       -0.728281
H        5.300687        0.672660       -1.265586
F        1.066267       -0.819169        1.350855
N        0.960404        1.608668       -0.240147
N       -0.163146        1.075837       -0.179034
C       -1.362131        0.554694       -0.111175
C       -1.740555       -0.803330       -0.297965
C       -2.609729        1.230069        0.159525
N       -3.615724        0.384687        0.151000
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N       -3.067602       -0.831449       -0.154428
C       -3.949787       -1.954690       -0.343166
H       -3.597243       -2.820408        0.223483
H       -4.931759       -1.655054        0.020639
H       -4.022463       -2.225085       -1.401790
C       -0.922766       -1.977103       -0.677688
H        0.116395       -1.666461       -0.786901
H       -0.968879       -2.761319        0.085694
H       -1.255689       -2.412747       -1.626429
C       -2.775407        2.670878        0.472658
H       -2.504656        2.879244        1.513345
H       -2.110510        3.267298       -0.158359
H       -3.810505        2.980438        0.317918
H        5.339683       -1.396576        0.116537
30
4pzMeF1A-ts-H-n ; E = -782.999191446 Hartree
C        2.284007       -0.401298        0.664476
C        3.510815       -1.042876        0.706158
C        2.088636        0.774887       -0.063992
H        3.608800       -1.948922        1.295219
C        4.585114       -0.502425        0.005087
C        3.192229        1.321773       -0.719850
H        3.040364        2.258432       -1.248689
C        4.425809        0.683509       -0.709087
H        5.264591        1.113268       -1.247541
F        1.270580       -0.919741        1.380611
N        0.873134        1.540195       -0.095214
N       -0.183643        0.880838       -0.109188
C       -1.321672        0.233486       -0.160217
C       -2.610309        0.785370        0.067439
C       -1.586709       -1.155493       -0.466756
N       -2.877263       -1.402713       -0.428123
N       -3.472904       -0.220536       -0.078531
C       -4.894597       -0.215013        0.152651
H       -5.329945        0.722698       -0.199189
H       -5.320513       -1.049140       -0.404279
H       -5.121637       -0.339955        1.216576
C       -2.957095        2.173574        0.439555
H       -2.047536        2.776008        0.375751
H       -3.710146        2.597901       -0.233033
H       -3.344984        2.241758        1.462119
C       -0.606743       -2.202161       -0.853990
H       -0.084036       -1.922920       -1.774297
H        0.148872       -2.320164       -0.074539
H       -1.118916       -3.152218       -1.014871
H        5.547696       -1.003564        0.029827
30
4pzMeF1B-ts-B-m ; E = -783.003123653 Hartree
C       -2.604040       -0.921906       -1.257202
C       -3.882693       -0.410816       -1.434168
C       -1.874587       -0.625023       -0.079736
H       -4.410789       -0.651671       -2.352371
C       -4.498478        0.377381       -0.466433
C       -2.518310        0.196748        0.876761
F       -1.807348        0.513317        1.982902
C       -3.794034        0.676827        0.702447
H       -4.219210        1.295644        1.486349
H       -2.137946       -1.545609       -2.011454
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N       -0.651541       -1.066832        0.139614
N        0.489115       -1.502079        0.278881
C        1.550428       -0.626805        0.060446
C        1.573796        0.755325       -0.169683
C        2.907263       -1.042622        0.072095
N        3.703172       -0.010203       -0.143034
N        2.877266        1.060138       -0.281844
C        3.469818        2.360099       -0.490837
H        4.540259        2.199417       -0.607436
H        3.071462        2.829254       -1.394005
H        3.293873        3.016037        0.366725
C        0.472096        1.748185       -0.233144
H       -0.162800        1.579881       -1.108678
H       -0.169787        1.648613        0.646659
H        0.852913        2.770924       -0.273529
C        3.441622       -2.416100        0.269617
H        3.029075       -2.865934        1.176673
H        3.169199       -3.067602       -0.566386
H        4.529668       -2.381151        0.346362
H       -5.503138        0.757423       -0.611311
30
4pzMeF1B-ts-B-n ; E = -783.004922906 Hartree
C        2.730967        1.074665       -1.139990
C        4.044569        0.655436       -1.302351
C        1.964776        0.608892       -0.044499
H        4.600520        1.021493       -2.160727
C        4.659204       -0.196457       -0.389673
C        2.608391       -0.276069        0.854255
F        1.868328       -0.745269        1.881528
C        3.919600       -0.658478        0.702014
H        4.344027       -1.333656        1.438310
H        2.263968        1.748857       -1.848894
N        0.706749        0.952964        0.153357
N       -0.460260        1.287838        0.336727
C       -1.456550        0.360747        0.037522
C       -2.805860        0.694595        0.147159
C       -1.424689       -1.002790       -0.380864
N       -2.658205       -1.456033       -0.515443
N       -3.474836       -0.419024       -0.193634
C       -4.901602       -0.594092       -0.294340
H       -5.399584       -0.167238        0.579582
H       -5.296301       -0.120776       -1.199252
H       -5.093438       -1.665330       -0.336336
C       -3.439245        1.975732        0.542195
H       -4.087404        1.851231        1.416473
H       -2.653510        2.690707        0.791397
H       -4.047247        2.393021       -0.267813
C       -0.249237       -1.883010       -0.612594
H        0.381129       -1.504206       -1.422944
H        0.377245       -1.931384        0.282842
H       -0.591345       -2.887731       -0.867663
H        5.690905       -0.502792       -0.518795
30
4pzMeF1B-ts-H-m ; E = -782.998764796 Hartree
C        1.817541       -0.791558        0.875763
C        2.884585       -1.660655        1.069013
C        1.963734        0.367755        0.110756
H        2.758646       -2.549280        1.680022
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C        4.120994       -1.378284        0.491271
C        3.221541        0.642684       -0.430446
F        3.391315        1.752824       -1.153469
C        4.291867       -0.221473       -0.264943
H        5.241117        0.024458       -0.728825
H        0.851833       -0.973190        1.339852
N        0.934676        1.355725       -0.039452
N       -0.230887        0.924301        0.012599
C       -1.465196        0.477598        0.028898
C       -1.940310       -0.830802       -0.260240
C       -2.665360        1.230999        0.306259
N       -3.732593        0.469198        0.211557
N       -3.271847       -0.761396       -0.163529
C       -4.230988       -1.795507       -0.457733
H       -4.028390       -2.694102        0.131901
H       -5.212390       -1.402677       -0.195494
H       -4.214066       -2.054628       -1.521113
C       -1.199352       -2.035348       -0.695334
H       -0.129693       -1.872874       -0.543665
H       -1.507331       -2.923986       -0.134041
H       -1.355987       -2.245774       -1.759934
C       -2.728133        2.657935        0.707566
H       -2.506951        2.778134        1.773645
H       -1.977041        3.230031        0.155603
H       -3.721766        3.066669        0.515675
H        4.959193       -2.053064        0.634386
30
4pzMeF1B-ts-H-n ; E = -782.999188949 Hartree
C       -1.966820        0.884034        0.718549
C       -3.122800        1.646912        0.820582
C       -1.994027       -0.390434        0.151027
H       -3.086466        2.631774        1.276232
C       -4.332326        1.138081        0.350022
C       -3.223476       -0.887945       -0.286438
F       -3.279670       -2.111292       -0.821622
C       -4.384783       -0.135974       -0.208867
H       -5.309968       -0.558974       -0.585483
H       -1.015372        1.245537        1.096669
N       -0.859342       -1.267512        0.097030
N        0.250265       -0.702035        0.061720
C        1.428060       -0.128392       -0.035560
C        2.677159       -0.774447        0.161591
C        1.790887        1.228743       -0.382843
N        3.097958        1.373442       -0.393409
N        3.610575        0.156542       -0.037133
C        5.037119        0.032864        0.122568
H        5.496149        0.868818       -0.404067
H        5.320423        0.072402        1.179414
H        5.386739       -0.908804       -0.306919
C        2.928618       -2.180556        0.541875
H        3.358748       -2.265369        1.546148
H        1.971494       -2.707876        0.530091
H        3.612579       -2.673297       -0.157381
C        0.889956        2.352440       -0.749716
H        0.095873        2.013842       -1.419550
H        0.403988        2.775047        0.136546
H        1.461730        3.145249       -1.235243
H       -5.240466        1.728274        0.423939
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30
4pzMeF2-ts-B-m ; E = -882.143178529 Hartree
C       -2.600534       -0.937043       -0.782663
C       -3.866910       -0.453508       -1.031242
C       -1.763493       -0.397486        0.223939
H       -4.440049       -0.912706       -1.829646
C       -4.387993        0.580671       -0.253135
C       -2.323980        0.668052        0.965445
F       -1.535651        1.219664        1.912597
C       -3.602689        1.137536        0.754882
H       -3.961553        1.947694        1.380680
F       -2.085078       -1.929741       -1.525895
N       -0.553284       -0.859090        0.455673
N        0.575785       -1.305128        0.652064
C        1.663483       -0.543704        0.241121
C        1.742282        0.745689       -0.304400
C        3.002430       -1.006191        0.340397
N        3.837521       -0.087341       -0.109453
N        3.054995        0.957926       -0.489062
C        3.698747        2.142310       -1.006730
H        3.327113        2.383359       -2.005999
H        3.540314        2.997860       -0.344004
H        4.763101        1.919799       -1.059708
C        0.683131        1.740873       -0.605329
H        0.028769        1.387358       -1.408275
H        0.053144        1.894362        0.275018
H        1.106256        2.702275       -0.903985
C        3.481049       -2.318700        0.848838
H        3.108908       -2.502872        1.860390
H        3.120644       -3.137334        0.218862
H        4.572158       -2.334395        0.858623
H       -5.390502        0.949730       -0.433566
30
4pzMeF2-ts-B-n ; E = -882.145235530 Hartree
C        2.433208        0.844680        0.793600
C        3.748891        1.183820        0.561423
C        1.841477       -0.331216        0.277029
H        4.131008        2.094426        1.010249
C        4.540928        0.372997       -0.250089
C        2.687224       -1.130002       -0.529208
F        2.144293       -2.238382       -1.058626
C        3.991548       -0.781768       -0.807178
H        4.569809       -1.438318       -1.448465
F        1.643349        1.632669        1.550128
N        0.593844       -0.662828        0.532657
N       -0.566666       -0.978787        0.784863
C       -1.587651       -0.243527        0.192906
C       -2.925109       -0.586560        0.394134
C       -1.603361        0.905432       -0.653815
N       -2.850885        1.230205       -0.940018
N       -3.631166        0.320660       -0.298802
C       -5.060808        0.383665       -0.468904
H       -5.303095        1.387542       -0.815017
H       -5.404166       -0.345831       -1.209583
H       -5.563156        0.192887        0.482139
C       -3.511699       -1.697101        1.182068
H       -4.090771       -2.378677        0.549803
H       -2.700969       -2.259081        1.648426
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H       -4.176129       -1.324726        1.969379
C       -0.461547        1.708850       -1.163909
H        0.148396        2.082065       -0.336426
H        0.194447        1.107595       -1.800928
H       -0.840513        2.553535       -1.742201
H        5.571864        0.639635       -0.450145
30
4pzMeF2-ts-H-m ; E = -882.139490459 Hartree
C        1.881563       -0.774770        0.752217
C        2.976028       -1.622711        0.816690
C        1.909149        0.448233        0.074527
H        2.891444       -2.552232        1.368668
C        4.156173       -1.244485        0.184422
C        3.126624        0.795816       -0.517795
F        3.203087        1.963006       -1.160163
C        4.238100       -0.030453       -0.491644
H        5.144370        0.287700       -0.994305
F        0.757697       -1.137300        1.391124
N        0.857083        1.427790        0.086758
N       -0.298988        0.971185        0.029203
C       -1.531125        0.532346       -0.013786
C       -1.984835       -0.764159       -0.382890
C       -2.744899        1.252478        0.293976
N       -3.799770        0.484904        0.140691
N       -3.314379       -0.722064       -0.288965
C       -4.255927       -1.756392       -0.635447
H       -3.977049       -2.702904       -0.165325
H       -5.230578       -1.438431       -0.267588
H       -4.305799       -1.895782       -1.720296
C       -1.219614       -1.936968       -0.861066
H       -0.161778       -1.676192       -0.904745
H       -1.335831       -2.793012       -0.187564
H       -1.541025       -2.250123       -1.860503
C       -2.836082        2.653668        0.773040
H       -2.571993        2.720797        1.833844
H       -2.128269        3.282293        0.225633
H       -3.849516        3.037591        0.644422
H        5.020405       -1.899380        0.221852
30
4pzMeF2-ts-H-n ; E = -882.140107338 Hartree
C       -2.052512       -0.782106       -0.727564
C       -3.238367       -1.498634       -0.709823
C       -1.924611        0.484652       -0.153094
H       -3.273288       -2.474124       -1.182032
C       -4.353814       -0.933928       -0.099376
C       -3.080582        1.021931        0.417921
F       -3.006904        2.240148        0.960304
C       -4.281107        0.332893        0.472705
H       -5.134220        0.795630        0.955726
F       -0.991510       -1.320417       -1.350584
N       -0.760534        1.324381       -0.256522
N        0.329055        0.743618       -0.097610
C        1.501800        0.189208        0.082622
C        2.763059        0.781980       -0.194137
C        1.837364       -1.115563        0.609377
N        3.140094       -1.282937        0.644203
N        3.677130       -0.128340        0.137230
C        5.105602       -0.062828       -0.037413
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H        5.454885        0.959681        0.118296
H        5.560080       -0.723170        0.700849
H        5.394423       -0.393654       -1.040362
C        3.037863        2.117843       -0.764976
H        2.086917        2.649660       -0.848729
H        3.712151        2.700568       -0.128320
H        3.488561        2.054193       -1.761505
C        0.903380       -2.154373        1.112829
H        0.315810       -1.771878        1.953341
H        0.198953       -2.441069        0.328798
H        1.461100       -3.032418        1.442423
H       -5.288312       -1.484498       -0.071500
34
4pzMeOMe1A-ts-B-m ; E = -798.262855518 Hartree
C        2.412689        0.229820        0.496066
C        3.692503        0.532637        0.071986
C        1.688809       -0.840628       -0.107280
H        4.234494        1.345013        0.544345
C        4.291838       -0.184768       -0.971275
C        2.305992       -1.557889       -1.153929
C        3.585580       -1.213771       -1.576841
H        4.033202       -1.778855       -2.389372
N        0.468900       -1.113742        0.320374
N       -0.667757       -1.408261        0.677778
C       -1.718008       -0.612697        0.216467
C       -1.716584        0.573349       -0.527620
C       -3.080642       -0.905759        0.478995
N       -3.859765        0.014905       -0.062146
N       -3.015125        0.895011       -0.660384
C       -3.580824        2.045952       -1.322602
H       -3.262378        2.091512       -2.367342
H       -4.662502        1.930236       -1.278339
H       -3.295320        2.972805       -0.816444
C       -0.592390        1.387929       -1.053244
H        0.112169        1.607795       -0.245404
H       -0.032402        0.841149       -1.818329
H       -0.942453        2.328078       -1.485220
C       -3.640310       -2.061620        1.228991
H       -3.440990       -3.002367        0.706787
H       -3.183543       -2.140271        2.219307
H       -4.719660       -1.942574        1.338437
H        5.295049        0.069616       -1.294559
H        1.760110       -2.372252       -1.616715
O        1.714072        0.882672        1.474368
C        2.391549        1.900456        2.168510
H        3.288909        1.515439        2.669715
H        2.683977        2.722913        1.501615
H        1.693792        2.276943        2.917879
34
4pzMeOMe1A-ts-B-n ; E = -798.264651160 Hartree
C       -2.487367        0.438370       -0.366438
C       -3.804931        0.535171        0.039565
C       -1.787810       -0.798773       -0.244499
H       -4.328843        1.479362       -0.064082
C       -4.464614       -0.563946        0.604346
C       -2.468527       -1.900785        0.312705
C       -3.783747       -1.764357        0.744238
H       -4.279311       -2.625451        1.183215
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N       -0.529235       -0.864421       -0.642264
N        0.633737       -0.928288       -1.026856
C        1.616729       -0.359201       -0.214633
C        2.964630       -0.433530       -0.558879
C        1.567229        0.367037        1.011519
N        2.790815        0.705521        1.379513
N        3.617912        0.215650        0.420102
C        5.040776        0.386421        0.566398
H        5.484432        0.717336       -0.376032
H        5.197284        1.147326        1.329738
H        5.522483       -0.545099        0.881291
C        3.613136       -1.072071       -1.729652
H        4.301892       -1.868251       -1.426728
H        2.837311       -1.505117       -2.363184
H        4.181590       -0.346226       -2.321488
C        0.382159        0.764138        1.816602
H       -0.308211        1.359757        1.212013
H       -0.175714       -0.110655        2.164520
H        0.707195        1.346766        2.680778
H       -5.495512       -0.466668        0.926266
H       -1.939636       -2.842333        0.408207
O       -1.733824        1.445936       -0.898041
C       -2.366621        2.688369       -1.076396
H       -3.221176        2.610228       -1.761133
H       -2.713905        3.107698       -0.122509
H       -1.618134        3.353551       -1.509263
34
4pzMeOMe1A-ts-H-m ; E = -798.257489312 Hartree
C       -2.987070        0.273925        0.133586
C       -3.946719       -0.728480       -0.017323
C       -1.674360        0.049891       -0.329897
H       -4.954571       -0.583368        0.353896
C       -3.615422       -1.928404       -0.645537
C       -1.369395       -1.152402       -0.962757
C       -2.329640       -2.145330       -1.126874
H       -2.081322       -3.070462       -1.637770
N       -0.742603        1.135637       -0.245194
N        0.456810        0.809798       -0.191655
C        1.725659        0.483902       -0.096026
C        2.293471       -0.726987        0.382601
C        2.870457        1.302637       -0.415957
N        3.992808        0.660888       -0.173417
N        3.618972       -0.548470        0.339063
C        4.643949       -1.444705        0.808742
H        4.557013       -2.423597        0.328331
H        5.601851       -0.996601        0.547897
H        4.585328       -1.573888        1.894244
C        1.630070       -1.930201        0.931379
H        1.717387       -1.981768        2.023234
H        0.565714       -1.893194        0.685865
H        2.058675       -2.851007        0.521583
C        2.833395        2.666808       -0.998563
H        3.772282        3.190477       -0.809620
H        2.672613        2.630243       -2.081567
H        2.000014        3.228809       -0.567420
H       -4.379025       -2.691734       -0.762666
H       -0.362644       -1.273332       -1.354186
O       -3.216785        1.462793        0.731837
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C       -4.525601        1.731779        1.172480
H       -5.248029        1.693821        0.346896
H       -4.842453        1.031867        1.956835
H       -4.503230        2.741829        1.583045
34
4pzMeOMe1A-ts-H-n ; E = -798.257844335 Hartree
C        3.013536       -0.419966        0.050158
C        4.059668        0.493657       -0.087477
C        1.708727       -0.038032       -0.323234
H        5.065032        0.226656        0.216711
C        3.818650        1.761682       -0.615044
C        1.494013        1.229366       -0.857560
C        2.538789        2.134722       -1.008455
H        2.358431        3.114121       -1.440506
N        0.678081       -1.030803       -0.254965
N       -0.477709       -0.589661       -0.118253
C       -1.702754       -0.158509        0.076778
C       -2.895544       -0.848478       -0.258363
C       -2.168552        1.078814        0.662048
N       -3.484529        1.125483        0.669540
N       -3.899586       -0.032191        0.077826
C       -5.307159       -0.214899       -0.165632
H       -5.550634       -0.051209       -1.220707
H       -5.617270       -1.223287        0.119829
H       -5.837064        0.516176        0.443900
C       -3.040541       -2.168414       -0.908637
H       -3.401065       -2.087253       -1.940745
H       -2.056872       -2.644667       -0.926875
H       -3.736533       -2.814056       -0.362542
C       -1.343438        2.144685        1.283964
H       -0.446602        2.338098        0.688205
H       -1.925054        3.062499        1.388104
H       -0.999502        1.840888        2.278663
H        4.647668        2.454822       -0.723617
H        0.485942        1.473044       -1.182094
O        3.152802       -1.665666        0.554840
C        4.447055       -2.085257        0.912396
H        5.133725       -2.060328        0.056263
H        4.864002       -1.472217        1.722206
H        4.344893       -3.113990        1.259802
34
4pzMeOMe1B-ts-B-m ; E = -798.262855555 Hartree
C       -2.305136       -1.557357       -1.154731
C       -3.584759       -1.213697       -1.577920
C       -1.688700       -0.840276       -0.107521
H       -4.031858       -1.778728       -2.390777
C       -4.291654       -0.185160       -0.972310
C       -2.413211        0.229714        0.495858
C       -3.692945        0.532224        0.071326
H       -4.235379        1.344314        0.543669
N       -0.468895       -1.113131        0.320612
N        0.667722       -1.407658        0.678109
C        1.718123       -0.612376        0.216668
C        1.717037        0.573559       -0.527611
C        3.080679       -0.905757        0.479268
N        3.860060        0.014634       -0.061958
N        3.015667        0.894877       -0.660340
C        3.581676        2.045754       -1.322409
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H        3.262907        2.091745       -2.367027
H        3.296758        2.972596       -0.815896
H        4.663315        1.929539       -1.278525
C        0.593084        1.388740       -1.052833
H        0.032968        0.842613       -1.818288
H       -0.111446        1.608301       -0.244881
H        0.943427        2.329064       -1.484199
C        3.639999       -2.061762        1.229312
H        4.719135       -1.942188        1.340282
H        3.181886       -2.141314        2.218925
H        3.441971       -3.002296        0.706217
H       -5.294858        0.068903       -1.295867
O       -1.715142        0.882660        1.474491
C       -2.393676        1.899104        2.169563
H       -2.686277        2.722234        1.503574
H       -3.291059        1.512841        2.669763
H       -1.696583        2.275101        2.919798
H       -1.758746       -2.371332       -1.617598
34
4pzMeOMe1B-ts-B-n ; E = -798.264651155 Hartree
C        2.468297       -1.900864        0.312575
C        3.783487       -1.764605        0.744246
C        1.787746       -0.798736       -0.244610
H        4.278915       -2.625784        1.183208
C        4.464493       -0.564252        0.604519
C        2.487449        0.438336       -0.366401
C        3.804979        0.534973        0.039755
H        4.328995        1.479120       -0.063765
N        0.529200       -0.864218       -0.642496
N       -0.633778       -0.928012       -1.027078
C       -1.616755       -0.359044       -0.214750
C       -2.964668       -0.433417       -0.558926
C       -1.567227        0.367061        1.011485
N       -2.790811        0.705419        1.379595
N       -3.617938        0.215587        0.420183
C       -5.040811        0.386224        0.566605
H       -5.484587        0.716959       -0.375830
H       -5.522385       -0.545308        0.881670
H       -5.197350        1.147212        1.329858
C       -3.613197       -1.071812       -1.729769
H       -4.180995       -0.345726       -2.321943
H       -2.837438       -1.505448       -2.362979
H       -4.302557       -1.867489       -1.426906
C       -0.382128        0.764195        1.816508
H        0.175713       -0.110584        2.164515
H        0.308254        1.359721        1.211843
H       -0.707128        1.346926        2.680629
H        5.495367       -0.467103        0.926554
O        1.734064        1.446025       -0.897999
C        2.367021        2.688395       -1.076226
H        2.714249        3.107640       -0.122281
H        3.221641        2.610190       -1.760874
H        1.618656        3.353683       -1.509141
H        1.939312       -2.842376        0.407936
34
4pzMeOMe1B-ts-H-m ; E = -798.257730523 Hartree
C        3.120486        1.463268       -0.791091
C        4.313096        0.757483       -0.891426
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C        1.997880        0.913743       -0.177868
H        5.168945        1.194216       -1.395964
C        4.396138       -0.510757       -0.328328
C        2.099410       -0.362186        0.420916
C        3.302688       -1.064597        0.334716
H        3.397918       -2.044877        0.787772
N        0.849615        1.770915       -0.119496
N       -0.259371        1.207698       -0.125321
C       -1.451278        0.667210       -0.113614
C       -1.820565       -0.628011       -0.564029
C       -2.691937        1.242933        0.347419
N       -3.688069        0.395768        0.203643
N       -3.143538       -0.713114       -0.379550
C       -4.025454       -1.772283       -0.796028
H       -3.626139       -2.745286       -0.498052
H       -4.983211       -1.605139       -0.304507
H       -4.170165       -1.763559       -1.881729
C       -1.000332       -1.666471       -1.226764
H       -1.281191       -1.802145       -2.277903
H        0.046218       -1.360555       -1.186003
H       -1.101085       -2.637983       -0.729923
C       -2.858790        2.578661        0.972034
H       -3.902514        2.895104        0.927635
H       -2.547250        2.565003        2.022178
H       -2.227024        3.309234        0.458695
H        5.320772       -1.077294       -0.387071
O        1.009375       -0.820267        1.086377
C        1.131522       -2.025040        1.801781
H        1.316109       -2.877483        1.134273
H        1.935233       -1.975413        2.547230
H        0.176833       -2.169115        2.309325
H        3.013905        2.464849       -1.198211
34
4pzMeOMe1B-ts-H-n ; E = -798.257532508 Hartree
C       -3.088793        1.680476        0.514380
C       -4.347018        1.100162        0.619087
C       -1.994240        0.964499        0.038127
H       -5.181946        1.667105        1.018143
C       -4.521370       -0.212602        0.196837
C       -2.185650       -0.357703       -0.421041
C       -3.453390       -0.934947       -0.332093
H       -3.617829       -1.949292       -0.677310
N       -0.767805        1.703259       -0.046210
N        0.280644        1.052166        0.109041
C        1.417502        0.420980        0.263433
C        2.688099        0.836483       -0.209349
C        1.682476       -0.843632        0.910856
N        2.960750       -1.150788        0.831779
N        3.540093       -0.140546        0.119510
C        4.928490       -0.261380       -0.242036
H        5.453447        0.681176       -0.067000
H        5.358509       -1.040389        0.386563
H        5.041073       -0.542451       -1.294617
C        3.030156        2.051031       -0.980448
H        3.275758        1.826422       -2.025044
H        2.161101        2.713772       -0.970186
H        3.883913        2.580546       -0.544176
C        0.719345       -1.670499        1.681778
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H       -0.276772       -1.582471        1.243641
H        1.033083       -2.716615        1.689076
H        0.655844       -1.331152        2.721593
H       -5.497356       -0.684405        0.262068
O       -1.112340       -0.983262       -0.964903
C       -1.304978       -2.260086       -1.524207
H       -1.605055       -2.994326       -0.765208
H       -2.056376       -2.243452       -2.323905
H       -0.339748       -2.552843       -1.938791
H       -2.908469        2.709148        0.813590
38
4pzMeOMe2-ts-B-m ; E = -912.662873854 Hartree
C        2.460387       -1.055712        0.140493
C        3.714023       -0.640407        0.568365
C        1.526342       -0.115680       -0.367849
H        4.416955       -1.365228        0.962702
C        4.082833        0.700853        0.472385
C        1.909853        1.249762       -0.415204
C        3.183417        1.641576       -0.024418
H        3.473147        2.684181       -0.089774
N        0.331732       -0.497006       -0.781014
N       -0.774837       -0.803808       -1.217725
C       -1.893327       -0.435906       -0.468249
C       -2.008214        0.235688        0.754382
C       -3.219612       -0.735599       -0.871633
N       -4.084957       -0.284830        0.020602
N       -3.330993        0.295281        0.990490
C       -4.005046        0.885343        2.121603
H       -5.071305        0.733611        1.961879
H       -3.705788        0.400614        3.055192
H       -3.797686        1.957149        2.188630
C       -0.970806        0.794617        1.656824
H       -0.289428        0.007843        1.994377
H       -0.363661        1.528585        1.119023
H       -1.412489        1.271240        2.534869
C       -3.662936       -1.443866       -2.101938
H       -4.749719       -1.544907       -2.098137
H       -3.359997       -0.896261       -2.999265
H       -3.210466       -2.437589       -2.164397
H        5.071778        1.013120        0.788809
O        0.929753        2.077124       -0.889327
C        1.265974        3.431471       -1.058795
H        1.537890        3.906856       -0.106506
H        2.097086        3.553796       -1.765143
H        0.376779        3.918842       -1.461377
O        1.981161       -2.329359        0.189305
C        2.861912       -3.324636        0.644840
H        3.764321       -3.383754        0.021944
H        3.162240       -3.154919        1.687696
H        2.317623       -4.267778        0.578329
38
4pzMeOMe2-ts-B-n ; E = -912.664763212 Hartree
C        2.497542       -1.133133        0.012137
C        3.796970       -0.824368        0.391763
C        1.593731       -0.103753       -0.357720
H        4.476350       -1.616195        0.685617
C        4.239427        0.497418        0.375397
C        2.056560        1.237014       -0.331300
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C         3.372484        1.523824        0.006809
H         3.721560        2.550057        0.001933
N         0.353758       -0.383234       -0.716345
N        -0.792370       -0.610673       -1.091621
C        -1.838651       -0.235449       -0.245877
C        -3.165332       -0.459254       -0.606067
C        -1.884034        0.373514        1.042595
N        -3.141006        0.511732        1.428777
N        -3.897821        0.007431        0.420299
C        -5.331485       -0.009396        0.556331
H        -5.807920        0.449188       -0.314696
H        -5.706646       -1.031484        0.671505
H        -5.574527        0.565889        1.448482
C        -3.727098       -1.070837       -1.834460
H        -4.360397       -0.365503       -2.384069
H        -2.900726       -1.371893       -2.480488
H        -4.333079       -1.954321       -1.605452
C        -0.760278        0.826807        1.903813
H        -0.095967       -0.005668        2.155507
H        -0.152772        1.571785        1.382289
H        -1.157643        1.257227        2.825245
H         5.261643        0.727974        0.654123
O         1.106512        2.150924       -0.688114
C         1.499854        3.499959       -0.720368
H         1.839678        3.848250        0.264241
H         2.300609        3.668814       -1.452080
H         0.616823        4.068171       -1.016239
O         1.946949       -2.378375       -0.008825
C         2.785254       -3.451309        0.336447
H         3.652376       -3.521486       -0.333841
H         3.143698       -3.369487        1.371420
H         2.181663       -4.354722        0.237247
38
4pzMeOMe2-ts-H-m ; E = -912.657076258 Hartree
C         2.934613       -0.616354        0.222884
C         3.965387        0.306212        0.412079
C         1.667570       -0.197941       -0.225630
H         4.933684       -0.008754        0.780722
C         3.735942        1.647186        0.127323
C         1.469807        1.165191       -0.519748
C         2.505016        2.087587       -0.340994
H         2.359127        3.136614       -0.567823
N         0.711656       -1.227432       -0.511491
N        -0.476582       -0.944637       -0.276935
C        -1.745942       -0.693325       -0.078280
C        -2.303948        0.319442        0.744959
C        -2.896875       -1.367677       -0.629020
N        -4.014669       -0.825204       -0.196509
N        -3.630479        0.174818        0.653363
C        -4.648484        0.878822        1.388642
H        -4.467207        1.956511        1.360776
H        -5.602159        0.656832        0.910943
H        -4.682445        0.550057        2.432912
C        -1.620192        1.296867        1.620150
H        -1.795525        1.090641        2.682544
H        -0.547046        1.236589        1.429287
H        -1.955784        2.321007        1.421896
C        -2.873479       -2.487887       -1.602153
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H       -3.826511       -3.020123       -1.599069
H       -2.685683       -2.122663       -2.617738
H       -2.061624       -3.177313       -1.353659
H        4.536947        2.365910        0.272135
O        0.249958        1.503845       -1.008755
C        0.059651        2.824207       -1.453043
H        0.133168        3.545779       -0.628391
H        0.780933        3.099449       -2.232817
H       -0.949194        2.857067       -1.866710
O        3.051768       -1.938637        0.476318
C        4.312984       -2.420273        0.870816
H        5.083577       -2.206428        0.118996
H        4.627100       -1.997577        1.834258
H        4.203062       -3.500413        0.974327
38
4pzMeOMe2-ts-H-n ; E = -912.656984075 Hartree
C        2.927085       -0.779551        0.082036
C        4.052398        0.028417        0.256099
C        1.682175       -0.216279       -0.253191
H        5.006341       -0.398638        0.539497
C        3.936525        1.400604        0.068158
C        1.598867        1.174827       -0.452406
C        2.727627        1.983061       -0.289565
H        2.669961        3.053829       -0.441849
N        0.614393       -1.130694       -0.536725
N       -0.520990       -0.764895       -0.184302
C       -1.744312       -0.433403        0.146214
C       -2.945489       -0.964071       -0.388313
C       -2.193861        0.554732        1.099045
N       -3.508907        0.612417        1.131354
N       -3.939355       -0.293790        0.203117
C       -5.349830       -0.378943       -0.072264
H       -5.868786        0.118476        0.746440
H       -5.600801        0.118994       -1.014991
H       -5.667232       -1.423499       -0.125919
C       -3.108399       -1.998375       -1.432395
H       -3.494643       -1.584359       -2.371098
H       -2.125979       -2.434947       -1.629575
H       -3.791065       -2.793306       -1.113141
C       -1.342279        1.359478        2.011012
H       -0.410078        1.622983        1.506212
H       -1.866304        2.264222        2.326195
H       -1.080671        0.788927        2.908940
H        4.810344        2.031130        0.202439
O        0.390299        1.655311       -0.839142
C        0.294947        3.020340       -1.165240
H        0.492148        3.660498       -0.295510
H        0.983317        3.293917       -1.974958
H       -0.732970        3.176871       -1.494496
O        2.930344       -2.121712        0.247136
C        4.159756       -2.742093        0.532409
H        4.903089       -2.553515       -0.252996
H        4.568186       -2.412197        1.496705
H        3.952745       -3.811911        0.580446
42
4pzMePyr1A-ts-B-m ; E = -895.029461975 Hartree
C        2.248342       -0.247790       -0.003120
C        3.470780       -0.589031        0.560752
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C        1.385049       -1.293878       -0.453866
H        4.121761        0.206373        0.909948
C        3.869820       -1.918258        0.713359
C        1.809891       -2.636392       -0.332387
C        3.029070       -2.929102        0.262843
H        3.319879       -3.970598        0.368338
N        0.196579       -0.997282       -0.956395
N       -0.928524       -0.812062       -1.415784
C       -1.954540       -0.513562       -0.518951
C       -1.926620       -0.244166        0.855439
C       -3.311657       -0.387930       -0.913177
N       -4.064300       -0.077258        0.127845
N       -3.207107        0.005533        1.179388
C       -3.737755        0.374553        2.469752
H       -3.461399       -0.361406        3.228971
H       -3.380304        1.362100        2.776604
H       -4.821296        0.400452        2.366296
C       -0.788228       -0.168152        1.803487
H       -1.087460        0.267037        2.759763
H       -0.361468       -1.158854        1.990239
H        0.008421        0.440105        1.357928
C       -3.891873       -0.579650       -2.269088
H       -3.830321       -1.627634       -2.578528
H       -4.940320       -0.276458       -2.268581
H       -3.345490        0.007812       -3.011913
H        4.824096       -2.151058        1.173122
C        1.079631        3.063068       -1.124306
C        1.576090        1.648495       -1.429181
N        1.761191        1.073475       -0.095648
C        2.433225        2.115374        0.658657
C        1.650517        3.375625        0.279090
H        1.412081        3.775875       -1.883112
H        0.874339        1.061631       -2.024333
H        2.415943        1.886450        1.728890
H        2.290828        4.261484        0.287121
H        2.537568        1.676764       -1.971277
H       -0.013314        3.085377       -1.108087
H        0.840697        3.550158        0.992763
H        3.490528        2.225626        0.354370
H        1.149905       -3.423291       -0.680175
42
4pzMePyr1A-ts-B-n ; E = -895.030481512 Hartree
C       -2.346148        0.114631       -0.052709
C       -3.639631        0.333003        0.403455
C       -1.572798        1.236491       -0.483207
H       -4.223323       -0.518975        0.738025
C       -4.191109        1.613902        0.472970
C       -2.152696        2.524221       -0.457687
C       -3.436023        2.698395        0.041793
H       -3.847462        3.702980        0.084518
N       -0.321642        1.053704       -0.876649
N        0.837738        0.884303       -1.245512
C        1.797904        0.612527       -0.269225
C        3.138337        0.442506       -0.610226
C        1.729644        0.435068        1.144672
N        2.935730        0.176172        1.619815
N        3.770821        0.189942        0.548103
C        5.172790       -0.076890        0.744205
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H         5.783169        0.733001        0.334556
H         5.336299       -0.147052        1.818505
H         5.465387       -1.019349        0.270529
C         3.800433        0.508919       -1.935323
H         4.302161       -0.432764       -2.183593
H         3.042364        0.711280       -2.693724
H         4.551421        1.305892       -1.972344
C         0.540766        0.484782        2.034757
H         0.074579        1.474870        2.021576
H        -0.214995       -0.226400        1.686101
H         0.838903        0.244683        3.057176
H        -5.196817        1.753272        0.854534
C        -0.718557       -3.068268       -0.936693
C        -1.379434       -1.751366       -1.347110
N        -1.709148       -1.142478       -0.059166
C        -2.289011       -2.222630        0.716436
C        -1.337304       -3.391942        0.443842
H        -0.895774       -3.854708       -1.674841
H        -0.728899       -1.107570       -1.941703
H        -2.357202       -1.942498        1.772219
H        -1.866698       -4.348297        0.454935
H        -2.297564       -1.937543       -1.932592
H         0.362886       -2.933664       -0.848375
H        -0.560148       -3.436972        1.211282
H        -3.306749       -2.479997        0.368318
H        -1.559017        3.368211       -0.790948
42
4pzMePyr1A-ts-H-m ; E = -895.026095654 Hartree
C         2.896350       -2.179812       -0.103201
C         4.008023       -1.867226        0.666878
C         1.891334       -1.246183       -0.344112
H         4.763806       -2.617093        0.876961
C         4.115383       -0.580904        1.188090
C         2.056888        0.100884        0.072370
C         3.165671        0.388609        0.889725
H         3.304712        1.393098        1.272915
N         0.721351       -1.800102       -0.978142
N        -0.361454       -1.368981       -0.536615
C        -1.530395       -0.937655       -0.125612
C        -1.811010       -0.182324        1.044211
C        -2.820169       -1.103919       -0.751636
N        -3.764418       -0.511928       -0.053024
N        -3.134650        0.014129        1.040090
C        -3.937969        0.625873        2.066809
H        -3.497691        1.574642        2.384293
H        -4.924075        0.805370        1.639922
H        -4.035332       -0.031189        2.937594
C        -0.905720        0.239496        2.136020
H        -1.139841       -0.268204        3.079094
H         0.118705       -0.008571        1.852644
H        -0.967947        1.318709        2.317118
C        -3.085111       -1.784030       -2.043944
H        -2.476936       -2.689891       -2.119117
H        -4.142522       -2.039179       -2.134026
H        -2.812636       -1.143042       -2.889876
H         4.962889       -0.313210        1.812819
C         0.459791        2.616273       -1.979344
C         0.602525        1.127938       -1.664228
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N        1.178760        1.098579       -0.314904
C        1.328117        2.445582        0.206721
C        0.311623        3.242549       -0.595480
H        1.369471        2.995187       -2.459018
H        1.251739        0.599434       -2.371654
H        1.147252        2.464919        1.288460
H       -0.697087        3.066222       -0.204374
H        2.341440        2.847139        0.032104
H        0.508028        4.317406       -0.575219
H       -0.382178        2.820324       -2.645595
H       -0.375298        0.636570       -1.684239
H        2.734387       -3.181426       -0.492254
42
4pzMePyr1A-ts-H-n ; E = -895.024254913 Hartree
C        3.175439       -2.012352       -0.114171
C        4.402927       -1.496558        0.278378
C        2.052546       -1.199140       -0.252058
H        5.258157       -2.150699        0.414673
C        4.509486       -0.128560        0.507569
C        2.174294        0.208364       -0.110252
C        3.418937        0.709438        0.300641
H        3.542710        1.778008        0.437687
N        0.846987       -1.928969       -0.537403
N       -0.196107       -1.439045       -0.065286
C       -1.339308       -0.941273        0.332708
C       -2.611456       -1.144195       -0.259131
C       -1.593227        0.000937        1.398730
N       -2.868303        0.333163        1.433578
N       -3.453121       -0.335446        0.398532
C       -4.831976       -0.058222        0.090578
H       -4.919775        0.586672       -0.790527
H       -5.378825       -0.986837       -0.091858
H       -5.258089        0.451923        0.953699
C       -2.960047       -1.975952       -1.431489
H       -3.172553       -1.374424       -2.323657
H       -2.108582       -2.624131       -1.654195
H       -3.837290       -2.602160       -1.237318
C       -0.619933        0.459411        2.421693
H       -0.632222       -0.197955        3.298135
H        0.386110        0.438343        1.997327
H       -0.860955        1.470025        2.759817
H        5.455880        0.301711        0.822618
C       -0.662701        2.087355       -1.532930
C        0.431877        1.022817       -1.658306
N        1.101652        1.064307       -0.362338
C        1.194410        2.467392       -0.012884
C       -0.189228        3.003226       -0.383107
H       -0.792652        2.629584       -2.473402
H        1.143758        1.285373       -2.459902
H        1.431667        2.584229        1.049378
H       -0.865605        2.911499        0.470481
H        1.977921        2.988899       -0.594158
H       -0.150110        4.057987       -0.667277
H       -1.619926        1.624529       -1.279939
H        0.040625        0.029584       -1.877948
H        3.029758       -3.076354       -0.279029
42
4pzMePyr1B-ts-B-m ; E = -895.029462007 Hartree
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C       -1.808410       -2.636613       -0.333061
C       -3.027375       -2.930182        0.262191
C       -1.384351       -1.293823       -0.454228
H       -3.317580       -3.971875        0.367414
C       -3.868655       -1.919947        0.713073
C       -2.248227       -0.248348       -0.003167
C       -3.470393       -0.590452        0.560772
H       -4.121800        0.204485        0.910237
N       -0.196089       -0.996430       -0.956780
N        0.928953       -0.810916       -1.416212
C        1.954938       -0.512775       -0.519236
C        1.926699       -0.243941        0.855246
C        3.312115       -0.386895       -0.913144
N        4.064511       -0.076599        0.128174
N        3.207094        0.005690        1.179583
C        3.737452        0.374302        2.470181
H        4.821056        0.399461        2.367214
H        3.380545        1.362081        2.776920
H        3.460249       -0.361499        3.229238
C        0.787963       -0.168377        1.802911
H       -0.008389        0.440391        1.357511
H        0.360882       -1.159144        1.988668
H        1.086905        0.265973        2.759660
C        3.892606       -0.578093       -2.269012
H        4.940889       -0.274338       -2.268351
H        3.831665       -1.626062       -2.578626
H        3.345977        0.009187       -3.011799
H       -4.822747       -2.153418        1.172878
C       -1.080932        3.063197       -1.123443
C       -1.577085        1.648664       -1.428808
N       -1.761880        1.073227       -0.095427
C       -2.434530        2.114568        0.659103
C       -1.652885        3.375533        0.279567
H        0.012005        3.085382       -1.106293
H       -0.875272        1.062159       -2.024243
H       -3.491968        2.224051        0.355014
H       -2.294218        4.260660        0.286928
H       -2.416906        1.885523        1.729304
H       -0.843672        3.551286        0.993625
H       -1.412671        3.776132       -1.882439
H       -2.538644        1.676902       -1.970771
H       -1.148008       -3.423039       -0.681130
42
4pzMePyr1B-ts-B-n ; E = -895.029972383 Hartree
C       -2.071177       -2.557382       -0.557601
C       -3.318233       -2.807510       -0.002578
C       -1.510990       -1.260390       -0.515690
H       -3.701640       -3.823588        0.003282
C       -4.072087       -1.764985        0.521232
C       -2.297909       -0.175373       -0.012667
C       -3.565952       -0.464598        0.488843
H       -4.165785        0.341828        0.895864
N       -0.256802       -1.073078       -0.908766
N        0.921952       -0.957628       -1.246410
C        1.847293       -0.586411       -0.264028
C        3.185141       -0.374577       -0.591573
C        1.754226       -0.369101        1.143562
N        2.942744       -0.045593        1.625090
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N        3.790106       -0.049505        0.564195
C        5.184213        0.244499        0.774856
H        5.804316       -0.644096        0.618504
H        5.519469        1.036442        0.099141
H        5.287659        0.578644        1.806153
C        3.868357       -0.465936       -1.904526
H        4.680527       -1.200964       -1.887210
H        3.137118       -0.771230       -2.654861
H        4.297071        0.496377       -2.206062
C        0.567884       -0.467231        2.035358
H       -0.216919        0.223298        1.711509
H        0.136203       -1.472413        2.007979
H        0.865172       -0.236115        3.060210
H       -5.054163       -1.948341        0.944515
C       -1.326814        3.146552       -1.130820
C       -0.999719        1.652324       -1.130365
N       -1.753218        1.110313        0.011627
C       -2.488781        2.174353        0.674443
C       -1.689620        3.419603        0.326558
H       -0.496228        3.754344       -1.499263
H        0.076833        1.497166       -0.994300
H       -3.517233        2.274206        0.284292
H       -2.260447        4.340525        0.470052
H       -2.559673        1.979253        1.750663
H       -0.786369        3.472399        0.944610
H       -2.196081        3.344307       -1.768121
H       -1.290921        1.161268       -2.066117
H       -1.467380       -3.357887       -0.971036
42
4pzMePyr1B-ts-H-m ; E = -895.028319125 Hartree
C        2.383951        0.714440       -0.199558
C        3.052384        1.959813       -0.240304
C        0.980429        0.732522       -0.432631
H        4.117938        1.998435       -0.049375
C        2.381564        3.142210       -0.506415
C        0.331351        1.939755       -0.704327
C        1.007796        3.147234       -0.745821
H        0.486340        4.068607       -0.984668
N        0.286863       -0.511674       -0.543930
N       -0.947709       -0.477303       -0.390997
C       -2.250018       -0.466082       -0.213961
C       -3.028523        0.434183        0.559142
C       -3.215801       -1.404245       -0.732009
N       -4.432883       -1.099999       -0.332613
N       -4.290865       -0.010931        0.474051
C       -5.449103        0.494641        1.163706
H       -5.601667        1.556145        0.947089
H       -6.305961       -0.074547        0.805474
H       -5.351079        0.363225        2.246288
C       -2.601614        1.570820        1.405678
H       -2.641624        1.324508        2.473741
H       -1.567081        1.827349        1.164094
H       -3.231654        2.452684        1.247050
C       -2.930415       -2.535590       -1.649131
H       -1.982264       -3.005440       -1.371527
H       -3.734477       -3.272869       -1.610045
H       -2.829410       -2.192625       -2.684742
H        2.944449        4.071144       -0.533055
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C        3.721235       -2.406454        1.154612
C        2.546712       -1.717848        0.466028
N        3.096473       -0.423570        0.066276
C        4.543606       -0.390070        0.204098
C        4.925366       -1.851890        0.400525
H        3.769919       -2.107338        2.208120
H        2.196068       -2.283882       -0.403600
H        5.013174        0.053370       -0.682518
H        5.871985       -1.966732        0.934540
H        1.682930       -1.584052        1.122887
H        3.645022       -3.496104        1.115834
H        5.021235       -2.346931       -0.572227
H        4.848402        0.213424        1.075382
H       -0.728916        1.885331       -0.936057
42
4pzMePyr1B-ts-H-n ; E = -895.028306661 Hartree
C        2.448784        0.627282       -0.241023
C        3.217625        1.811200       -0.313991
C        1.039985        0.768047       -0.380000
H        4.293069        1.756003       -0.196890
C        2.633803        3.050756       -0.518964
C        0.479389        2.030192       -0.590962
C        1.252495        3.176405       -0.662385
H        0.796568        4.142989       -0.851083
N        0.237652       -0.410678       -0.462986
N       -0.977749       -0.271585       -0.232876
C       -2.258185       -0.166003        0.043539
C       -3.296509       -0.987770       -0.459817
C       -2.942872        0.774066        0.901582
N       -4.240905        0.543893        0.905275
N       -4.434989       -0.495655        0.047839
C       -5.783080       -0.897586       -0.257803
H       -5.888098       -1.983352       -0.183183
H       -6.434057       -0.418184        0.472391
H       -6.072539       -0.579930       -1.265206
C       -3.198979       -2.114286       -1.412972
H       -3.588288       -1.858941       -2.405803
H       -2.142763       -2.374830       -1.520323
H       -3.746057       -2.994274       -1.057929
C       -2.327432        1.803980        1.776716
H       -1.924242        1.352580        2.690089
H       -1.489482        2.292451        1.270851
H       -3.070969        2.549303        2.065636
H        3.271046        3.929050       -0.573783
C        3.594582       -2.603593        1.021986
C        2.443114       -1.814437        0.405829
N        3.076014       -0.572532       -0.034424
C        4.526169       -0.662526        0.018573
C        4.792957       -2.152214        0.193493
H        3.733958       -2.312587        2.069611
H        1.990543       -2.347633       -0.437187
H        4.979381       -0.256354       -0.894025
H        5.757361       -2.349425        0.668349
H        1.637774       -1.606596        1.115765
H        3.422971       -3.682656        0.991033
H        4.785843       -2.650510       -0.782340
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H       -0.594805        2.069081       -0.749075
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54
4pzMePyr2-ts-B-m ; E = -1106.20170178 Hartree
C       -2.541255        0.693174        0.307505
C       -3.082953        1.851553        0.895004
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H       -4.115646        1.866259        1.222750
C       -2.308835        2.994410        1.018634
C       -0.405630        1.934680       -0.006144
C       -0.997350        3.069483        0.552328
H       -0.455024        4.005322        0.616676
N       -0.501182       -0.460791       -0.188031
N        0.077637       -1.570072       -0.239949
C        1.437798       -1.593687        0.138229
C        2.146160       -0.852597        1.085245
C        2.358818       -2.556516       -0.349712
N        3.546728       -2.406201        0.219008
N        3.396857       -1.378448        1.082180
C        4.491146       -1.021134        1.944874
H        5.373627       -1.541924        1.575328
H        4.667991        0.058307        1.920775
H        4.302113       -1.324093        2.980894
C        1.733277        0.196221        2.054694
H        2.311820        1.118602        1.930972
H        0.682616        0.446066        1.915165
H        1.874364       -0.145709        3.087487
C        2.109477       -3.590598       -1.390377
H        2.060298       -3.146932       -2.391039
H        2.910580       -4.332527       -1.383068
H        1.150689       -4.085220       -1.211698
H       -2.757574        3.882026        1.457001
C        2.373260        1.988376       -2.334677
C        1.248779        1.165668       -1.705147
N        0.864366        1.945107       -0.517531
C        1.721762        3.105638       -0.355698
C        2.969927        2.725256       -1.138126
H        3.094998        1.361905       -2.864531
H        1.604709        0.170504       -1.428302
H        1.265178        4.013955       -0.783651
H        3.576347        3.592002       -1.412559
C       -4.336544       -2.162687       -1.040434
C       -2.985031       -1.479828       -0.828517
N       -3.287223       -0.430770        0.153307
C       -4.645414       -0.529130        0.654551
C       -5.050059       -1.952255        0.292461
H       -4.893720       -1.661950       -1.840779
H       -2.226767       -2.172374       -0.451920
H       -4.675586       -0.334160        1.732739
H       -6.134223       -2.077404        0.234433
H       -2.590309       -1.040273       -1.750782
H       -4.228954       -3.215100       -1.314571
H       -4.664518       -2.650621        1.043386
H       -5.311164        0.202420        0.165658
H        1.908676        3.298830        0.707506
H        3.589946        2.042646       -0.545377
H        1.966313        2.713888       -3.048394
H        0.386578        1.044047       -2.370531
54
4pzMePyr2-ts-B-n ; E = -1106.20126235 Hartree
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C       -2.616508        0.413022        0.277167
C       -3.351051        1.448939        0.879973
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H       -4.382203        1.289215        1.171750
C       -2.772891        2.695939        1.058740
C       -0.691628        1.976474        0.077154
C       -1.478885        2.987547        0.634847
H       -1.093141        3.994438        0.739003
N       -0.426741       -0.412916       -0.185258
N        0.305216       -1.424709       -0.252493
C        1.614837       -1.308243        0.262810
C        2.654465       -2.123211       -0.169466
C        2.148197       -0.566059        1.356035
N        3.421329       -0.889346        1.552000
N        3.711675       -1.819867        0.617374
C        5.050228       -2.338593        0.528955
H        5.040381       -3.431867        0.495738
H        5.569346       -1.962598       -0.359720
H        5.581405       -2.008804        1.421025
C        2.674782       -3.122006       -1.266515
H        3.064336       -4.089668       -0.931252
H        1.650083       -3.262513       -1.617109
H        3.286593       -2.794728       -2.115581
C        1.454658        0.365265        2.289302
H        1.150517        1.288154        1.791240
H        0.546769       -0.095748        2.690858
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C        2.123393        2.502423       -2.146742
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N        0.569326        2.221600       -0.396515
C        1.190819        3.524116       -0.226504
C        2.516363        3.377955       -0.959719
H        2.974736        2.021664       -2.635353
H        1.715011        0.606239       -1.170929
H        0.583014        4.322855       -0.683497
H        2.945612        4.341221       -1.246401
C       -3.945607       -2.594170       -1.265104
C       -2.713457       -1.732294       -0.984280
N       -3.174328       -0.810363        0.062023
C       -4.517810       -1.126381        0.507674
C       -4.702979       -2.569923        0.059935
H       -4.559596       -2.134895       -2.048583
H       -1.862707       -2.328323       -0.642192
H       -4.606274       -0.996290        1.592360
H       -5.755748       -2.849043       -0.031518
H       -2.384915       -1.176963       -1.869893
H       -3.679291       -3.601324       -1.595802
H       -4.230151       -3.246211        0.780583
H       -5.269993       -0.473079        0.032171
H        1.305538        3.761045        0.837876
H        3.237803        2.852614       -0.324027
H        1.599858        3.107127       -2.896282
H        0.388535        1.150546       -2.208449
54
4pzMePyr2-ts-H-m ; E = -1106.19254424 Hartree
C        2.596031        0.562717        0.361256
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C        1.227096        0.521539       -0.035561
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C        2.177428        2.760555        1.316463
C        0.412488        1.684558        0.081588
C        0.883309        2.782558        0.815839
H        0.267091        3.661412        0.955426
N        0.722931       -0.734895       -0.494372
N       -0.440700       -1.007378       -0.132124
C       -1.682211       -1.322059        0.146465
C       -2.519651       -0.729420        1.127488
C       -2.521778       -2.322304       -0.468503
N       -3.723871       -2.327222        0.067190
N       -3.690225       -1.377447        1.047936
C       -4.837506       -1.232163        1.904940
H       -5.112396       -0.178727        2.006469
H       -5.657052       -1.779259        1.440156
H       -4.644556       -1.646541        2.900367
C       -2.201179        0.307061        2.133586
H       -2.187773       -0.099810        3.151863
H       -1.211769        0.712706        1.911364
H       -2.930519        1.125076        2.115873
C       -2.147257       -3.201249       -1.604526
H       -1.127552       -3.572953       -1.467791
H       -2.839057       -4.041784       -1.684823
H       -2.163013       -2.650941       -2.552293
H        2.541134        3.611610        1.885939
C       -2.067494        2.110293       -2.523149
C       -1.037338        1.182448       -1.880754
N       -0.824399        1.746068       -0.543115
C       -1.684614        2.897776       -0.337006
C       -2.822274        2.660974       -1.316682
H       -1.568973        2.931544       -3.050853
H       -0.091257        1.138821       -2.432695
H       -2.008232        2.958435        0.708839
H       -3.508453        1.904063       -0.919587
C        4.552234       -2.510387       -0.238651
C        3.251363       -1.751281       -0.474603
N        3.494186       -0.454697        0.153318
C        4.909784       -0.255777        0.434782
C        5.602910       -1.408500       -0.282307
H        4.537504       -2.976866        0.753235
H        3.034674       -1.639078       -1.545613
H        5.249494        0.719638        0.065957
H        6.551210       -1.681725        0.187748
H        2.383461       -2.243140       -0.035358
H        4.712481       -3.298226       -0.979275
H        5.809127       -1.128361       -1.321467
H        5.108432       -0.283678        1.518310
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H       -1.430191        0.162549       -1.821763
54
4pzMePyr2-ts-H-n ; E = -1106.19088792 Hartree
C        2.741646        0.541301        0.037642
C        3.370589        1.760343        0.374619
C        1.327021        0.544729       -0.124761
H        4.437053        1.786849        0.555594
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C	2.636006	2.921458	0.520582
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H	0.724106	3.880291	0.351340
N	0.719100	-0.713374	-0.420978
N	-0.421481	-0.894666	0.050945
C	-1.664813	-1.103915	0.399101
C	-2.610407	-1.946892	-0.236966
C	-2.418340	-0.463697	1.451439
N	-3.673283	-0.867840	1.443540
N	-3.774252	-1.732121	0.392827
C	-5.075674	-2.232931	0.036624
H	-5.030100	-3.304205	-0.175753
H	-5.732574	-2.057870	0.888019
H	-5.475449	-1.712200	-0.840541
C	-2.422930	-2.810044	-1.423447
H	-2.907838	-2.402229	-2.318920
H	-1.350591	-2.883310	-1.622748
H	-2.819961	-3.817938	-1.261510
C	-1.871853	0.451548	2.483874
H	-1.558967	-0.099926	3.377510
H	-0.994317	0.962028	2.078939
H	-2.621975	1.184614	2.790270
H	3.148163	3.840018	0.793820
C	-2.709300	1.610865	-1.695654
C	-1.192489	1.380067	-1.709602
N	-0.763359	1.799981	-0.378595
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C	-2.947302	2.581992	-0.519540
H	-3.049210	2.022784	-2.649969
H	-0.710063	2.008926	-2.478123
H	-1.473063	3.231880	0.984603
H	-3.457314	2.063133	0.296102
C	4.359512	-2.751102	0.274199
C	3.085924	-1.980451	-0.062446
N	3.522102	-0.583876	-0.081365
C	4.972820	-0.482683	-0.038209
C	5.449631	-1.893073	-0.356558
H	4.499856	-2.793354	1.360627
H	2.677060	-2.281202	-1.033137
H	5.335485	0.258906	-0.760135
H	6.451049	-2.092289	0.033584
H	2.293405	-2.131612	0.673820
H	4.334804	-3.776877	-0.102946
H	5.469862	-2.045375	-1.441551
H	5.326116	-0.171287	0.959346
H	-1.200019	3.866567	-0.655059
H	-3.551051	3.449817	-0.798266
H	-3.244098	0.671770	-1.531252
H	-0.917844	0.344764	-1.913406

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