Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Why Water Makes 2-Aminopurine Fluorescent

Mario Barbatti and Hans Lischka

TABLE OF CONTENTS

SECTION S1. SINGLET STATES

Table S1. Vertical excitation energies (ΔE_v) and oscillator strengths (f) at the S_0 minimum for 2AP and 2AP-water clusters computed at ADC(2)/aug-cc-pVDZ. The three main orbital-transition contributions (c_i) and their percentages are given as well. Rs and Rp indicate Rydberg orbitals with s or p character.

2AP	ΔE_v (eV)	f	c_1	%	c_2	%	c_3	%
S_1	4.32	0.155	π-π*	46.0	π-π*	29.1	π-Rp	4.5
S_2	4.46	0.003	n-π*	48.7	n-π*	33.1	n-Rp	5.3
S_3	5.21	0.004	π-Rs	51.5	π-Rs	21.0	π-Rs	5.0
S_4	5.37	0.057	π-π*	21.5	π-π*	20.9	π-π*	13.0
2AP-1W	ΔE_v (eV)	f	c_1	%	c_2	%	c_3	%
S_1	4.31	0.165	π-π*	47.5	π-Rp	18.7	π-Rp	7.2
S_2	4.53	0.002	n-π*	50.0	n-Rp	21.0	n-Rp	8.0
S_3	5.23	0.008	π-Rs	42.5	π-π*	6.8	π-Rs	5.5
S_4	5.32	0.011	π-π*	27.8	π-Rs	13.1	π-Rp	10.8
2AP-1WT	ΔE_v (eV)	f	c_1	%	c_2	%	c_3	%
S_1	4.17	0.146	π-π*	48.7	π-π*	20.4	π-Rp	10.9
S_2	4.57	0.002	n-π*	52.4	n-π*	23.1	n-Rp	12.1
S_3	5.21	0.001	π-Rp	62.8	π-Rp	10.6	π-Rs	5.8
S_4	5.31	0.080	π-π*	21.7	π-Rp	12.1	π-Rp	9.5
2AP-2W	ΔE_v (eV)	f	c_1	%	c_2	%	c_3	%
S_1	4.28	0.167	π-π*	49.4	π-π*	17.7	π-π*	9.6
S_2	4.55	0.002	n-π*	52.5	n-π*	19.7	n-π*	10.3
S_3	5.21	0.005	π-Rs	27.8	π-π*	18.5	π-Rp	6.3
S_4	5.28	0.008	π-Rs	29.1	π-π*	19.4	π-π*	6.7
2AP-2WT	ΔE_v (eV)	f	c_1	%	c_2	%	c_3	%
S_1	4.17	0.157	π-π*	50.3	π-Rp	9.5	π-Rp	8.9
S_2	4.66	0.002	n-π*	53.9	n-Rp	10.6	n-Rp	10.0
S_3	5.24	0.015	π-π*	31.7	π-π*	11.8	π-π*	8.9
S_4	5.31	0.004	π-Rs	48.9	π-Rs	6.5	π-Rp	4.6
2AP-3W	ΔE_v (eV)	f	c_1	%	c_2	%	c_3	%
S_1	4.25	0.163	π-π*	48.6	π-Rp	12.1	π-Rp	8.2
S_2	4.54	0.003	n-π*	51.6	n-Rp	13.4	n-Rp	9.1
S_3	5.21	0.004	π-Rs	21.6	π-π*	17.6	π-Rs	7.7
S_4	5.27	0.006	π-Rs	21.2	π-π*	19.2	π-Rs	8.4
2AP-3WT	ΔE_v (eV)	f	c_1	%	c_2	%	c_3	%
S_1	4.12	0.159	π-π*	52.8	π-Rp	11.5	π-Rp	6.6
S_2	4.69	0.002	n-π*	57.0	n-Rp	12.5	n-Rp	7.2
S_3	5.20	0.006	π-π*	37.2	π-Rp	8.1	π-Rp	7.8
S_4	5.29	0.004	π-Rs	44.5	π-Rs	13.6	π-Rs	9.8
2AP-4WT	ΔE_v (eV)	f	c_1	%	c_2	%	c_3	%
S_1	4.10	0.155	π-π*	30.7	π-Rp	12.8	π-π*	12.5
S_2	4.68	0.002	n-π*	33.1	n-Rp	14.1	n-π*	13.7
S_3	5.19	0.005	π-π*	21.5	π-Rp	9.0	π-π*	8.7
S_4	5.26	0.003	π-Rs	37.8	π-Rs	13.3	π-Rp	13.0

Table S2. Vertical emission energies (ΔE_e) and oscillator strengths (f) at the S_1 minimum for 2AP and 2AP-W clusters computed at ADC(2)/aug-cc-pVDZ. The three main orbital-transition contributions (c_i) and their percentages are given as well. Rs and Rp indicate Rydberg orbitals with s or p character. τ_{rad} is the calculated radiative lifetime (Eq. 1). τ_{es} is the experimental excited-state lifetime after 0_0^0 excitation.[1]

	ΔE_e (eV)	f	c_1	%	c_2	%	c_3	%	τ_{rad} (ns)	τ_{es} (ns)
2AP (nπ*)	2.99	0.006	n-π*	53.2	n-Rp	10.1	π–π*	9.8	429	0.156
2AP (ππ*)	3.14	0.098	π–π*	31.5	π-Rp	23.8	π-Rs	6.8	24	
2AP-1W (nπ*)	2.75	0.022	n-π*	23.2	n-π*	17.0	π–π*	15.5	138	0.584
2AP-1W (ππ*)	3.37	0.135	π–π*	64.4	π-Rp	7.3	π-Rs	3.1	15	
2AP-1W-T	3.33	0.122	π–π*	70.1	π-Rp	5.5	π-Rp	2.7	19	14.5
2AP-2W (nπ*)	2.73	0.035	n-π*	24.5	π–π*	19.6	π–π*	15.6	88	2.46
2AP-2W (ππ*)	3.49	0.148	π–π*	60.1	π-Rp	9.0	π-Rp	7.6	13	
2AP-2W-T	3.37	0.136	π–π*	60.6	π-Rp	9.1	π-Rp	6.2	15	15.9
2AP-3W	3.25	0.127	π–π*	47.7	π-Rp	11.6	π-Rp	9.0	17	7.8
2AP-3W-T	3.29	0.133	π–π*	48.3	π-Rp	26.4	π-Rp	3.7	16	17.0
2AP-4W-T	3.23	0.126	π–π*	46.9	π-Rp	14.7	π-Rp	9.3	18	-

Table S3. Vertical excitation energies (ΔE_v) and oscillator strengths (f) at the S_0 minimum for 2AP and 2AP-water clusters computed with different methods.

	ADC(2) (Present work)			TD-B3LYP [a]		CASPT2 [b]		DFT/MRCI [c]	
2AP	ΔE_v (eV)	f	c_1	ΔE_v (eV)	f	ΔE_v (eV)	f	ΔE_v (eV)	f
S_1	4.32	0.155	π-π*	4.41	0.130	4.33	0.070	4.31	0.18
S_2	4.46	0.003	n-π*	4.45	0.002	4.46	0.008	4.53	
S_3	5.21	0.004	π-Rs					5.16	
S_4	5.37	0.057	π-π*	5.46	0.054	5.33	0.148	5.16	
2AP-1W	ΔE_v (eV)	f	c_1	ΔE_v (eV)	f				
S_1	4.31	0.165	π-π*	4.42	0.135				
S_2	4.53	0.002	n-π*	4.52	0.002				
S_3	5.23	0.008	π-Rs						
S_4	5.32	0.011	π-π*	5.40	0.010				
2AP-1WT	ΔE_v (eV)	f	c_1	ΔE_v (eV)	f				
S_1	4.17	0.146	π-π*	4.26	0.120				
S_2	4.57	0.002	n-π*	4.56	0.002				
S_3	5.21	0.001	π-Rp						
S_4	5.31	0.080	π-π*	5.41	0.06				
2AP-2W	ΔE_v (eV)	f	c_1	ΔE_v (eV)	f				
S_1	4.28	0.167	π-π*	4.41	0.135				
S_2	4.55	0.002	n-π*	4.53	0.002				
S_3	5.21	0.005	π-Rs						
S_4	5.28	0.008	π-Rs						
2AP-2WT	ΔE_v (eV)	f	c_1	ΔE_v (eV)	f				
S_1	4.17	0.157	π-π*	4.27	0.126				
S_2	4.66	0.002	n-π*	4.66	0.001				
S_3	5.24	0.015	π-π*	5.38	0.011				
S_4	5.31	0.004	π-Rs						
2AP-3W	ΔE_v (eV)	f	c_1	ΔE_v (eV)	f				
S_1	4.25	0.163	π-π*	4.38	0.132				
S_2	4.54	0.003	n-π*	4.54	0.001				
S_3	5.21	0.004	π-Rs						
S_4	5.27	0.006	π-Rs						
2AP-3WT	ΔE_v (eV)	f	c_1	ΔE_v (eV)	f				
S_1	4.12	0.159	π-π*	4.26	0.125				
S_2	4.69	0.002	n-π*	4.67	0.002				
S_3	5.20	0.006	π-π*	5.33	0.002				
S_4	5.29	0.004	π-Rs						

[a] TDDFT/B3LYP/TZVP.[1]

[b] CASPT2//CASSCF(16,13)/6-31G(d,p).[2]

[c] DFT(BHLYP)/MRCI //B3LYP/TZVP+Ryd.[3]

SECTION S2. STATIONARY POINTS AND CONICAL INTERSECTIONS

Table S4. Absolute (au) and relative (eV) energies of the ground (S_0) and first (S_1) excited singlet states. Computed adiabatic energies (ΔE_a). Energy barries computed between the S_1 transition state and the lowest (9H) S_1 minimum. All data for 2AP and 2AP-W clusters computed at ADC(2)/aug-cc-pVDZ.

2AP	S_0 (au)	S_1 (au)	S_0 (eV)	S_1 (eV)	ΔE_a (eV)	Barrier (eV)
S_0 Min	-466.091282	-465.932551	0.00	4.32		
S_1 Min nπ*	-466.058308	-465.948396	0.90	3.89	3.89	
S_1 Min ππ*	-466.062064	-465.946830	0.80	3.93	3.93	
C2 S_1 TS	-466.005798	-465.929397	2.33	4.41		0.52
C2 X	-465.946273	-465.945808	3.95	3.96		
C6 S_1 TS	-466.035461	-465.944321	1.52	4.00		0.11
C6 X	-465.944314	-465.943725	4.00	4.02		0.13
2AP-1W	S_0 (au)	S_1 (au)	S_0 (eV)	S_1 (eV)	ΔE_a (eV)	Barrier (eV)
S_0 Min	-542.370211	-542.211805	0.00	4.31		
S_1 Min nπ*	-542.326795	-542.225672	1.18	3.93	3.93	
S_1 Min ππ*	-542.349603	-542.225908	0.56	3.93	3.93	
C2 S_1 TS	-542.285889	-542.209823	2.29	4.36		0.43
C2 X	-542.227163	-542.226699	3.89	3.91		
C6 S_1 TS	-542.315072	-542.221696	1.50	4.04		0.11
C6 X	-542.221801	-542.221183	4.04	4.06		0.13
3H S_1 TS	-542.315617	-542.194702	1.49	4.78		0.84
3H S_1 Min	-542.316105	-542.232053	1.47	3.76		
2AP-1WT	S_0 (au)	S_1 (au)	S_0 (eV)	S_1 (eV)	ΔE_a (eV)	Barrier (eV)
S_0 Min	-542.367770	-542.214378	0.00	4.17		
S_1 Min ππ*	-542.350517	-542.228279	0.47	3.80	3.80	
C2 S_1 TS	-542.282275	-542.206574	2.33	4.39		0.59
C2 X	-542.221456	-542.220974	3.98	3.99		
C6 S_1 TS	-542.308688	-542.218223	1.61	4.07		0.27
C6 X	-542.219015	-542.218446	4.05	4.06		
1H S_1 TS	-542.315912	-542.213159	1.41	4.21		0.41
1H S_1 Min	-542.305746	-542.250937	1.69	3.18		
2AP-2W	S_0 (au)	S_1 (au)	S_0 (eV)	S_1 (eV)	ΔE_a (eV)	Barrier (eV)
S_0 Min	-618.651238	-618.494077	0.00	4.28		
S_1 Min nπ*	-618.607824	-618.507355	1.18	3.92	3.92	
S_1 Min ππ*	-618.635979	-618.507762	0.42	3.90	3.90	
C2 S_1 TS	-618.568123	-618.492757	2.26	4.31		0.41
C2 X	-618.510189	-618.509733	3.84	3.85		
C6 S_1 TS	-618.595546	-618.502249	1.52	4.05		0.15
C6 X	-618.501906	-618.501299	4.06	4.08		0.18
3H S_1 TS	-618.603478	-618.482079	1.30	4.60		0.70
3H S_1 Min	-618.602356	-618.513638	1.33	3.74		
2AP-2WT	S_0 (au)	S_1 (au)	S_0 (eV)	S_1 (eV)	ΔE_a (eV)	Barrier (eV)
S_0 Min	-618.646844	-618.493763	0.00	4.17		
S_1 Min ππ*	-618.631375	-618.507602	0.42	3.79	3.79	
C2 S_1 TS	-618.562501	-618.486844	2.30	4.35		0.56
C2 X	-618.500144	-618.499670	3.99	4.00		
C6 S_1 TS	-618.588565	-618.495824	1.59	4.11		0.32
C6 X	-618.497182	-618.496575	4.07	4.09		

3H S_1 TS	-618.592050	-618.475458	1.49	4.66		0.87
3H S_1 Min	-618.592094	-618.511054	1.49	3.70		
1H S_1 TS	-618.596270	-618.491916	1.38	4.22		0.43
1H S_1 Min	-618.588103	-618.529322	1.60	3.20		
2AP-3W	S_0 (au)	S_1 (au)	S_0 (eV)	S_1 (eV)	ΔE_a (eV)	Barrier (eV)
S_0 Min	-694.927199	-694.771158	0.00	4.25		
S_1 Min ππ*	-694.905044	-694.785711	0.60	3.85	3.85	
C2 S_1 TS	-694.845213	-694.768935	2.23	4.31		0.46
C2 X	-694.783738	-694.783208	3.90	3.92		
C6 S_1 TS	-694.871053	-694.778327	1.53	4.05		0.20
C6 X	-694.777957	-694.777334	4.06	4.08		
3H S_1 Min	-694.881350	-694.789223	1.25	3.75		
2AP-3WT	S_0 (au)	S_1 (au)	S_0 (eV)	S_1 (eV)	ΔE_a (eV)	Barrier (eV)
S_0 Min	-694.928091	-694.776545	0.00	4.12		
S_1 Min ππ*	-694.910850	-694.789833	0.47	3.76	3.76	
C2 S_1 TS	-694.844384	-694.769698	2.28	4.31		0.55
C2 X	-694.783073	-694.782607	3.95	3.96		
C6 S_1 TS	-694.869040	-694.776415	1.61	4.13		0.37
C6 X	-694.777248	-694.776588	4.10	4.12		
3H S_1 TS	-694.879621	-694.762637	1.32	4.50		0.74
3H S_1 Min	-694.881539	-694.791865	1.27	3.71		
1H S_1 TS	-694.876755	-694.772513	1.40	4.23		0.47
1H S_1 Min	-694.870507	-694.810213	1.57	3.21		
2AP-4WT	S_0 (au)	S_1 (au)	S_0 (eV)	S_1 (eV)	ΔE_a (eV)	Barrier (eV)
S_0 Min	-771.204019	-771.053304	0.00	4.10		
S_1 Min ππ*	-771.185842	-771.067063	0.49	3.73	3.73	
C2 S_1 TS	-771.121417	-771.045671	2.25	4.31		0.58
C2 X	-771.058595	-771.058062	3.96	3.97		
C6 S_1 TS	-771.144474	-771.052284	1.62	4.13		0.40
C6 X	-771.053179	-771.052566	4.10	4.12		
3H S_1 Min	-771.165434	-771.068458	1.05	3.69		
1H S_1 TS	-771.151272	-771.048990	1.44	4.22		0.49
1H S_1 Min	-771.144119	-771.086036	1.63	3.21		

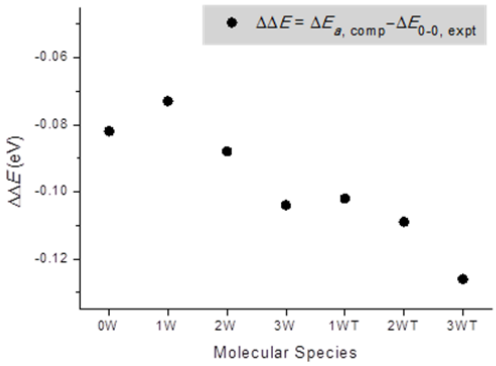

Fig. S1 Energy differences between computed adiabatic excitations into the ππ* state and measured[1] band origin.

SECTION S3. TRIPLET STATES

Table S5. Energy gaps (ΔE) between S_0 and T_1 (ground triplet state) and between S_0 and T_2 (first excited triplet state) at the S_1 minimum for 2AP and 2AP-W clusters computed at ADC(2)/aug-cc-pVDZ. The three main orbital-transition contributions (c_i) and their percentages are given as well. Rs and Rp indicate Rydberg orbitals with s or p character.

2AP	ΔE (eV)	c_1	%	c_2	%	c_3	%
T_1	2.79	n-π*	47.7	π-π*	10.8	n-Rp	8.9
T_2	3.10	π-π*	51.2	π-Rp	9.7	π-π*	8.5
2AP-1W	ΔE (eV)	c_1	%	c_2	%	c_3	%
T_1	2.50	π-π*	22.6	π-Rp	16.9	n-π*	15.9
T_2	2.91	π-π*	25.7	π-Rp	18.5	π-π*	15.5
2AP-1WT	ΔE (eV)	c_1	%	c_2	%	c_3	%
T_1	2.66	π-π*	75.0	π-Rp	5.8	π-Rp	2.7
T_2	4.01	n-π*	64.0	π-π*	6.6	n-Rp	5.2
2AP-2W	ΔE (eV)	c_1	%	c_2	%	c_3	%
T_1	2.43	π-π*	40.4	n-π*	13.1	π-Rp	8.0
T_2	2.92	π-π*	24.1	π-π*	19.1	n-π*	15.1
2AP-2WT	ΔE (eV)	c_1	%	c_2	%	c_3	%
T_1	2.67	π-π*	64.1	π-Rp	9.4	π-Rp	7.1
T_2	4.15	n-π*	60.6	n-Rp	8.9	n-Rp	6.8
2AP-3W	ΔE (eV)	c_1	%	c_2	%	c_3	%
T_1	2.59	π-π*	52.7	π-Rp	12.0	π-Rp	10.7
T_2	3.80	n-π*	38.1	π-π*	8.6	n-Rp	8.5
2AP-3WT	ΔE (eV)	c_1	%	c_2	%	c_3	%
T_1	2.60	π-π*	52.6	π-Rp	27.1	π-Rp	3.9
T_2	4.10	n-π*	43.4	n-Rp	22.5	π-π*	6.0
2AP-4WT	ΔE (eV)	c_1	%	c_2	%	c_3	%
T_1	2.56	π-π*	50.7	π-Rp	14.8	π-Rp	9.8
T_2	4.08	n-π*	34.6	π-π*	11.4	n-Rp	10.1

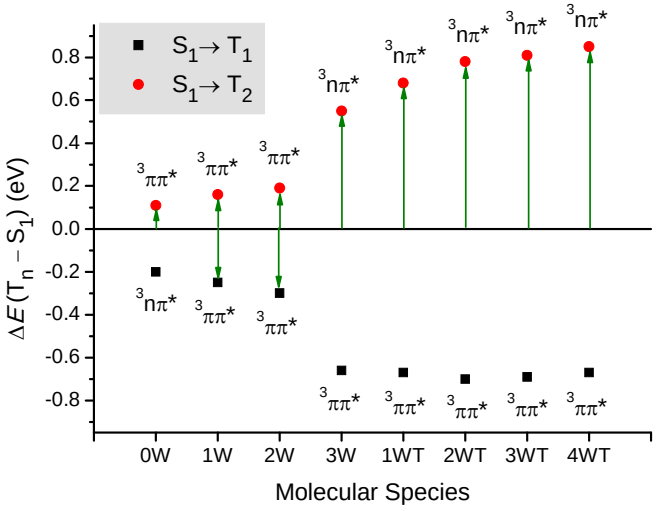

Fig. S2 Energy gaps between T_1 and S_1 and between T_2 and S_1. The arrows indicate the allowed transitions according to El-Sayed's rule.

SECTION S4. REACTION PATH TO C6 X

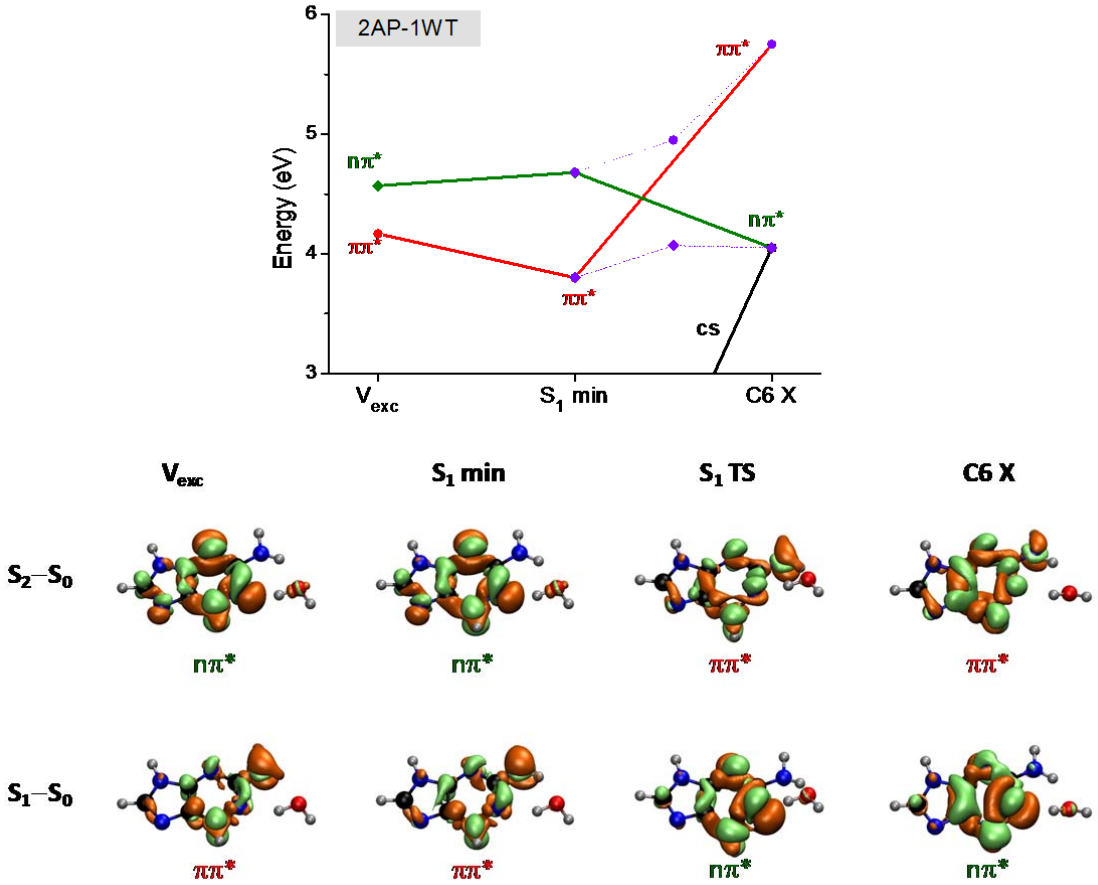

Fig. S3 Diabatic connection of the energies at the S_0 minimum (V_{exc}), the S_1 minimum, and C6 X for 2AP-1WT. Dotted lines indicated the adiabatic connections through the S_1 transition state. The S_1-S_0 electron density difference for all structures are shown as well. Orange regions are electron donor and green regions are electron acceptor.

SECTION S5. MOLECULAR ORBITALS

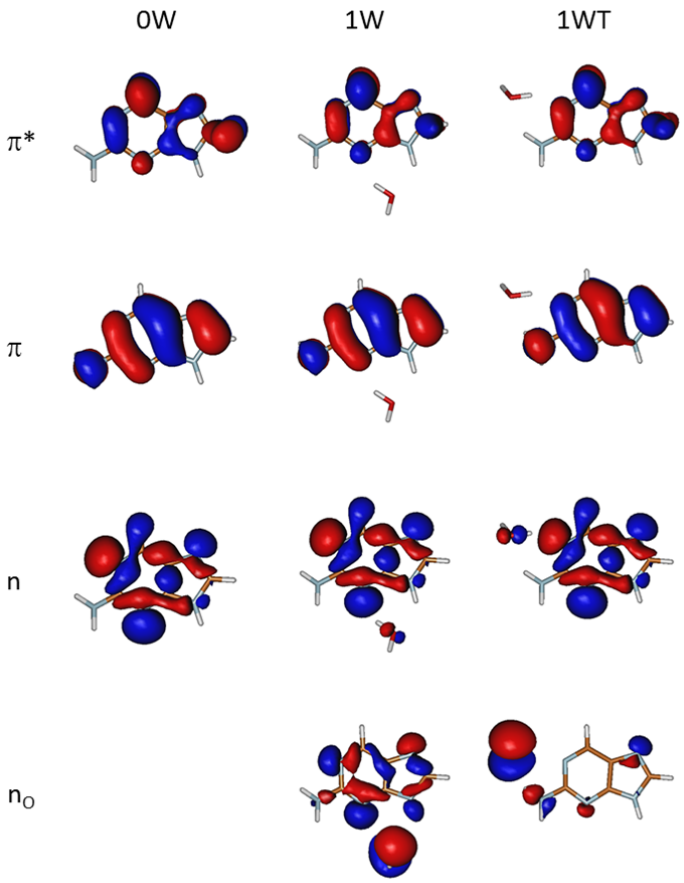

Fig. S4 Canonical Hartree-Fock molecular orbitals for the ground state minimum of 2AP (0W), 2AP-1W, and 2AP-1WT.

–

SECTION S6. ADDITIONAL REFERENCES

1 S. Lobsiger, S. Blaser, R. K. Sinha, H.-M. Frey and S. Leutwyler, *Nat Chem*, 2014, **6**, 989.

2 L. Serrano-Andrés, M. Merchán and A. C. Borin, *Proc. Natl. Acad. Sci. USA*, 2006, **103**, 8691.

3 K. A. Seefeld, C. Plutzer, D. Lowenich, T. Haber, R. Linder, K. Kleinermanns, J. Tatchen and C. M. Marian, *Phys. Chem. Chem. Phys.*, 2005, **7**, 3021.

SECTION S7. CARTESIAN COORDINATES

XYZ format in Angstrom.

```
15
0W S0
N     0.522144     0.110680    -1.972021
C     1.721424     0.024925    -1.319948
N     1.934536    -0.088190     0.008326
C     0.785453    -0.085222     0.699157
C    -0.523219     0.012916     0.165533
C    -0.599467     0.104889    -1.236206
N    -1.482679    -0.014942     1.173112
C    -0.763022    -0.127642     2.287114
N     0.602826    -0.177350     2.064571
N     2.842620     0.117313    -2.127925
H    -1.176299    -0.178388     3.292815
H     1.333955    -0.254728     2.762703
H     3.697108    -0.245836    -1.721158
H     2.682047    -0.110479    -3.102557
H    -1.553450     0.170437    -1.768487
15
0W S1 (np*)
N     0.553369     0.083090    -1.856431
C     1.774859     0.051856    -1.357883
N     1.935691     0.007159    -0.001874
C     0.750443    -0.046361     0.698149
C    -0.566092     0.043810     0.186562
C    -0.696923     0.282732    -1.238380
N    -1.493588    -0.037452     1.195535
C    -0.768299    -0.158901     2.315478
N     0.595349    -0.160302     2.054097
N     2.893175     0.109615    -2.164437
H    -1.164030    -0.252678     3.323745
H     1.345760    -0.249934     2.730382
H     3.714401    -0.299496    -1.726524
H     2.740337    -0.189442    -3.122708
H    -1.590478     0.074687    -1.830684
15
0W S1 (pp*)
N     0.251961     0.073081     1.623608
C     1.502012    -0.092459     2.133631
N     2.707675    -0.248357     1.494151
C     2.481051    -0.080088     0.156073
C     1.231125    -0.061350    -0.523127
C     0.012394    -0.240895     0.276025
N     1.407590     0.079255    -1.874665
C     2.744256     0.099440    -2.040489
N     3.425056    -0.023496    -0.850444
N     1.572794    -0.077452     3.490063
H     3.254800     0.182861    -2.997633
H     4.430535    -0.004385    -0.719109
H     2.463741    -0.267617     3.935403
H     0.723627     0.044520     4.030684
H    -0.978633     0.001135    -0.119552
15
0W C2 X
N     0.528812    -0.190517    -2.040683
C     1.795530    -0.028111    -1.297494
N     1.873413    -0.718895    -0.023836
C     0.890403    -0.202769     0.716280
C    -0.342959     0.267818     0.154643
C    -0.493989     0.128176    -1.302532
N    -1.307794     0.395004     1.109086
C    -0.696346     0.033303     2.257100
N     0.598895    -0.364264     2.069187
N     2.138815     1.354405    -1.212253
H    -1.164346     0.058631     3.240789
H     1.245905    -0.685247     2.782449
H     3.103413     1.464206    -0.894753
H     2.032269     1.797138    -2.127283
H    -1.499378     0.138191    -1.744759
15
0W C6 X
N     0.494643    -0.406339    -1.825702
C     1.792790    -0.197900    -1.288381
N     1.936088    -0.279721     0.006772
C     0.698834    -0.204938     0.697340
C    -0.558029     0.092413     0.184990
C    -0.554116     0.443890    -1.261147
N    -1.479689     0.270316     1.192836
C    -0.782436     0.038188     2.318092
N     0.543185    -0.245281     2.060110
N     2.837188    -0.128221    -2.169340
H    -1.195291     0.014707     3.322412
H     1.270601    -0.432331     2.743062
H     3.744871    -0.375347    -1.785493
H     2.646314    -0.482285    -3.100909
H    -0.534854     1.514009    -1.538553
15
0W TS S1 - C2 X
N     0.447442    -0.054648    -2.158660
C     1.619912    -0.158946    -1.425109
N     1.777669    -0.942327    -0.206008
C     0.832828    -0.321867     0.577224
C    -0.441334     0.029004     0.080179
C    -0.642099    -0.071973    -1.402112
N    -1.303966     0.357187     1.077471
C    -0.568385     0.226557     2.211315
N     0.708542    -0.196436     1.956407
N     2.604824     0.747701    -1.662525
H    -0.931503     0.433965     3.215336
H     1.435512    -0.379383     2.641219
H     3.545209     0.539515    -1.350303
H     2.460441     1.489829    -2.339149
H    -1.631693    -0.053052    -1.866910
15
```

```
0W TS S1 - C6 X
N     0.539880    -0.106735    -1.875794
C     1.786998     0.062673    -1.334574
N     1.940296     0.008289    -0.008580
C     0.732886    -0.076564     0.691438
C    -0.571987     0.015724     0.185977
C    -0.683882     0.309001    -1.249599
N    -1.500339    -0.009403     1.200075
C    -0.769176    -0.128802     2.318911
N     0.588531    -0.164876     2.051832
N     2.868846     0.206355    -2.169455
H    -1.163569    -0.219320     3.327419
H     1.341022    -0.244158     2.727850
H     3.754411    -0.060573    -1.748207
H     2.728787    -0.129435    -3.117070
H    -1.463465     0.888284    -1.763552
18
1W S0
N     0.629984     0.140922    -1.845479
C     1.759754    -0.015291    -1.094453
N     1.842563    -0.159712     0.245032
C     0.634283    -0.121018     0.837756
C    -0.612729     0.042636     0.185488
C    -0.554150     0.170532    -1.213914
N    -1.657535     0.036597     1.101733
C    -1.041523    -0.124794     2.273810
N     0.332671    -0.227039     2.176242
N     2.952116     0.034311    -1.799633
H    -1.548571    -0.173381     3.235620
H     1.031384    -0.349867     2.911467
H     3.745449    -0.402060    -1.344014
H     2.856612    -0.158851    -2.790491
H    -1.450121     0.294249    -1.829859
O     3.049338    -0.355976     2.817961
H     3.012783    -0.326756     1.838979
H     3.817045    -0.899348     3.033776
18
1W S1 (np*)
N     0.585370    -0.028854    -1.757469
C     1.789184    -0.044879    -1.174144
N     1.911720    -0.095931     0.178965
C     0.668250    -0.112675     0.789860
C    -0.606590     0.079716     0.198222
C    -0.645730     0.433886    -1.208311
N    -1.604912     0.000371     1.145445
C    -0.950002    -0.196454     2.296476
N     0.423217    -0.262484     2.126659
N     2.920249    -0.018770    -1.950354
H    -1.414795    -0.299388     3.274315
H     1.158498    -0.408683     2.821497
H     3.759395    -0.361947    -1.493745
H     2.806621    -0.274360    -2.924542
H    -1.533314     0.335401    -1.839081
O     3.188851    -0.391264     2.713872
H     3.826258    -1.105816     2.837863
H     3.103709    -0.292338     1.742457
18
1W S1 (pp*)
N     0.617187     0.010007    -1.921379
C     1.739933    -0.013658    -1.154429
N     1.925941    -0.019411     0.216041
C     0.684818    -0.106603     0.792023
C    -0.580817     0.013896     0.155273
C    -0.608549     0.234498    -1.300811
N    -1.588472    -0.075608     1.065961
C    -0.955585    -0.223373     2.262342
N     0.401605    -0.223178     2.142958
N     2.897575    -0.044825    -1.864362
H    -1.462051    -0.317706     3.220477
H     1.122399    -0.321790     2.862219
H     3.785490    -0.008991    -1.375520
H     2.847320    -0.050096    -2.878168
H    -1.514761     0.127796    -1.902005
O     3.141269    -0.253578     2.772725
H     3.779709    -0.962492     2.920098
H     3.066016    -0.176298     1.797099
18
1W C2 X
N     0.709815    -0.375820    -1.895773
C     1.878938    -0.028407    -1.078731
N     1.914995    -0.610107     0.259924
C     0.822177    -0.134881     0.854204
C    -0.388126     0.214212     0.152653
C    -0.402378    -0.076468    -1.287735
N    -1.416764     0.415783     1.018905
C    -0.865739     0.212055     2.241018
N     0.446550    -0.151702     2.192235
N     2.093292     1.383898    -1.066357
H    -1.405406     0.318316     3.178972
H     1.094312    -0.393324     2.949380
H     2.978026     1.601319    -0.603913
H     2.100235     1.755984    -2.018497
H    -1.356940    -0.209016    -1.812532
O     3.004740    -0.992940     2.854077
H     3.398297    -1.832878     3.121860
H     2.970026    -1.028614     1.872749
18
1W C6 X
N     0.514383    -0.464116    -1.766279
C     1.781315    -0.210486    -1.168901
N     1.862122    -0.245461     0.131241
C     0.578979    -0.174442     0.750436
C    -0.643179     0.110322     0.153735
C    -0.574048     0.404359    -1.300237
N    -1.616979     0.322806     1.104364
C    -0.977833     0.130391     2.273120
N     0.353322    -0.164121     2.102093
N     2.847644    -0.114322    -2.015944
H    -1.442918     0.150171     3.254500
H     1.078355    -0.329972     2.802614
H     3.765328    -0.250690    -1.603218
H     2.718678    -0.492552    -2.948936
H    -0.553634     1.456671    -1.636972
O     3.054937    -0.629235     2.778041
H     3.359468    -1.536786     2.909213
H     3.009481    -0.524006     1.806590
18
1W S1 3H
N     0.679669     0.195524    -1.807454
C     1.749103    -0.047853    -1.078525
N     1.744852    -0.303437     0.303140
C     0.516996    -0.144896     0.911671
C    -0.633839     0.081578     0.199961
C    -0.573958     0.264554    -1.236671
N    -1.669935    -0.103582     1.129898
C    -1.064765    -0.169232     2.398980
N     0.237941    -0.366790     2.298532
N     3.025123    -0.031824    -1.650448
H    -1.646365    -0.238279     3.315109
H     2.117678    -0.567238     3.074631
H     3.617949    -0.805902    -1.353210
H     2.956049     0.013324    -2.664955
H    -1.430598     0.489140    -1.872849
O     3.048893    -0.417639     2.822347
H     3.573697    -0.935168     3.445385
H     2.595397    -0.297030     0.873774
18
1W TS S1 - C2 X
N     0.447442    -0.054648    -2.158660
C     1.619913    -0.158946    -1.425109
N     1.777669    -0.942327    -0.206008
C     0.832828    -0.321867     0.577224
C    -0.441334     0.029004     0.080179
C    -0.642099    -0.071973    -1.402112
N    -1.303966     0.357187     1.077472
C    -0.568385     0.226557     2.211315
N     0.708542    -0.196436     1.956407
N     2.604824     0.747701    -1.662525
H    -0.931503     0.433965     3.215337
H     1.435512    -0.379383     2.641219
H     3.545209     0.539515    -1.350303
H     2.460441     1.489829    -2.339150
H    -1.631693    -0.053052    -1.866910
O     3.344202    -1.217973     2.136976
H     3.802215    -2.041236     2.348070
H     3.057694    -1.318600     1.202683
```

18
1W TS S1 - C6
N 0.539880 -0.106735 -1.875795
C 1.786998 0.062673 -1.334575
N 1.940297 0.008289 -0.008580
C 0.732887 -0.076564 0.691438
C -0.571987 0.015724 0.185977
C -0.683882 0.309001 -1.249599
N -1.500340 -0.009403 1.200075
C -0.769176 -0.128802 2.318912
N 0.588531 -0.164876 2.051833
N 2.868847 0.206355 -2.169456
H -1.163569 -0.219320 3.327421
H 1.341022 -0.244158 2.727851
H 3.754412 -0.060572 -1.748208
H 2.728788 -0.129435 -3.117071
H -1.463465 0.888284 -1.763553
O 3.412673 -0.306456 2.439899
H 3.999380 -1.068617 2.526172
H 3.238725 -0.230318 1.479314
18
1W TS S1 - S1 3H
N 0.635175 0.044663 -1.818664
C 1.748680 -0.086847 -1.069417
N 1.880321 -0.184900 0.317395
C 0.636401 -0.082016 0.893851
C -0.602426 0.021169 0.254021
C -0.605524 0.070518 -1.222291
N -1.583609 -0.007871 1.191015
C -0.886033 -0.107672 2.415614
N 0.438039 -0.172844 2.282459
N 2.926906 -0.147852 -1.745664
H -1.405253 -0.132220 3.371772
H 1.686427 -0.351789 2.751435
H 3.804980 -0.161773 -1.242455
H 2.906649 -0.041639 -2.753276
H -1.483469 0.267753 -1.839353
O 2.840945 -0.444863 2.545803
H 3.131556 -1.341267 2.775932
H 2.691037 -0.378346 1.391045
18
1WT S0
N 0.683834 -0.026693 -1.781573
C 1.824848 -0.060493 -1.016845
N 1.894435 -0.089070 0.332735
C 0.682864 -0.064491 0.902581
C -0.569044 -0.020911 0.239317
C -0.507332 -0.009141 -1.163583
N -1.623530 -0.011568 1.147095
C -1.016034 -0.048432 2.330335
N 0.366536 -0.082470 2.245927
N 3.011121 -0.019885 -1.708558
H -1.527837 -0.052515 3.290999
H 1.026937 -0.110435 3.015016
H 3.836152 -0.285217 -1.186075
H 2.975477 -0.242154 -2.701986
H -1.402789 0.010026 -1.792169
O 1.747526 -0.498008 -4.372899
H 1.140915 -0.272791 -3.633641
H 1.597736 0.189118 -5.034421
18
1WT S1
N 0.636615 -0.080973 -1.850885
C 1.766578 -0.132358 -1.086314
N 1.964522 -0.111081 0.276299
C 0.731918 -0.112419 0.873984
C -0.536118 0.011714 0.254469
C -0.583117 0.135138 -1.207010
N -1.534673 0.026888 1.183984
C -0.893361 -0.074370 2.377824
N 0.462191 -0.142385 2.235410
N 2.923468 -0.230522 -1.793063
H -1.385260 -0.096810 3.347676
H 1.149867 -0.229724 2.976376
H 3.790968 -0.267433 -1.264664
H 2.886776 -0.272872 -2.822832
H -1.501483 0.051650 -1.791904
O 1.820053 -0.418327 -4.346651
H 1.120904 -0.278929 -3.661412
H 1.634779 0.231440 -5.036595
18
1WT C2 X
N 0.682240 -0.652332 -1.761978
C 1.886493 -0.248148 -0.989681
N 1.889559 -0.671680 0.399333
C 0.827224 -0.083034 0.951532
C -0.388352 0.163170 0.228415
C -0.414807 -0.278751 -1.173055
N -1.432863 0.398984 1.070714
C -0.889699 0.326298 2.304088
N 0.438751 0.003140 2.286204
N 2.127773 1.142794 -1.164982
H -1.431423 0.509734 3.229708
H 1.043298 -0.124791 3.093147
H 3.010675 1.400583 -0.720799
H 2.156433 1.366877 -2.166219
H -1.378123 -0.426400 -1.678153
O 1.605677 0.458562 -4.246284
H 1.247136 -0.218299 -3.640367
H 2.176958 -0.028566 -4.854041
18
1WT C6 X
N 0.599678 -0.346399 -1.695007
C 1.860962 -0.223390 -1.041841
N 1.867183 -0.380414 0.258293
C 0.576329 -0.244917 0.822126
C -0.600044 0.188891 0.213284
C -0.448736 0.552546 -1.213423
N -1.571780 0.469688 1.152192
C -0.995074 0.167588 2.324385
N 0.307581 -0.264018 2.166431
N 2.965599 -0.143922 -1.809974
H -1.481431 0.207218 3.296995
H 0.957243 -0.530514 2.897125
H 3.867620 -0.241098 -1.360437
H 2.868198 -0.158585 -2.822962
H -0.354706 1.618606 -1.485795
O 1.639871 -0.196387 -4.344385
H 0.954258 -0.719011 -3.896034
H 1.640740 -0.497632 -5.263093
18
1WT S1 imino
N 0.801542 -0.107201 -1.719637
C 1.933030 -0.178368 -0.953220
N 2.006942 -0.180224 0.358361
C 0.711179 -0.108724 0.921129
C -0.505568 -0.012273 0.255981
C -0.500202 0.044416 -1.191489
N -1.553856 0.036852 1.147079
C -0.963337 -0.028725 2.357164
N 0.402010 -0.113820 2.265726
N 3.104963 -0.263099 -1.730992
H -1.486782 -0.016836 3.310245
H 1.065642 -0.174412 3.030333
H 3.880737 -0.319888 -1.050586
H 2.691636 -0.268157 -3.713323
H -1.348072 -0.113637 -1.857949
O 1.938567 -0.311815 -4.337241
H 0.953153 -0.123123 -2.738527
H 2.102382 0.382564 -4.988489
18
1WT TS S1 - C2 X
N 0.447442 -0.054648 -2.158660
C 1.619913 -0.158946 -1.425109
N 1.777669 -0.942327 -0.206008
C 0.832828 -0.321867 0.577224
C -0.441334 0.029004 0.080179
C -0.642099 -0.071973 -1.402112
N -1.303966 0.357187 1.077472
C -0.568385 0.226557 2.211315
N 0.708542 -0.196436 1.956407
N 2.604824 0.747701 -1.662525
H -0.931503 0.433965 3.215337
H 1.435512 -0.379383 2.641219
H 3.545209 0.539515 -1.350303
H 2.460441 1.489829 -2.339150

```
H    -1.631693    -0.053052    -1.866910
O     1.191918     2.149048    -3.794981
H     0.719775     1.324862    -3.555365
H     1.272789     2.121888    -4.756780
18
1WT TS S1 - C6 X
N     0.539880    -0.106735    -1.875795
C     1.786998     0.062673    -1.334575
N     1.940297     0.008289    -0.008580
C     0.732887    -0.076564     0.691438
C    -0.571987     0.015724     0.185977
C    -0.683882     0.309001    -1.249599
N    -1.500340    -0.009403     1.200075
C    -0.769176    -0.128802     2.318912
N     0.588531    -0.164876     2.051833
N     2.868847     0.206355    -2.169456
H    -1.163569    -0.219320     3.327421
H     1.341022    -0.244158     2.727851
H     3.754412    -0.060572    -1.748208
H     2.728788    -0.129435    -3.117071
H    -1.463465     0.888284    -1.763553
O     1.542768    -1.453985    -4.228450
H     0.871095    -1.388194    -3.526600
H     1.040236    -1.599489    -5.040274
18
1WT TS S1 - S1 imino
N     0.687063    -0.148834    -1.881602
C     1.824340    -0.203189    -1.120511
N     1.992544    -0.189719     0.216711
C     0.742555    -0.124848     0.816368
C    -0.512965    -0.033222     0.190766
C    -0.566144     0.002508    -1.264997
N    -1.517933     0.036412     1.119557
C    -0.879584    -0.007941     2.313870
N     0.475737    -0.097733     2.176361
N     2.959985    -0.294348    -1.890929
H    -1.370811     0.022201     3.283772
H     1.163580    -0.146659     2.920271
H     3.826591    -0.344590    -1.349508
H     2.689309    -0.282818    -3.076422
H    -1.466202    -0.115303    -1.869334
O     1.830839    -0.309173    -4.047886
H     1.052395    -0.196508    -3.163580
H     1.820995     0.496751    -4.585562
21
2W S0
N     0.700896     0.131407    -1.804891
C     1.811970     0.090905    -1.014277
N     1.857372    -0.033556     0.329735
C     0.632959    -0.081918     0.891269
C    -0.597869    -0.039933     0.188120
C    -0.501127     0.060717    -1.211051
N    -1.671651    -0.122513     1.064626
C    -1.084536    -0.207834     2.260173
N     0.296103    -0.191733     2.218878
N     3.018513     0.246599    -1.673994
H    -1.618699    -0.286956     3.205427
H     0.954503    -0.200079     3.017972
H     3.848910    -0.044363    -1.171398
H     2.995117     0.034958    -2.664547
H    -1.383285     0.083039    -1.858097
O     4.003332    -0.660520     2.013084
H     3.298164    -0.448104     1.349935
H     4.222883    -1.588654     1.858007
O     2.334365    -0.229703     4.145030
H     3.069143    -0.373534     3.503834
H     2.593777     0.547455     4.655677
21
2W S1 (np*)
N     0.630784    -0.184058    -1.763687
C     1.805488    -0.061054    -1.134559
N     1.908972     0.019418     0.219972
C     0.653547    -0.047869     0.801997
C    -0.609881    -0.000222     0.153208
C    -0.637425     0.246435    -1.279203
N    -1.634377    -0.106997     1.068509
C    -1.006559    -0.168933     2.249882
N     0.372945    -0.125706     2.136958
N     2.965292    -0.126349    -1.872200
H    -1.499110    -0.243657     3.217028
H     1.070422    -0.159108     2.900343
H     3.780100     0.270209    -1.412942
H     2.879020     0.063946    -2.865889
H    -1.503156     0.023667    -1.909543
O     4.105438    -0.677059     1.781623
H     4.293809    -1.608724     1.606308
H     3.370822    -0.447919     1.156808
O     2.506543    -0.261388     3.976286
H     3.213997    -0.406603     3.305745
H     2.807465     0.491813     4.499816
21
2W S1 (pp*)
N     0.625813     0.010198    -1.929179
C     1.732799     0.004866    -1.145528
N     1.906328    -0.019685     0.231971
C     0.665392    -0.082191     0.809768
C    -0.594456    -0.031554     0.151450
C    -0.615729     0.088626    -1.315255
N    -1.607251    -0.083164     1.054349
C    -0.978508    -0.153830     2.267656
N     0.374615    -0.141144     2.165452
N     2.908655     0.025806    -1.827569
H    -1.495510    -0.209056     3.223305
H     1.072331    -0.162557     2.931562
H     3.785033     0.080213    -1.317850
H     2.882169     0.055910    -2.842021
H    -1.514033    -0.017735    -1.925290
O     4.113175    -0.661621     1.758062
H     4.273791    -1.606558     1.633163
H     3.354062    -0.451379     1.149555
O     2.525453    -0.254719     3.961685
H     3.232507    -0.375700     3.284607
H     2.827488     0.475116     4.516558
21
2W C2 X
N     0.921494    -0.495848    -1.792585
C     2.016534    -0.055260    -0.924629
N     1.992912    -0.570604     0.441122
C     0.843608    -0.129958     0.950620
C    -0.327880     0.136617     0.151305
C    -0.238590    -0.213191    -1.271747
N    -1.420256     0.326424     0.933806
C    -0.945514     0.192259     2.198301
N     0.380262    -0.111020     2.258611
N     2.180503     1.359054    -0.976612
H    -1.554531     0.302995     3.094209
H     0.964614    -0.252980     3.108726
H     3.041527     1.639210    -0.503266
H     2.190130     1.689949    -1.943564
H    -1.154319    -0.410902    -1.843984
O     3.903454    -1.301956     2.353475
H     4.243812    -2.194862     2.212519
H     3.316840    -1.127714     1.573960
O     2.161085    -0.600103     4.310965
H     2.883390    -0.916001     3.712875
H     2.553564     0.142932     4.787683
21
2W C6 X
N     0.605292    -0.503800    -1.668761
C     1.875698    -0.240084    -1.081233
N     1.961793    -0.280385     0.217961
C     0.680716    -0.209830     0.851336
C    -0.540885     0.080592     0.251834
C    -0.491629     0.360386    -1.204880
N    -1.513775     0.303666     1.200079
C    -0.871937     0.111360     2.367618
N     0.457988    -0.192942     2.203808
N     2.931063    -0.125911    -1.937344
H    -1.335254     0.140132     3.350533
H     1.149057    -0.341663     2.958568
H     3.862599    -0.221468    -1.543794
H     2.793979    -0.495565    -2.871980
H    -0.486952     1.407771    -1.554260
O     4.160707    -0.779022     1.935821
H     4.425814    -1.697428     1.791622
H     3.443826    -0.612809     1.276792
```

```
O     2.490346    -0.600888     4.131413
H     3.217382    -0.636685     3.469084
H     2.719611     0.122996     4.727965
21
2W S1 3H
N     0.655748    -0.018878    -1.943599
C     1.742691    -0.018071    -1.200314
N     1.777913     0.032298     0.206613
C     0.534804     0.032676     0.801516
C    -0.637022    -0.016383     0.082163
C    -0.597661    -0.044522    -1.365757
N    -1.638003    -0.226121     1.039690
C    -1.037053    -0.025611     2.296070
N     0.282640    -0.019674     2.206694
N     3.003221    -0.141070    -1.781088
H    -1.606070    -0.060917     3.222343
H     1.681477    -0.220779     3.463624
H     3.731112     0.408049    -1.327272
H     2.965512     0.006269    -2.786419
H    -1.476088    -0.037960    -2.011645
O     4.062203    -0.680799     1.685499
H     4.413097    -1.579355     1.637843
H     2.626351    -0.285034     0.712111
O     2.531621    -0.368667     3.937067
H     3.665110    -0.607029     2.583798
H     2.638002     0.400831     4.510779
21
2W TS S1 - C2 X
N     0.447442    -0.054648    -2.158660
C     1.619913    -0.158946    -1.425109
N     1.777669    -0.942327    -0.206008
C     0.832828    -0.321867     0.577224
C    -0.441334     0.029004     0.080179
C    -0.642099    -0.071973    -1.402112
N    -1.303966     0.357187     1.077472
C    -0.568385     0.226557     2.211315
N     0.708542    -0.196436     1.956407
N     2.604824     0.747701    -1.662525
H    -0.931503     0.433965     3.215337
H     1.435512    -0.379383     2.641219
H     3.545209     0.539515    -1.350303
H     2.460441     1.489829    -2.339150
H    -1.631693    -0.053052    -1.866910
O     4.066992    -1.744233     1.098453
H     4.243358    -2.685572     0.971037
H     3.264263    -1.556582     0.542001
O     2.984466    -0.859314     3.456107
H     3.495816    -1.215602     2.690950
H     3.583024    -0.237377     3.887830
21
2W TS S1 - C6 X
N     0.539880    -0.106735    -1.875795
C     1.786998     0.062673    -1.334575
N     1.940297     0.008289    -0.008580
C     0.732887    -0.076564     0.691438
C    -0.571987     0.015724     0.185977
C    -0.683882     0.309001    -1.249599
N    -1.500340    -0.009403     1.200075
C    -0.769176    -0.128802     2.318912
N     0.588531    -0.164876     2.051833
N     2.868847     0.206355    -2.169456
H    -1.163569    -0.219320     3.327421
H     1.341022    -0.244158     2.727851
H     3.754412    -0.060572    -1.748208
H     2.728788    -0.129435    -3.117071
H    -1.463465     0.888284    -1.763553
O     4.236668    -0.946549     1.260321
H     4.258566    -1.901615     1.111386
H     3.445602    -0.632033     0.755133
O     2.931338    -0.405777     3.645238
H     3.554528    -0.579332     2.904664
H     3.323713     0.325500     4.138331
21
2W TS S1 - S1 3H
N     0.665823     0.054228    -1.885180
C     1.771413    -0.017360    -1.120659
N     1.892498    -0.127584     0.264924
C     0.656868    -0.107178     0.864994
C    -0.574536    -0.067252     0.187381
C    -0.572835    -0.016878    -1.292291
N    -1.584942    -0.109629     1.084012
C    -0.929755    -0.160240     2.325371
N     0.402586    -0.173370     2.239245
N     2.967459     0.013141    -1.763776
H    -1.471346    -0.194457     3.268903
H     1.350417    -0.197775     3.067131
H     3.833327     0.045903    -1.236417
H     2.966968     0.120140    -2.771942
H    -1.464961     0.115103    -1.906069
O     3.846068    -0.573692     1.731020
H     4.155553    -1.490685     1.703933
H     2.905819    -0.388545     0.907943
O     2.424757    -0.283236     3.668683
H     3.202643    -0.422592     2.782817
H     2.627612     0.531122     4.150054
21
2WT S0
N     0.619258    -0.023284    -1.842144
C     1.765881    -0.121559    -1.094664
N     1.843707    -0.187581     0.252901
C     0.637718    -0.124040     0.845091
C    -0.614793    -0.007155     0.192428
C    -0.564194     0.032372    -1.210179
N    -1.655150     0.033865     1.112858
C    -1.031595    -0.056056     2.288126
N     0.343412    -0.155438     2.188120
N     2.944805    -0.106916    -1.799941
H    -1.531812    -0.053700     3.254706
H     1.048695    -0.239040     2.923240
H     3.770607    -0.414028    -1.302908
H     2.886666    -0.293450    -2.800074
H    -1.463089     0.104332    -1.829927
O     3.061763    -0.291274     2.830074
H     3.018748    -0.307853     1.851134
H     3.777394    -0.893951     3.066855
O     1.654122    -0.480639    -4.447600
H     1.050637    -0.250078    -3.707641
H     1.510710     0.207622    -5.109328
21
2WT S1
N     0.567190    -0.120621    -1.917094
C     1.707698    -0.198363    -1.174662
N     1.918694    -0.206217     0.189880
C     0.693628    -0.156497     0.807829
C    -0.579725    -0.016591     0.203258
C    -0.647193     0.062204    -1.261318
N    -1.555993     0.052503     1.148086
C    -0.889219    -0.037467     2.337093
N     0.453861    -0.149751     2.175175
N     2.853235    -0.285116    -1.899018
H    -1.367740    -0.020858     3.313660
H     1.194825    -0.238074     2.875569
H     3.732046    -0.335624    -1.392507
H     2.799726    -0.285892    -2.928770
H    -1.570723     0.005719    -1.839606
O     3.205626    -0.364569     2.717337
H     3.763788    -1.130880     2.900439
H     3.097843    -0.355602     1.741798
O     1.720141    -0.363013    -4.441465
H     1.026317    -0.243219    -3.747966
H     1.536086     0.310452    -5.108623
21
2WT C2 X
N     0.660558    -0.380123    -1.856382
C     1.854980    -0.029882    -1.064436
N     1.887339    -0.583508     0.282847
C     0.809963    -0.083830     0.883757
C    -0.406726     0.253904     0.190608
C    -0.440393    -0.056873    -1.243634
N    -1.436236     0.419429     1.061311
C    -0.880069     0.210026     2.279533
N     0.440198    -0.120659     2.222341
N     2.086634     1.373209    -1.095077
H    -1.426019     0.287189     3.217884
H     1.091302    -0.377747     2.970761
H     2.960948     1.601645    -0.618774
```

```
H     2.124030     1.705046    -2.061432
H    -1.405654    -0.182538    -1.753259
O     2.982238    -1.028961     2.855125
H     3.465747    -1.814301     3.141368
H     2.953563    -1.086076     1.876509
O     1.876477    -0.207308    -4.497243
H     1.366581    -0.459812    -3.704552
H     1.284740    -0.404438    -5.233716
21
2WT C6 X
N     0.594280    -0.399158    -1.742117
C     1.858834    -0.206518    -1.100219
N     1.883541    -0.288864     0.203856
C     0.581206    -0.196312     0.773417
C    -0.614619     0.142248     0.147670
C    -0.502756     0.473495    -1.291582
N    -1.604682     0.381011     1.077353
C    -1.006850     0.150009     2.258391
N     0.317718    -0.197166     2.117464
N     2.943038    -0.158032    -1.897826
H    -1.493192     0.186316     3.229822
H     1.016719    -0.402256     2.834576
H     3.863090    -0.189523    -1.477439
H     2.814087    -0.191213    -2.908239
H    -0.457508     1.532617    -1.599768
O     3.039250    -0.680839     2.806037
H     3.480179    -1.527852     2.949595
H     2.981010    -0.591775     1.831755
O     1.512102    -0.262846    -4.386309
H     0.768559    -0.711087    -3.951604
H     1.415544    -0.456734    -5.328276
21
2WT S1 3H
N     0.611173    -0.080910    -1.830314
C     1.691956    -0.332231    -1.109889
N     1.692508    -0.530764     0.282188
C     0.460450    -0.378102     0.887054
C    -0.681162    -0.066449     0.192208
C    -0.627513     0.096597    -1.246146
N    -1.631676     0.222995     1.180603
C    -1.074883    -0.181470     2.406607
N     0.226040    -0.394153     2.297044
N     2.948995    -0.368089    -1.690481
H    -1.629275    -0.125575     3.340425
H     2.138545    -0.202160     3.041158
H     3.573978    -1.071895    -1.305573
H     2.914771    -0.360961    -2.713260
H    -1.486500     0.299646    -1.886215
O     3.051701    -0.059819     2.727437
H     3.623201    -0.431320     3.410652
H     2.537445    -0.366806     0.841286
O     1.761627    -0.228000    -4.401096
H     1.127069    -0.101365    -3.658306
H     1.667702     0.564814    -4.944089
21
2WT S1 imino
N     0.718248    -0.112807    -1.812595
C     1.868940    -0.209239    -1.082810
N     1.968528    -0.227303     0.230776
C     0.689544    -0.140028     0.831644
C    -0.540876    -0.015050     0.194383
C    -0.569418     0.052859    -1.251430
N    -1.561003     0.050135     1.113526
C    -0.934217    -0.033085     2.308138
N     0.422074    -0.143836     2.184611
N     3.015632    -0.298635    -1.887309
H    -1.434401    -0.015719     3.273430
H     1.140375    -0.230243     2.906555
H     3.812933    -0.364900    -1.234181
H     2.552121    -0.275285    -3.878023
H    -1.433143    -0.085087    -1.901739
O     3.179292    -0.367012     2.815619
H     3.749125    -1.114492     3.035994
H     3.101414    -0.384049     1.839187
O     1.769775    -0.313401    -4.463533
H     0.843447    -0.118975    -2.835416
H     1.917533     0.360937    -5.139178
21
2WT TS S1 - C2 X
N     0.447442    -0.054648    -2.158660
C     1.619913    -0.158946    -1.425109
N     1.777669    -0.942327    -0.206008
C     0.832828    -0.321867     0.577224
C    -0.441334     0.029004     0.080179
C    -0.642099    -0.071973    -1.402112
N    -1.303966     0.357187     1.077472
C    -0.568385     0.226557     2.211315
N     0.708542    -0.196436     1.956407
N     2.604824     0.747701    -1.662525
H    -0.931503     0.433965     3.215337
H     1.435512    -0.379383     2.641219
H     3.545209     0.539515    -1.350303
H     2.460441     1.489829    -2.339150
H    -1.631693    -0.053052    -1.866910
O     3.345366    -1.196530     2.143609
H     3.834215    -2.001403     2.356332
H     3.069174    -1.305610     1.207710
O     1.344235     2.020415    -3.927822
H     0.781058     1.282282    -3.617492
H     0.731425     2.747119    -4.097773
21
2WT TS S1 - C6 X
N     0.539880    -0.106735    -1.875795
C     1.786998     0.062673    -1.334575
N     1.940297     0.008289    -0.008580
C     0.732887    -0.076564     0.691438
C    -0.571987     0.015724     0.185977
C    -0.683882     0.309001    -1.249599
N    -1.500340    -0.009403     1.200075
C    -0.769176    -0.128802     2.318912
N     0.588531    -0.164876     2.051833
N     2.868847     0.206355    -2.169456
H    -1.163569    -0.219320     3.327421
H     1.341022    -0.244158     2.727851
H     3.754412    -0.060572    -1.748208
H     2.728788    -0.129435    -3.117071
H    -1.463465     0.888284    -1.763553
O     3.394515    -0.125765     2.465330
H     4.101240    -0.773980     2.576869
H     3.241781    -0.080965     1.499237
O     1.551067    -1.408941    -4.250440
H     0.860953    -1.382691    -3.564972
H     1.073927    -1.541794    -5.079657
21
2WT TS S1 - S1 3H
N     0.635175     0.044663    -1.818664
C     1.748680    -0.086847    -1.069417
N     1.880321    -0.184900     0.317395
C     0.636401    -0.082016     0.893851
C    -0.602426     0.021169     0.254021
C    -0.605524     0.070518    -1.222291
N    -1.583609    -0.007871     1.191015
C    -0.886033    -0.107672     2.415614
N     0.438039    -0.172844     2.282459
N     2.926906    -0.147852    -1.745664
H    -1.405253    -0.132220     3.371772
H     1.686427    -0.351789     2.751435
H     3.804980    -0.161773    -1.242455
H     2.906649    -0.041639    -2.753276
H    -1.483469     0.267753    -1.839353
O     2.840945    -0.444863     2.545803
H     3.131556    -1.341267     2.775932
H     2.691037    -0.378346     1.391045
O     1.818573     0.079959    -4.351595
H     1.134622     0.124561    -3.641463
H     1.623114     0.819626    -4.940447
21
2WT TS S1 - S1 imino
N     0.617394    -0.158244    -1.944122
C     1.766426    -0.242333    -1.205133
N     1.941777    -0.247431     0.135891
C     0.700514    -0.160049     0.752946
C    -0.559361    -0.036404     0.139885
C    -0.626426     0.004989    -1.316399
N    -1.546426     0.055396     1.080596
C    -0.887646    -0.007341     2.269107
```

```
N     0.457767    -0.129074     2.117213
N     2.886326    -0.339824    -1.989570
H    -1.368686     0.033497     3.243628
H     1.192685    -0.202454     2.824466
H     3.762737    -0.405347    -1.467486
H     2.593559    -0.310200    -3.177865
H    -1.532980    -0.077406    -1.916429
O     3.219309    -0.338573     2.684894
H     3.785222    -1.090605     2.900174
H     3.117276    -0.366913     1.710190
O     1.727415    -0.313933    -4.128568
H     0.964228    -0.197541    -3.235089
H     1.727333     0.498429    -4.656713
24
3W S0
N     0.441004     0.247043    -2.048708
C     1.623576     0.207153    -1.368585
N     1.798302     0.028357    -0.039665
C     0.636263    -0.079930     0.633425
C    -0.655844    -0.046611     0.049329
C    -0.695823     0.113922    -1.347270
N    -1.640014    -0.197832     1.016936
C    -0.940487    -0.313845     2.147806
N     0.429883    -0.256162     1.979740
N     2.759366     0.418873    -2.127500
H    -1.381789    -0.445931     3.134268
H     1.143458    -0.257085     2.732645
H     3.640975     0.129695    -1.716100
H     2.645958     0.258772    -3.121266
H    -1.636397     0.134589    -1.906315
O     4.353495    -0.860261     0.502611
H     3.418559    -0.534166     0.406607
H     4.282733    -1.818891     0.397893
O     2.291415    -0.171553     4.069338
H     3.235264    -0.166228     3.782353
H     2.207949     0.620885     4.615146
O     4.834785    -0.068492     3.090847
H     5.611893    -0.499167     3.466196
H     4.789545    -0.372279     2.155080
24
3W S1
N     0.548406     0.193852    -1.961483
C     1.684884     0.000329    -1.244617
N     1.887319    -0.267014     0.100101
C     0.682112    -0.145023     0.740169
C    -0.598142    -0.063173     0.128789
C    -0.672136    -0.063490    -1.343732
N    -1.577292    -0.009337     1.071508
C    -0.906808    -0.077220     2.255571
N     0.442604    -0.186062     2.101804
N     2.835853     0.084311    -1.960854
H    -1.384097    -0.063667     3.233286
H     1.158497    -0.184097     2.852213
H     3.728858    -0.104468    -1.505672
H     2.769816     0.296439    -2.951512
H    -1.584264     0.192020    -1.889194
O     4.452261    -1.033426     0.414471
H     3.468329    -0.839634     0.442750
H     4.508418    -1.997448     0.360769
O     2.414316    -0.097278     4.101629
H     3.329322    -0.097790     3.735176
H     2.382592     0.694901     4.653101
O     4.909372    -0.028261     2.954099
H     5.695339    -0.415048     3.358317
H     4.874050    -0.401181     2.044407
24
3W C2 X
N     0.459221    -0.171692    -2.073513
C     1.706020     0.038119    -1.327482
N     1.811733    -0.661360    -0.047606
C     0.809485    -0.175991     0.689683
C    -0.438689     0.255234     0.111475
C    -0.581136     0.112087    -1.344624
N    -1.393017     0.408071     1.064543
C    -0.749649     0.107102     2.221821
N     0.545538    -0.277292     2.048732
N     2.035133     1.421044    -1.229018
H    -1.211282     0.146834     3.208157
H     1.243048    -0.397081     2.812488
H     2.982852     1.529819    -0.859129
H     1.974661     1.869065    -2.145991
H    -1.580938     0.079749    -1.796180
O     4.498598    -0.980947     0.600791
H     3.536485    -1.027848     0.366689
H     4.873806    -1.824954     0.319498
O     2.343033    -0.266265     4.146500
H     3.282663    -0.241833     3.842462
H     2.249500     0.549751     4.655054
O     4.864911    -0.053125     3.149797
H     5.648421    -0.466849     3.532162
H     4.817825    -0.394727     2.225722
24
3W C6 X
N     0.457865    -0.420300    -1.837675
C     1.750561    -0.183023    -1.294252
N     1.882897    -0.246644     0.002052
C     0.636980    -0.186099     0.694077
C    -0.608893     0.103365     0.151420
C    -0.620427     0.427728    -1.299533
N    -1.545796     0.284607     1.142331
C    -0.856625     0.067318     2.278137
N     0.468461    -0.218257     2.052626
N     2.787842    -0.082243    -2.172668
H    -1.283881     0.060940     3.278105
H     1.196330    -0.321794     2.782334
H     3.717978    -0.244746    -1.791849
H     2.610438    -0.434162    -3.107183
H    -0.617384     1.488734    -1.608065
O     4.498872    -0.957551     0.476946
H     3.529433    -0.741510     0.438416
H     4.528696    -1.923797     0.488423
O     2.359952    -0.225784     4.147016
H     3.290922    -0.186413     3.829529
H     2.250269     0.590795     4.650567
O     4.899371    -0.057568     3.096332
H     5.670852    -0.487674     3.484709
H     4.880976    -0.354913     2.160362
24
3W S1 3H
N     0.540546     0.239484    -2.016347
C     1.658489     0.130605    -1.325894
N     1.754003     0.027600     0.084299
C     0.535124    -0.052090     0.721892
C    -0.667862     0.020754     0.055573
C    -0.685704     0.195265    -1.388054
N    -1.641409    -0.304331     0.999992
C    -0.967486    -0.316822     2.245542
N     0.344727    -0.293149     2.117422
N     2.885546     0.186688    -1.951708
H    -1.502201    -0.466785     3.181400
H     1.686402    -0.128876     3.395776
H     3.676734    -0.215821    -1.453812
H     2.851033     0.045829    -2.955211
H    -1.589927     0.319798    -1.984940
O     4.312373    -1.150269     0.462922
H     2.598082    -0.430701     0.459456
H     4.385661    -2.112620     0.496333
O     2.424825     0.063690     4.020305
H     4.043022    -0.094511     3.365325
H     2.237927     0.956036     4.340213
O     4.914009    -0.170113     2.908723
H     5.520902    -0.528274     3.567370
H     4.657713    -0.841756     1.336205
24
3W TS S1 - C2 X
N     0.447442    -0.054648    -2.158660
C     1.619913    -0.158946    -1.425109
N     1.777669    -0.942327    -0.206008
C     0.832828    -0.321867     0.577224
C    -0.441334     0.029004     0.080179
C    -0.642099    -0.071973    -1.402112
N    -1.303966     0.357187     1.077472
C    -0.568385     0.226557     2.211315
N     0.708542    -0.196436     1.956407
N     2.604824     0.747701    -1.662525
H    -0.931503     0.433965     3.215337
```

```
H     1.435512    -0.379383     2.641219
H     3.545209     0.539515    -1.350303
H     2.460441     1.489829    -2.339150
H    -1.631693    -0.053052    -1.866910
O     4.476722    -1.029687     0.014440
H     3.483927    -1.157036     0.043101
H     4.821842    -1.856886    -0.347520
O     2.724017    -0.659362     3.859373
H     3.614182    -0.503356     3.464667
H     2.732860    -0.165756     4.688685
O     5.095061    -0.203031     2.565240
H     5.908311    -0.625772     2.867032
H     4.971024    -0.522978     1.641973
24
3W TS S1 - C6 X
N     0.539880    -0.106735    -1.875795
C     1.786998     0.062673    -1.334575
N     1.940297     0.008289    -0.008580
C     0.732887    -0.076564     0.691438
C    -0.571987     0.015724     0.185977
C    -0.683882     0.309001    -1.249599
N    -1.500340    -0.009403     1.200075
C    -0.769176    -0.128802     2.318912
N     0.588531    -0.164876     2.051833
N     2.868847     0.206355    -2.169456
H    -1.163569    -0.219320     3.327421
H     1.341022    -0.244158     2.727851
H     3.754412    -0.060572    -1.748208
H     2.728788    -0.129435    -3.117071
H    -1.463465     0.888284    -1.763553
O     4.462897    -1.012440     0.378904
H     3.524948    -0.681645     0.370133
H     4.374499    -1.975636     0.375987
O     2.641983    -0.266403     4.008413
H     3.565745    -0.204260     3.673727
H     2.574542     0.452642     4.649440
O     5.148050    -0.059483     2.887984
H     5.940468    -0.488459     3.232719
H     5.039880    -0.408150     1.975114
24
3WT S0
N     0.648008    -0.053572    -1.803452
C     1.779865    -0.053627    -1.029048
N     1.827519    -0.095250     0.321493
C     0.609679    -0.099308     0.895826
C    -0.629800    -0.087430     0.206239
C    -0.549133    -0.075979    -1.195245
N    -1.694242    -0.102778     1.097635
C    -1.093877    -0.122722     2.288925
N     0.287293    -0.123405     2.230476
N     2.970169     0.029303    -1.703134
H    -1.618062    -0.136738     3.242778
H     0.956268    -0.118032     3.021055
H     3.821673    -0.116908    -1.178173
H     2.963258    -0.136211    -2.707836
H    -1.437317    -0.087372    -1.834163
O     4.013612    -0.603105     1.988362
H     3.292953    -0.431090     1.330356
H     4.271067    -1.522775     1.841007
O     2.348686    -0.199038     4.127643
H     3.080365    -0.336824     3.481230
H     2.639533     0.531368     4.687734
O     1.803279    -0.412850    -4.372593
H     1.151791    -0.237046    -3.658718
H     1.612381     0.244063    -5.053778
24
3WT S1
N     0.581590    -0.186023    -1.916872
C     1.708684    -0.202671    -1.151245
N     1.880391    -0.244828     0.218373
C     0.648212    -0.145312     0.815090
C    -0.614860    -0.192733     0.175927
C    -0.651779    -0.322897    -1.289097
N    -1.617920    -0.130837     1.090021
C    -0.973935    -0.051700     2.293950
N     0.377282    -0.075052     2.174515
N     2.876201    -0.168630    -1.843038
H    -1.478591     0.016693     3.255246
H     1.086828    -0.007800     2.926933
H     3.745213    -0.170062    -1.316044
H     2.849289    -0.108629    -2.871628
H    -1.557203    -0.198670    -1.886441
O     4.095891    -0.773786     1.787748
H     4.259262    -1.726292     1.773088
H     3.333380    -0.636311     1.165266
O     2.559121    -0.005968     3.932812
H     3.247256    -0.257721     3.272711
H     2.902819     0.783891     4.368539
O     1.810558    -0.150574    -4.418748
H     1.091019    -0.126796    -3.742598
H     1.589555     0.539543    -5.056944
24
3WT C2 X
N     0.870149    -0.497173    -1.770173
C     1.991695    -0.055248    -0.920473
N     1.964446    -0.548598     0.448272
C     0.827234    -0.086803     0.970146
C    -0.354897     0.161026     0.180491
C    -0.281624    -0.205103    -1.237509
N    -1.447088     0.316466     0.970776
C    -0.960599     0.189833     2.232048
N     0.373205    -0.082748     2.283861
N     2.166520     1.351091    -1.000793
H    -1.565532     0.285060     3.133145
H     0.966946    -0.221520     3.132115
H     3.009057     1.633493    -0.497925
H     2.221920     1.660170    -1.973987
H    -1.203954    -0.392432    -1.803410
O     3.887064    -1.318393     2.334493
H     4.248767    -2.203687     2.201331
H     3.297970    -1.156133     1.556342
O     2.175691    -0.582159     4.308619
H     2.896298    -0.901861     3.712245
H     2.580911     0.119412     4.834176
O     1.877859    -0.196137    -4.490857
H     1.452547    -0.504341    -3.667605
H     1.232165    -0.388176    -5.182427
24
3WT C6 X
N     0.665145    -0.396820    -1.756779
C     1.915491    -0.149558    -1.114690
N     1.942589    -0.245231     0.189386
C     0.646458    -0.201402     0.777827
C    -0.559919     0.095716     0.148602
C    -0.459801     0.429550    -1.292002
N    -1.552215     0.328465     1.076626
C    -0.939300     0.138940     2.257991
N     0.393413    -0.177411     2.124072
N     2.996208    -0.011629    -1.907371
H    -1.424663     0.170830     3.230583
H     1.082540    -0.280412     2.886524
H     3.913348    -0.011705    -1.478554
H     2.873255    -0.102365    -2.914080
H    -0.443096     1.493509    -1.588940
O     4.123158    -0.683507     1.861365
H     3.387398    -0.552081     1.210443
H     4.407918    -1.597598     1.729535
O     2.459553    -0.400519     4.049124
H     3.194348    -0.471261     3.397931
H     2.683028     0.356152     4.605705
O     1.629534    -0.410842    -4.418599
H     0.837979    -0.722677    -3.949814
H     1.300723     0.055986    -5.197944
24
3WT S1 3H
N     0.606699    -0.219869    -1.916252
C     1.706758    -0.213997    -1.178904
N     1.734052    -0.109394     0.221183
C     0.496542    -0.038348     0.819901
C    -0.680900    -0.092315     0.111304
C    -0.648280    -0.193904    -1.334312
N    -1.686418    -0.232341     1.073665
C    -1.060624    -0.003223     2.319573
N     0.255735    -0.020655     2.230112
N     2.947009    -0.378449    -1.754890
H    -1.626655     0.022254     3.248233
```

```
H     1.700854    -0.083827     3.450525
H     3.732065     0.023639    -1.251496
H     2.959912    -0.277501    -2.772045
H    -1.527013    -0.190453    -1.979711
O     4.070070    -0.679106     1.661932
H     4.423197    -1.577294     1.703209
H     2.590269    -0.380091     0.740340
O     2.576874    -0.160656     3.892885
H     3.692314    -0.510983     2.556492
H     2.673648     0.651691     4.405822
O     1.810831    -0.230939    -4.459239
H     1.148336    -0.206883    -3.729493
H     1.579574     0.511446    -5.031351
24
3WT S1 imino
N     0.724388    -0.171304    -1.828177
C     1.868185    -0.198438    -1.084673
N     1.944930    -0.218456     0.232484
C     0.661074    -0.163817     0.823801
C    -0.564939    -0.178661     0.162402
C    -0.577779    -0.253154    -1.282876
N    -1.601945    -0.129825     1.061224
C    -0.986986    -0.084470     2.265356
N     0.374806    -0.107833     2.172181
N     3.030983    -0.182771    -1.866702
H    -1.503676    -0.035772     3.221206
H     1.064142    -0.053574     2.941273
H     3.824830    -0.231751    -1.207445
H     2.597158    -0.094968    -3.858838
H    -1.422413    -0.060940    -1.944016
O     4.113359    -0.744805     1.913910
H     4.281539    -1.696095     1.885816
H     3.387185    -0.594261     1.258000
O     2.500378    -0.032670     4.029073
H     3.210475    -0.262044     3.385966
H     2.802000     0.775938     4.461580
O     1.829134    -0.165878    -4.460193
H     0.862874    -0.145126    -2.849209
H     1.929048     0.555446    -5.094808
24
3WT TS S1 - C2 X
N     0.447442    -0.054648    -2.158660
C     1.619913    -0.158946    -1.425109
N     1.777669    -0.942327    -0.206008
C     0.832828    -0.321867     0.577224
C    -0.441334     0.029004     0.080179
C    -0.642099    -0.071973    -1.402112
N    -1.303966     0.357187     1.077472
C    -0.568385     0.226557     2.211315
N     0.708542    -0.196436     1.956407
N     2.604824     0.747701    -1.662525
H    -0.931503     0.433965     3.215337
H     1.435512    -0.379383     2.641219
H     3.545209     0.539515    -1.350303
H     2.460441     1.489829    -2.339150
H    -1.631693    -0.053052    -1.866910
O     3.983298    -1.928431     1.132950
H     4.079282    -2.881393     1.007331
H     3.218190    -1.670202     0.554870
O     2.947362    -0.940407     3.468193
H     3.437254    -1.341851     2.711416
H     3.589477    -0.369002     3.907056
O     1.203117     2.152369    -3.795786
H     0.723009     1.330595    -3.566619
H     1.279703     2.138631    -4.758415
24
3WT TS S1 - C6 X
N     0.539880    -0.106735    -1.875795
C     1.786998     0.062673    -1.334575
N     1.940297     0.008289    -0.008580
C     0.732887    -0.076564     0.691438
C    -0.571987     0.015724     0.185977
C    -0.683882     0.309001    -1.249599
N    -1.500340    -0.009403     1.200075
C    -0.769176    -0.128802     2.318912
N     0.588531    -0.164876     2.051833
N     2.868847     0.206355    -2.169456
H    -1.163569    -0.219320     3.327421
H     1.341022    -0.244158     2.727851
H     3.754412    -0.060572    -1.748208
H     2.728788    -0.129435    -3.117071
H    -1.463465     0.888284    -1.763553
O     4.230357    -0.940562     1.284502
H     4.279068    -1.888006     1.098380
H     3.450396    -0.622664     0.765249
O     2.908713    -0.451893     3.663040
H     3.535652    -0.618084     2.923376
H     3.317677     0.247372     4.187831
O     1.567250    -1.422594    -4.243684
H     0.862545    -1.393605    -3.573829
H     1.109517    -1.566846    -5.081898
24
3WT TS S1 - S1 3H
N     0.665823     0.054228    -1.885180
C     1.771413    -0.017360    -1.120659
N     1.892498    -0.127584     0.264924
C     0.656868    -0.107178     0.864994
C    -0.574536    -0.067252     0.187381
C    -0.572835    -0.016878    -1.292291
N    -1.584942    -0.109629     1.084012
C    -0.929755    -0.160240     2.325371
N     0.402586    -0.173370     2.239245
N     2.967459     0.013141    -1.763776
H    -1.471346    -0.194457     3.268903
H     1.350417    -0.197775     3.067131
H     3.833327     0.045903    -1.236417
H     2.966968     0.120140    -2.771942
H    -1.464961     0.115103    -1.906069
O     3.846068    -0.573692     1.731020
H     4.155553    -1.490685     1.703933
H     2.905819    -0.388545     0.907943
O     2.424757    -0.283236     3.668683
H     3.202643    -0.422592     2.782817
H     2.627612     0.531122     4.150054
O     1.935658     0.174418    -4.386758
H     1.210291     0.181512    -3.720303
H     1.727467     0.889409    -5.001153
24
3WT TS S1 - S1 imino
N     0.687063    -0.148834    -1.881602
C     1.824340    -0.203189    -1.120511
N     1.992544    -0.189719     0.216711
C     0.742555    -0.124848     0.816368
C    -0.512965    -0.033222     0.190766
C    -0.566144     0.002508    -1.264997
N    -1.517933     0.036412     1.119557
C    -0.879584    -0.007941     2.313870
N     0.475737    -0.097733     2.176361
N     2.959985    -0.294348    -1.890929
H    -1.370811     0.022201     3.283772
H     1.163580    -0.146659     2.920271
H     3.826591    -0.344590    -1.349508
H     2.689309    -0.282818    -3.076422
H    -1.466202    -0.115303    -1.869334
O     4.228942    -0.800316     1.769288
H     4.376566    -1.751851     1.684800
H     3.468543    -0.608171     1.164309
O     2.655315    -0.269609     3.983956
H     3.356948    -0.430431     3.312857
H     2.985223     0.458217     4.525391
O     1.830839    -0.309173    -4.047886
H     1.052395    -0.196508    -3.163580
H     1.820995     0.496751    -4.585562
27
4WT S0
N     0.519511     0.076599    -2.055218
C     1.704182     0.070681    -1.363872
N     1.849279    -0.035895    -0.022011
C     0.677910    -0.110663     0.637150
C    -0.607187    -0.108079     0.035483
C    -0.628560    -0.018631    -1.365315
N    -1.605429    -0.210252     0.994936
C    -0.921409    -0.268060     2.139022
N     0.451969    -0.217204     1.986905
N     2.841871     0.217470    -2.113115
H    -1.375560    -0.352307     3.124791
```

```
H     1.153193    -0.191744     2.751555
H     3.731103     0.053718    -1.656830
H     2.762768     0.097603    -3.120956
H    -1.560843    -0.025252    -1.938289
O     4.430522    -0.793992     0.617897
H     3.485416    -0.515707     0.486623
H     4.420835    -1.748162     0.461746
O     2.250476    -0.087838     4.123361
H     3.205499    -0.128816     3.878696
H     2.177197     0.715026     4.655082
O     4.832152    -0.105545     3.251025
H     5.565661    -0.600413     3.635154
H     4.803647    -0.369830     2.302521
O     1.485653    -0.161192    -4.717319
H     0.888221    -0.026367    -3.949368
H     1.223449     0.509874    -5.359932
27
4WT S1
N     0.553186    -0.012550    -1.997896
C     1.696755    -0.149641    -1.272874
N     1.898478    -0.301474     0.086653
C     0.694285    -0.162256     0.728849
C    -0.585330    -0.101896     0.124537
C    -0.668392    -0.140707    -1.342854
N    -1.560178    -0.037819     1.069660
C    -0.880970    -0.064103     2.254839
N     0.464075    -0.159260     2.096142
N     2.848507    -0.137038    -1.993526
H    -1.354374    -0.021170     3.233314
H     1.181506    -0.134840     2.845696
H     3.730982    -0.266776    -1.497244
H     2.791971    -0.000952    -3.013221
H    -1.581881     0.072813    -1.901796
O     4.471027    -1.032564     0.483631
H     3.488802    -0.834643     0.486157
H     4.523732    -1.998058     0.458802
O     2.407223    -0.009862     4.110197
H     3.331263    -0.035207     3.767390
H     2.371576     0.801857     4.632243
O     4.922780    -0.012585     3.019176
H     5.686318    -0.430411     3.435427
H     4.887063    -0.383910     2.108734
O     1.702745     0.144176    -4.530194
H     1.011691     0.156353    -3.824292
H     1.507901     0.902932    -5.094744
27
4WT C2 X
N     0.556312    -0.421177    -1.989349
C     1.763692     0.018654    -1.264999
N     1.893731    -0.500402     0.089158
C     0.830931    -0.041275     0.751257
C    -0.434618     0.201199     0.103972
C    -0.524957    -0.146573    -1.319301
N    -1.425873     0.364335     1.015792
C    -0.793348     0.250164     2.212696
N     0.534910    -0.031572     2.107579
N     1.926936     1.424972    -1.358007
H    -1.285421     0.371505     3.178545
H     1.212135    -0.130904     2.895317
H     2.804855     1.703557    -0.916372
H     1.934108     1.716234    -2.339464
H    -1.508952    -0.324789    -1.772897
O     4.578933    -1.061381     0.595473
H     3.610981    -0.997838     0.406528
H     4.880917    -1.850661     0.129344
O     2.335928    -0.270030     4.208778
H     3.270614    -0.287040     3.887069
H     2.339089     0.384901     4.917916
O     4.840681    -0.200182     3.158070
H     5.625864    -0.558507     3.588737
H     4.853833    -0.570640     2.244160
O     1.738526     0.125772    -4.556111
H     1.246047    -0.281754    -3.817641
H     1.484926    -0.398317    -5.325117
27
4WT C6 X
N     0.525200    -0.392091    -1.834177
C     1.809538    -0.177049    -1.248773
N     1.891257    -0.284583     0.054944
C     0.627807    -0.221245     0.707683
C    -0.605025     0.081723     0.139090
C    -0.567478     0.438321    -1.302398
N    -1.556123     0.293340     1.112695
C    -0.889524     0.083104     2.262077
N     0.437057    -0.226973     2.062784
N     2.863351    -0.066908    -2.082959
H    -1.334448     0.105055     3.253774
H     1.159701    -0.323814     2.796630
H     3.791951    -0.175383    -1.682672
H     2.694744    -0.205772    -3.079557
H    -0.544914     1.510427    -1.572166
O     4.497424    -0.970007     0.512966
H     3.523038    -0.766254     0.492212
H     4.538824    -1.935520     0.471288
O     2.374298    -0.236545     4.131498
H     3.305148    -0.188881     3.814107
H     2.267672     0.562106     4.664426
O     4.915313    -0.046523     3.092725
H     5.683023    -0.472729     3.492693
H     4.887883    -0.378427     2.167372
O     1.492426    -0.550242    -4.590411
H     0.709735    -0.823235    -4.083807
H     1.156054     0.041595    -5.276202
27
4WT S1 3H
N     0.540109     0.095901    -2.026166
C     1.669082    -0.050197    -1.336365
N     1.763554    -0.114881     0.071108
C     0.551990    -0.119975     0.722585
C    -0.655651    -0.004522     0.068320
C    -0.682095     0.125857    -1.388205
N    -1.657857    -0.178547     1.006429
C    -0.948362    -0.267508     2.242819
N     0.361887    -0.293988     2.127716
N     2.866609    -0.135381    -1.970504
H    -1.484511    -0.357225     3.186407
H     1.673956    -0.109528     3.416291
H     3.710851    -0.277164    -1.424892
H     2.870509    -0.110863    -2.991142
H    -1.584139     0.286007    -1.980110
O     4.384381    -1.060613     0.506124
H     2.628410    -0.512215     0.469768
H     4.537390    -2.014309     0.498705
O     2.405404     0.074031     4.053830
H     4.023562    -0.068693     3.422988
H     2.205470     0.953545     4.399710
O     4.906177    -0.138214     2.986123
H     5.487531    -0.536308     3.645059
H     4.696274    -0.761852     1.396562
O     1.686624    -0.039907    -4.590459
H     1.031456     0.069680    -3.861729
H     1.522663     0.700125    -5.188271
27
4WT S1 imino
N     0.661777    -0.121204    -1.932521
C     1.839651    -0.215254    -1.251746
N     1.980097    -0.291899     0.058945
C     0.732139    -0.217625     0.719151
C    -0.525307    -0.184656     0.119493
C    -0.613043    -0.204980    -1.324957
N    -1.515958    -0.151738     1.069851
C    -0.840571    -0.164184     2.241911
N     0.514576    -0.212439     2.080717
N     2.963099    -0.204220    -2.091272
H    -1.307795    -0.140612     3.223955
H     1.226954    -0.167144     2.831652
H     3.789646    -0.341486    -1.485270
H     2.433768    -0.020909    -4.040190
H    -1.484479     0.039966    -1.931982
O     4.495333    -1.170442     0.746773
H     3.554430    -0.879233     0.607704
H     4.445716    -2.135553     0.779693
O     2.393514     0.013986     4.165194
H     3.337139     0.000978     3.880431
H     2.303173     0.845396     4.648106
O     4.953701     0.015693     3.191302
```

```
H     5.710776    -0.374826     3.644013
H     4.910393    -0.434560     2.316711
O     1.642018    -0.050800    -4.614754
H     0.749457    -0.058312    -2.957566
H     1.737611     0.689600    -5.227635
27
4WT TS S1 - C2 X
N     0.447442    -0.054648    -2.158660
C     1.619913    -0.158946    -1.425109
N     1.777669    -0.942327    -0.206008
C     0.832828    -0.321867     0.577224
C    -0.441334     0.029004     0.080179
C    -0.642099    -0.071973    -1.402112
N    -1.303966     0.357187     1.077472
C    -0.568385     0.226557     2.211315
N     0.708542    -0.196436     1.956407
N     2.604824     0.747701    -1.662525
H    -0.931503     0.433965     3.215337
H     1.435512    -0.379383     2.641219
H     3.545209     0.539515    -1.350303
H     2.460441     1.489829    -2.339150
H    -1.631693    -0.053052    -1.866910
O     4.486524    -1.054848     0.017820
H     3.493903    -1.171151     0.040268
H     4.826125    -1.891417    -0.327265
O     2.728636    -0.658433     3.859484
H     3.620316    -0.516273     3.463376
H     2.738129    -0.138009     4.672356
O     5.106516    -0.222125     2.568419
H     5.929024    -0.629527     2.866019
H     4.985317    -0.539021     1.644017
O     1.181827     2.159226    -3.804220
H     0.711730     1.334800    -3.564036
H     1.271149     2.126056    -4.765251
27
4WT TS S1 - C6 X
N     0.539880    -0.106735    -1.875795
C     1.786998     0.062673    -1.334575
N     1.940297     0.008289    -0.008580
C     0.732887    -0.076564     0.691438
C    -0.571987     0.015724     0.185977
C    -0.683882     0.309001    -1.249599
N    -1.500340    -0.009403     1.200075
C    -0.769176    -0.128802     2.318912
N     0.588531    -0.164876     2.051833
N     2.868847     0.206355    -2.169456
H    -1.163569    -0.219320     3.327421
H     1.341022    -0.244158     2.727851
H     3.754412    -0.060572    -1.748208
H     2.728788    -0.129435    -3.117071
H    -1.463465     0.888284    -1.763553
O     4.466299    -1.014294     0.391482
H     3.530571    -0.680884     0.372724
H     4.376123    -1.976800     0.361434
O     2.640189    -0.266663     4.005463
H     3.564712    -0.208685     3.671099
H     2.576731     0.453067     4.646071
O     5.146208    -0.059500     2.891269
H     5.941427    -0.484330     3.234569
H     5.034694    -0.414934     1.980918
O     1.565932    -1.430051    -4.246354
H     0.864749    -1.386712    -3.573241
H     1.102027    -1.568556    -5.082204
27
4WT TS S1 - S1 imino
N     0.687063    -0.148834    -1.881602
C     1.824340    -0.203189    -1.120511
N     1.992544    -0.189719     0.216711
C     0.742555    -0.124848     0.816368
C    -0.512965    -0.033222     0.190766
C    -0.566144     0.002508    -1.264997
N    -1.517933     0.036412     1.119557
C    -0.879584    -0.007941     2.313870
N     0.475737    -0.097733     2.176361
N     2.959985    -0.294348    -1.890929
H    -1.370811     0.022201     3.283772
H     1.163580    -0.146659     2.920271
H     3.826591    -0.344590    -1.349508
H     2.689309    -0.282818    -3.076422
H    -1.466202    -0.115303    -1.869334
O     4.537298    -1.011331     0.776392
H     3.578066    -0.745980     0.720844
H     4.516544    -1.978018     0.805811
O     2.382202    -0.100488     4.274529
H     3.322747    -0.064345     3.985480
H     2.288059     0.660579     4.861411
O     4.955508     0.049003     3.305793
H     5.719587    -0.347574     3.741361
H     4.943475    -0.335014     2.400745
O     1.830839    -0.309173    -4.047886
H     1.052395    -0.196508    -3.163580
H     1.820995     0.496751    -4.585562
```