



FOUNDATIONS
ADVANCES

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Supporting information for article:

X-ray molecular orbital analysis. II. Application to diformohydrazide, (NHCHO)₂

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Supporting information

Table S1(a) MO coefficients of valence a_g orbitals

a_g		MO		7		9		11		14		15		18		21	
		E(RHF)		-1.45581		-1.34608		-0.91704		-0.75259		-0.70332		-0.61821		-0.46629	
		E(XMO)		-1.17697		-1.06452		-0.20293		-0.11673		-0.39140		-0.26202		-0.26554	
		E(diag)		-1.28129		-1.07150		-0.75673		-0.55088		-0.52212		-0.49548		-0.23439	
		Method		XMO	RHF	XMO	RHF	XMO	RHF	XMO	RHF	XMO	RHF	XMO	RHF	XMO	RHF
SO	so	atoms	GTO	$a_{7,so}$	$a_{7,so}$	$a_{9,so}$	$a_{9,so}$	$a_{11,so}$	$a_{11,so}$	$a_{14,so}$	$a_{14,so}$	$a_{15,so}$	$a_{15,so}$	$a_{18,so}$	$a_{18,so}$	$a_{21,so}$	$a_{21,so}$
$N_{so}S+$	1	N+N'	1 S	-0.028	-0.013	0.066	0.016	-0.016	0.002	0.000	0.000	-0.009	0.001	0.004	-0.002	-0.004	0.002
	2	N+N'	2 S	-0.104	-0.183	0.054	0.226	0.051	0.041	0.031	-0.025	-0.005	-0.002	0.001	-0.011	0.053	0.050
	3	N+N'	3 S	-0.051	-0.034	0.019	0.040	-0.003	0.007	0.012	-0.010	-0.004	-0.002	0.027	0.003	0.008	0.008
	4	N+N'	4 S	-0.498	-0.303	0.389	0.379	0.131	0.067	0.045	-0.017	-0.060	-0.009	0.016	-0.033	0.055	0.068
	5	N+N'	5 S	-0.061	-0.219	0.286	0.316	0.086	0.094	0.052	-0.092	-0.125	0.055	-0.041	-0.041	0.207	0.292
	6	N+N'	6 S	0.213	-0.002	0.118	0.057	0.030	-0.128	0.047	-0.100	-0.077	-0.133	-0.072	0.009	0.677	0.357
$N_{so}p(x,y)-$	28	N-N'	1 X	0.011	-0.009	0.010	0.016	-0.067	0.067	0.063	0.053	0.042	0.078	-0.052	-0.035	0.046	-0.032
	29	N-N'	1 Y	-0.002	-0.009	-0.017	0.001	0.023	-0.037	0.051	0.081	-0.025	-0.031	-0.021	-0.040	-0.040	0.026
	31	N-N'	2 X	0.025	-0.015	0.002	0.022	-0.122	0.102	0.070	0.084	0.075	0.119	-0.060	-0.053	0.056	-0.046

	32	N-N'	2	Y	-0.055	-0.012	-0.001	-0.002	0.063	-0.056	0.133	0.125	-0.027	-0.049	-0.047	-0.061	-0.026	0.032
	34	N-N'	3	X	0.072	-0.036	-0.045	0.067	-0.282	0.254	0.279	0.185	0.261	0.283	-0.226	-0.130	0.123	-0.120
	35	N-N'	3	Y	0.232	-0.030	0.005	0.004	0.081	-0.104	0.207	0.227	-0.191	-0.088	-0.256	-0.109	-0.090	0.089
	37	N-N'	4	X	0.030	-0.011	0.014	0.001	-0.040	0.076	0.070	0.114	0.030	0.130	-0.067	-0.070	0.232	-0.125
	38	N-N'	4	Y	-0.400	0.013	0.003	0.001	-0.045	-0.045	0.178	0.103	-0.025	-0.011	-0.048	-0.098	-0.334	0.098
	40	N-N'	5	X	0.028	-0.002	0.038	-0.018	-0.004	0.070	0.013	0.066	-0.001	0.071	-0.038	-0.031	0.295	-0.133
	41	N-N'	5	Y	0.214	0.005	0.050	-0.025	-0.030	-0.056	-0.222	0.078	-0.037	-0.039	-0.059	-0.049	-0.236	0.122
H(N) _{so} S+	43	H+H'	1	S	0.009	0.021	-0.023	-0.030	-0.024	-0.012	-0.050	0.088	-0.006	0.009	0.021	-0.049	-0.069	0.005
	44	H+H'	2	S	0.102	0.033	-0.054	-0.059	0.017	-0.024	-0.219	0.205	0.018	0.018	0.057	-0.113	0.005	0.009
	45	H+H'	3	S	0.032	-0.005	0.031	0.025	0.049	0.006	-0.244	0.037	-0.011	0.015	0.034	-0.033	0.005	0.019
	46	H+H'	4	S	-0.003	0.005	0.009	0.026	0.020	0.001	0.003	-0.030	-0.030	0.012	0.012	-0.007	0.001	-0.008
C _{so} S+	51	C+C'	1	S	0.040	0.011	0.002	0.001	0.050	0.011	-0.001	-0.003	0.010	0.001	0.006	0.000	0.017	0.000
	52	C+C'	2	S	-0.019	-0.166	0.038	-0.038	-0.045	-0.204	-0.015	0.068	-0.012	0.049	-0.007	0.045	0.001	-0.017
	53	C+C'	3	S	-0.057	-0.031	-0.020	-0.010	-0.011	-0.028	0.009	0.005	-0.007	0.010	-0.009	0.006	-0.047	-0.007
	54	C+C'	4	S	-0.126	-0.273	0.106	-0.062	-0.439	-0.372	-0.118	0.151	-0.150	0.070	-0.094	0.099	-0.005	0.027
	55	C+C'	5	S	-0.163	-0.046	-0.012	0.005	-0.136	-0.112	-0.045	0.037	0.009	0.097	0.031	0.116	-0.286	-0.281
	56	C+C'	6	S	0.018	-0.005	-0.025	0.026	-0.050	0.068	-0.040	-0.008	0.046	0.101	-0.023	0.001	-0.376	-0.209
C _{so} p(x,y)-	78	C-C'	1	X	-0.001	0.019	0.061	0.003	0.028	-0.027	-0.048	-0.043	0.058	0.057	-0.046	-0.042	0.007	-0.027
	79	C-C'	1	Y	0.007	0.010	-0.030	0.040	0.010	-0.032	-0.008	0.006	-0.020	-0.051	-0.037	-0.050	-0.009	0.002

	81	C-C'	2	X	-0.035	0.040	0.024	0.005	0.068	-0.044	-0.102	-0.076	0.067	0.091	-0.050	-0.069	0.108	-0.060
	82	C-C'	2	Y	0.014	0.024	-0.101	0.081	0.036	-0.057	-0.043	0.008	-0.029	-0.090	-0.159	-0.097	-0.012	0.011
	84	C-C'	3	X	-0.173	0.054	-0.005	0.012	0.088	-0.084	0.107	-0.149	0.293	0.189	-0.179	-0.154	0.071	-0.064
	85	C-C'	3	Y	0.041	0.016	-0.057	0.107	0.060	-0.101	0.000	0.015	-0.194	-0.177	-0.207	-0.163	0.037	-0.013
	87	C-C'	4	X	0.006	0.000	0.021	-0.024	0.049	-0.074	-0.014	-0.030	0.127	0.088	-0.116	-0.104	-0.130	0.050
	88	C-C'	4	Y	0.154	-0.013	0.049	-0.023	0.039	-0.015	0.021	0.004	-0.140	-0.037	-0.091	-0.038	0.248	-0.159
	90	C-C'	5	X	0.110	-0.005	0.015	-0.001	-0.018	0.023	-0.013	0.009	-0.008	0.034	-0.073	-0.027	0.036	-0.097
	91	C-C'	5	Y	-0.090	-0.002	0.019	0.005	-0.056	0.029	0.142	0.014	-0.011	0.032	-0.021	-0.028	0.025	-0.096
H(C) _{so} S+	93	H+H'	1	S	0.004	0.010	0.019	0.001	0.101	0.060	-0.049	0.022	0.058	-0.058	-0.003	0.035	0.053	0.051
	94	H+H'	2	S	-0.158	0.019	-0.105	0.004	0.190	0.128	0.033	0.039	0.099	-0.131	-0.002	0.077	0.105	0.173
	95	H+H'	3	S	0.210	0.004	0.018	-0.011	0.135	0.059	-0.025	0.045	0.011	-0.082	-0.090	0.050	0.342	0.150
	96	H+H'	4	S	-0.016	-0.006	0.021	0.008	-0.023	0.040	-0.015	0.009	0.000	0.008	-0.004	0.009	-0.128	-0.036
O _{so} S+	101	O+O'	1	S	0.016	-0.007	0.027	-0.006	-0.075	-0.001	-0.025	0.001	-0.055	0.002	-0.049	0.006	0.007	0.001
	102	O+O'	2	S	-0.221	-0.205	-0.204	-0.209	0.089	0.096	0.090	-0.073	0.105	-0.070	0.125	-0.116	-0.046	0.007
	103	O+O'	3	S	-0.028	-0.077	-0.074	-0.080	0.014	0.042	0.013	-0.034	0.015	-0.034	0.048	-0.064	-0.003	0.001
	104	O+O'	4	S	-0.540	-0.305	-0.406	-0.306	-0.003	0.126	0.106	-0.088	0.012	-0.077	0.167	-0.106	-0.085	0.021
	105	O+O'	5	S	-0.077	-0.200	-0.212	-0.238	0.082	0.121	0.019	-0.143	0.116	-0.139	0.040	-0.260	-0.002	-0.001
	106	O+O'	6	S	-0.081	-0.053	-0.098	-0.052	0.099	0.050	-0.124	-0.052	0.022	-0.035	0.149	-0.158	-0.060	-0.087
O _{so} p(x,y)-	128	O-O'	1	X	-0.001	-0.010	-0.018	-0.013	0.002	-0.016	0.023	-0.003	0.072	0.068	0.034	0.030	-0.092	0.128

129	O-O'	1	Y	-0.026	-0.026	-0.011	-0.019	0.074	-0.010	0.061	0.044	0.012	0.009	0.065	0.109	0.070	-0.056
131	O-O'	2	X	0.050	-0.013	-0.001	-0.018	0.016	-0.024	0.028	-0.003	0.197	0.105	0.017	0.044	-0.123	0.195
132	O-O'	2	Y	0.110	-0.037	0.018	-0.024	0.050	-0.014	0.076	0.070	-0.003	0.015	0.076	0.163	0.060	-0.087
134	O-O'	3	X	0.027	-0.035	0.059	-0.041	-0.006	-0.035	0.048	-0.011	0.144	0.157	0.072	0.074	-0.257	0.289
135	O-O'	3	Y	0.055	-0.081	0.026	-0.067	0.119	-0.023	0.294	0.094	-0.012	0.016	0.270	0.261	0.121	-0.119
137	O-O'	4	X	-0.035	0.001	-0.024	-0.002	-0.096	-0.022	0.056	-0.011	0.094	0.095	0.045	0.015	-0.301	0.271
138	O-O'	4	Y	-0.022	-0.010	-0.012	-0.007	-0.041	-0.015	0.082	0.050	-0.044	-0.001	0.132	0.114	0.131	-0.140
140	O-O'	5	X	0.012	-0.008	0.000	-0.014	-0.010	-0.001	-0.030	-0.001	0.047	0.046	0.002	0.027	-0.065	0.103
141	O-O'	5	Y	-0.037	-0.019	-0.022	-0.013	-0.027	-0.006	0.103	0.014	-0.003	0.003	0.042	0.068	-0.024	-0.053

Table S1(b) MO coefficients of valence a_u π -orbitals

a_u		MO		16		20	
		E(RHF)		-0.66999			
		E(XMO)		-0.35825		-0.32543	
		E(diag)		-0.51916		-0.32670	
		Method		XMO	RHF	XMO	RHF
SO	so	atoms	GTO	$a_{16,so}$	$a_{16,so}$	$a_{20,so}$	$a_{20,so}$
$N_{so}p_z+$	9	N+N'	1 Z	0.170	0.102	-0.104	-0.069
	12	N+N'	2 Z	0.166	0.163	-0.084	-0.112
	15	N+N'	3 Z	0.291	0.295	-0.053	-0.192
	18	N+N'	4 Z	0.240	0.292	-0.585	-0.257
	21	N+N'	5 Z	-0.023	0.089	0.113	-0.090
$C_{so}p_z+$	59	C+C'	1 Z	-0.100	-0.052	-0.073	-0.041
	62	C+C'	2 Z	-0.132	-0.083	-0.003	-0.063
	65	C+C'	3 Z	-0.041	-0.171	-0.070	-0.135
	68	C+C'	4 Z	-0.464	-0.090	-0.206	-0.108
	71	C+C'	5 Z	0.129	-0.015	-0.081	-0.028
$O_{so}p_z+$	109	O+O'	1 Z	-0.003	-0.048	-0.158	-0.121
	112	O+O'	2 Z	-0.132	-0.074	-0.188	-0.185
	115	O+O'	3 Z	-0.186	-0.112	-0.134	-0.272
	118	O+O'	4 Z	-0.137	-0.087	-0.370	-0.271
	121	O+O'	5 Z	0.314	-0.028	-0.053	-0.113

Table S1(c) MO coefficients of valence $b_g(\text{XMO})$ and $a_g(\text{RHF})$ π -orbitals

$a_g(\text{RHF})$ & $b_g(\text{XMO})$		MO		19		23		
		E(RHF)		-0.57726		-0.37697		
		E(XMO)		-0.44193		-0.10304		
		E(diag)		-0.34427		-0.21921		
		Method		XMO	RHF	XMO	RHF	
SO	so	atoms	GTO	$a_{19,so}$	$a_{19,so}$	$a_{23,so}$	$a_{23,so}$	
$N_{so}p_z-$	30	N-N'	1	Z	0.034	0.052	0.198	0.115
	33	N-N'	2	Z	0.074	0.084	0.197	0.190
	36	N-N'	3	Z	0.185	0.131	0.179	0.275
	39	N-N'	4	Z	0.162	0.107	0.377	0.312
	42	N-N'	5	Z	-0.080	0.020	0.124	0.153
$C_{so}p_z-$	80	C-C'	1	Z	-0.123	-0.072	-0.013	-0.013
	83	C-C'	2	Z	-0.126	-0.114	-0.071	-0.019
	86	C-C'	3	Z	-0.214	-0.236	0.050	-0.046
	89	C-C'	4	Z	-0.244	-0.154	0.020	0.005
	92	C-C'	5	Z	0.149	-0.037	-0.033	0.007
$O_{so}p_z-$	130	O-O'	1	Z	-0.133	-0.101	0.172	0.086
	133	O-O'	2	Z	-0.151	-0.155	0.236	0.134
	136	O-O'	3	Z	-0.283	-0.232	0.114	0.191
	139	O-O'	4	Z	-0.206	-0.206	0.189	0.217
	142	O-O'	5	Z	-0.002	-0.066	0.004	0.112

Table S1(d) MO coefficients of valence $b_u(\text{XMO})$ and $a_u(\text{RHF})$ orbitals

		MO		8		10		12		13		17		22	
		E(RHF)		-1.42331		-1.17805		-0.89338		-0.78805		-0.63817		-0.46248	
		E(XMO)		-1.19006		-0.52344		-0.24487		-0.05476		-0.50611		-0.24496	
		E(diag)		-1.27801		-0.93637		-0.63278		-0.58223		-0.50282		-0.22464	
		Method		XMO	RHF	XMO	RHF	XMO	RHF	XMO	RHF	XMO	RHF	XMO	RHF
SO	so	atoms	GTO	$a_{8,so}$	$a_{8,so}$	$a_{10,so}$	$a_{10,so}$	$a_{12,so}$	$a_{12,so}$	$a_{13,so}$	$a_{13,so}$	$a_{17,so}$	$a_{17,so}$	$a_{22,so}$	$a_{22,so}$
$N_{so}p(x,y)+$	7	N+N'	1 X	0.043	-0.006	-0.042	0.037	-0.017	-0.011	-0.015	-0.006	-0.031	-0.007	0.006	-0.004
	8	N+N'	1 Y	-0.035	0.012	0.037	-0.015	-0.070	-0.093	-0.018	0.021	0.022	0.021	0.036	0.039
	10	N+N'	2 X	0.060	-0.010	-0.057	0.056	-0.007	-0.017	-0.032	-0.010	-0.011	-0.007	-0.006	0.000
	11	N+N'	2 Y	-0.060	0.021	0.036	-0.020	-0.197	-0.144	-0.044	0.031	0.042	0.030	0.028	0.046
	13	N+N'	3 X	0.035	-0.011	-0.114	0.091	-0.045	-0.023	-0.025	-0.011	0.111	-0.023	-0.022	-0.020
	14	N+N'	3 Y	-0.093	0.032	0.034	-0.053	-0.278	-0.296	0.098	0.069	0.108	0.073	0.084	0.154
	16	N+N'	4 X	0.030	-0.015	-0.016	0.012	-0.027	-0.032	-0.217	-0.023	0.085	0.016	0.014	0.006
	17	N+N'	4 Y	-0.022	0.025	-0.018	-0.006	-0.200	-0.180	0.084	0.029	0.027	0.037	-0.030	0.130
	19	N+N'	5 X	0.071	0.009	-0.065	0.106	-0.021	-0.041	0.006	-0.014	-0.021	-0.072	0.146	0.135
20	N+N'	5 Y	-0.003	0.014	-0.080	-0.033	-0.027	-0.104	0.013	0.023	0.027	0.048	0.123	0.029	
$N_{so}S-$	22	N-N'	1 S	0.015	0.004	0.021	-0.013	0.006	0.002	-0.082	0.003	0.004	-0.001	-0.001	0.002

	23	N-N'	2	S	0.058	0.047	-0.245	-0.246	-0.080	0.080	0.058	0.081	0.002	-0.006	-0.048	0.045
	24	N-N'	3	S	0.042	0.008	-0.071	-0.051	-0.021	0.019	-0.046	0.016	0.006	0.000	-0.038	0.007
	25	N-N'	4	S	0.116	0.075	-0.293	-0.347	-0.116	0.104	-0.048	0.122	0.031	-0.016	-0.042	0.053
	26	N-N'	5	S	0.067	0.030	-0.111	-0.263	-0.151	0.103	-0.001	0.084	-0.041	0.006	-0.128	0.177
	27	N-N'	6	S	-0.009	0.027	-0.009	-0.017	0.020	-0.012	-0.004	0.072	0.014	-0.047	-0.113	0.154
H(N) _{so} S-	47	H-H'	1	S	-0.012	-0.002	0.040	0.044	0.067	-0.085	0.016	-0.002	0.012	0.019	0.090	0.014
	48	H-H'	2	S	0.057	-0.007	0.118	0.091	0.289	-0.171	0.058	-0.019	-0.136	0.049	0.015	0.028
	49	H-H'	3	S	-0.097	0.005	-0.017	-0.004	-0.051	-0.038	-0.002	0.036	-0.030	0.012	-0.422	0.028
	50	H-H'	4	S	-0.021	-0.004	0.007	0.003	0.005	-0.002	0.042	-0.014	-0.003	0.020	0.081	-0.039
C _{so} p(x,y)+	57	C+C'	1	X	0.045	-0.019	-0.027	0.004	0.025	0.014	-0.048	-0.072	0.022	0.045	0.005	-0.017
	58	C+C'	1	Y	-0.012	-0.025	0.041	-0.045	-0.004	-0.027	0.016	0.021	0.037	0.056	0.002	0.000
	60	C+C'	2	X	0.091	-0.038	0.017	0.007	0.007	0.026	-0.159	-0.120	0.045	0.078	-0.026	-0.038
	61	C+C'	2	Y	-0.023	-0.054	0.037	-0.086	0.005	-0.051	0.035	0.041	0.145	0.107	0.001	0.013
	63	C+C'	3	X	0.014	-0.054	-0.090	0.017	0.062	0.040	-0.172	-0.232	0.153	0.163	-0.047	-0.042
	64	C+C'	3	Y	-0.063	-0.059	0.335	-0.134	-0.107	-0.065	-0.007	0.066	0.238	0.187	0.081	-0.028
	66	C+C'	4	X	-0.032	0.018	-0.001	-0.016	0.016	0.006	-0.039	-0.117	0.081	0.067	-0.008	0.079
	67	C+C'	4	Y	-0.013	-0.001	-0.366	0.016	-0.052	-0.023	0.144	-0.022	0.118	0.066	-0.011	-0.068
	69	C+C'	5	X	-0.027	-0.006	-0.182	0.010	-0.116	-0.044	0.054	-0.019	0.091	0.046	-0.076	-0.070
	70	C+C'	5	Y	0.001	-0.004	0.093	0.025	-0.042	-0.016	-0.156	-0.028	0.011	0.014	0.007	-0.027

$C_{30}S^-$	72	C-C'	1	S	0.022	-0.011	-0.034	0.009	-0.015	0.003	0.016	0.005	-0.028	0.001	0.030	0.002
	73	C-C'	2	S	0.096	0.174	-0.159	-0.111	0.042	-0.109	0.150	-0.135	0.003	-0.060	0.016	-0.019
	74	C-C'	3	S	0.020	0.033	-0.021	-0.013	-0.009	-0.021	0.038	-0.020	-0.004	-0.005	-0.005	-0.001
	75	C-C'	4	S	0.139	0.289	-0.296	-0.204	0.193	-0.179	0.274	-0.229	0.190	-0.144	-0.155	-0.021
	76	C-C'	5	S	-0.004	0.012	-0.110	-0.042	0.034	-0.070	0.081	-0.174	0.092	-0.067	0.003	-0.108
	77	C-C'	6	S	-0.018	-0.009	-0.221	0.040	-0.066	0.009	0.090	-0.064	0.068	-0.026	0.016	-0.013
$H(C)_{30}S^-$	97	H-H'	1	S	-0.025	-0.010	0.021	0.016	0.017	0.011	-0.085	0.087	0.030	-0.034	0.006	0.038
	98	H-H'	2	S	-0.054	-0.023	0.121	0.031	0.052	0.037	-0.386	0.191	0.066	-0.076	-0.023	0.146
	99	H-H'	3	S	-0.054	0.000	-0.027	0.010	-0.120	0.007	0.024	0.100	0.029	-0.053	-0.463	0.137
	100	H-H'	4	S	-0.027	-0.006	-0.020	0.009	0.031	-0.029	0.008	0.010	0.003	0.010	0.009	-0.016
$O_{30}p(x,y)^+$	107	O+O'	1	X	-0.007	0.015	0.024	0.004	0.051	0.010	-0.073	-0.053	-0.021	-0.048	0.137	0.131
	108	O+O'	1	Y	0.014	0.032	-0.004	0.001	-0.057	-0.020	-0.028	-0.002	-0.073	-0.111	-0.085	-0.069
	110	O+O'	2	X	-0.014	0.020	0.028	0.007	0.044	0.015	-0.141	-0.080	-0.084	-0.072	0.178	0.201
	111	O+O'	2	Y	-0.009	0.044	-0.021	0.001	-0.089	-0.034	-0.058	-0.003	-0.127	-0.167	-0.067	-0.104
	113	O+O'	3	X	-0.021	0.051	0.010	0.013	0.048	0.027	-0.127	-0.123	-0.111	-0.113	0.212	0.293
	114	O+O'	3	Y	-0.083	0.103	-0.043	0.011	-0.132	-0.032	0.010	-0.005	-0.330	-0.263	-0.101	-0.160
	116	O+O'	4	X	0.002	-0.002	0.011	-0.001	0.064	0.020	-0.063	-0.071	-0.034	-0.046	0.427	0.281
	117	O+O'	4	Y	0.032	0.013	-0.166	0.002	-0.090	-0.038	0.081	-0.005	-0.084	-0.110	-0.166	-0.149
	119	O+O'	5	X	-0.031	0.011	0.066	0.006	-0.136	0.003	-0.153	-0.033	0.006	-0.033	-0.046	0.119

	120	O+O'	5	Y	0.011	0.016	-0.006	0.009	0.087	0.000	0.056	-0.003	-0.048	-0.060	-0.023	-0.069
O _{so} S ⁻	122	O-O'	1	S	-0.002	0.009	0.021	0.002	0.015	0.001	0.009	-0.002	0.007	-0.006	-0.006	-0.001
	123	O-O'	2	S	0.215	0.275	0.092	0.106	-0.073	0.090	-0.028	0.075	-0.121	0.134	-0.004	0.006
	124	O-O'	3	S	0.082	0.104	0.060	0.042	-0.041	0.037	-0.026	0.035	-0.061	0.072	-0.010	0.005
	125	O-O'	4	S	0.591	0.407	0.281	0.150	-0.060	0.129	-0.012	0.093	-0.151	0.126	-0.020	0.002
	126	O-O'	5	S	0.180	0.286	0.242	0.123	-0.054	0.136	-0.004	0.105	-0.163	0.297	-0.031	0.016
	127	O-O'	6	S	0.052	0.052	0.368	0.065	-0.052	0.015	-0.116	0.017	-0.142	0.175	0.009	-0.060

Table S1 (e) Energies of core MOs (E_h)

MO	1	2	3	4	5	6
E (RHF)	-20.55702	-20.55702	-15.66363	-15.66309	-11.39851	-11.39851
E (XMO)	-20.16710	-20.27236	-14.80847	-14.99254	-11.08789	-11.16772

Table S2 (a) Coefficients($a_{mo,so}$), e.s.d.'s and shifts of a_g XMO-MOs

a_g	mo	2	3	5	7	9	11	14	15	18	21
	E(RHF)	-20.55702	-15.66363	-11.39851	-1.45581	-1.34608	-0.91704	-0.75259	-0.70332	-0.61821	-0.46629
	E(XMO)	-20.27236	-14.80847	-11.08789	-1.17697	-1.06452	-0.20293	-0.11673	-0.39140	-0.26202	-0.26554
	E(diag.)	-20.37783	-15.03804	-11.22117	-1.28129	-1.07150	-0.75673	-0.55088	-0.52212	-0.49548	-0.23439
so	N _{so} S ⁺										
1	$a_{mo,so}$	0.00209	-0.99337	0.00113	-0.02817	0.06571	-0.01567	-0.00050	-0.00861	0.00374	-0.00410
	e.s.d.	0.00000	0.00000	0.00000	0.01652	0.00847	0.01033	0.00712	0.01048	0.01046	0.01036

	shift	0.00000	0.00000	0.00000	0.01046	0.00576	-0.00225	0.00204	0.00193	-0.00340	0.00037
2	a _{mo,so}	0.00679	-0.02814	-0.00255	-0.10392	0.05425	0.05106	0.03121	-0.00494	0.00129	0.05281
	e.s.d.	0.00000	0.00000	0.00000	0.00558	0.00957	0.00698	0.00814	0.00851	0.00854	0.01139
	shift	0.00000	0.00000	0.00000	-0.00285	-0.00129	-0.00101	-0.00235	0.00122	-0.00311	0.00308
3	a _{mo,so}	0.00046	0.01828	0.00001	-0.05057	0.01942	-0.00339	0.01231	-0.00433	0.02692	0.00774
	e.s.d.	0.00000	0.00000	0.00000	0.00299	0.00393	0.00308	0.00441	0.00374	0.00563	0.00544
	shift	0.00000	0.00000	0.00000	0.00111	-0.00186	0.00010	-0.00122	0.00022	0.00516	0.00388
4	a _{mo,so}	0.00928	-0.08533	0.00373	-0.49799	0.38861	0.13117	0.04462	-0.05980	0.01571	0.05476
	e.s.d.	0.00000	0.00000	0.00000	0.00382	0.00335	0.00246	0.00367	0.00536	0.00348	0.00605
	shift	0.00000	0.00000	0.00000	0.00068	0.00024	-0.00001	-0.00553	-0.00092	0.00501	-0.00183
5	a _{mo,so}	0.01168	-0.04634	-0.01604	-0.06141	0.28594	0.08622	0.05235	-0.12479	-0.04090	0.20670
	e.s.d.	0.00000	0.00000	0.00000	0.00434	0.00347	0.00372	0.00629	0.00630	0.00373	0.00706
	shift	0.00000	0.00000	0.00000	0.00054	0.00050	0.00134	-0.00177	-0.00368	0.00288	-0.00214
6	a _{mo,so}	0.00956	0.01599	0.00334	0.21298	0.11835	0.02989	0.04695	-0.07714	-0.07245	0.67723
	e.s.d.	0.00000	0.00000	0.00000	0.00600	0.00716	0.00471	0.00603	0.00749	0.00993	0.01388
	shift	0.00000	0.00000	0.00000	0.00353	0.00127	0.00313	-0.00599	-0.00047	0.01325	-0.00357
so	N _{so} px-,py-										
28	a _{so,mo(px-)}	0.00291	0.00383	0.00338	0.01099	0.00972	-0.06696	0.06297	0.04203	-0.05196	0.04632
	e.s.d.	0.00000	0.00000	0.00000	0.00416	0.00335	0.00289	0.00590	0.00223	0.00621	0.00505
	shift	0.00000	0.00000	0.00000	-0.00209	-0.00034	-0.00096	-0.00361	0.00088	0.00498	-0.00179
29	a _{mo,so(py-)}	-0.00047	-0.00105	-0.00478	-0.00237	-0.01668	0.02336	0.05135	-0.02509	-0.02060	-0.03971
	e.s.d.	0.00000	0.00000	0.00000	0.00393	0.00630	0.00868	0.00380	0.00689	0.00662	0.00875
	shift	0.00000	0.00000	0.00000	0.00000	0.00229	-0.00350	0.00036	0.00120	-0.00260	0.00146

31	a _{so,mo} (px-)	0.00474	0.00736	0.00472	0.02480	0.00191	-0.12203	0.07048	0.07527	-0.06028	0.05598
	e.s.d.	0.00000	0.00000	0.00000	0.00294	0.00204	0.00306	0.00515	0.00205	0.00323	0.00540
	shift	0.00000	0.00000	0.00000	-0.00185	0.00075	0.00158	-0.00394	0.00055	0.00137	-0.00782
32	a _{mo,so} (py-)	-0.00331	-0.00330	-0.00920	-0.05528	-0.00073	0.06301	0.13317	-0.02731	-0.04730	-0.02610
	e.s.d.	0.00000	0.00000	0.00000	0.00385	0.00619	0.00731	0.00212	0.00580	0.00470	0.00549
	shift	0.00000	0.00000	0.00000	-0.00282	0.00000	-0.00299	0.00315	-0.00042	-0.00366	-0.00024
34	a _{so,mo} (px-)	0.01124	0.01919	0.01143	0.07171	-0.04537	-0.28243	0.27931	0.26130	-0.22633	0.12333
	e.s.d.	0.00000	0.00000	0.00000	0.00242	0.00385	0.00177	0.00253	0.00407	0.00348	0.00486
	shift	0.00000	0.00000	0.00000	-0.00203	-0.00027	0.00039	-0.00006	-0.00271	0.00108	-0.00686
35	a _{mo,so} (py-)	0.01055	0.00803	-0.01399	0.23165	0.00481	0.08090	0.20727	-0.19138	-0.25597	-0.09036
	e.s.d.	0.00000	0.00000	0.00000	0.00297	0.00306	0.00698	0.00460	0.00647	0.00860	0.00816
	shift	0.00000	0.00000	0.00000	-0.00265	0.00000	-0.00153	0.00445	-0.00381	-0.00231	-0.00376
37	a _{so,mo} (px-)	0.00264	0.00655	0.00368	0.02955	0.01422	-0.04047	0.07044	0.02987	-0.06679	0.23180
	e.s.d.	0.00000	0.00000	0.00000	0.00550	0.00338	0.00365	0.00355	0.00556	0.00499	0.00936
	shift	0.00000	0.00000	0.00000	-0.00119	0.00108	-0.00022	-0.00076	-0.00479	0.01277	-0.01091
38	a _{mo,so} (py-)	-0.01691	-0.01782	-0.00115	-0.40006	0.00329	-0.04518	0.17782	-0.02526	-0.04820	-0.33384
	e.s.d.	0.00000	0.00000	0.00000	0.00681	0.00388	0.01257	0.00309	0.00933	0.00791	0.00533
	shift	0.00000	0.00000	0.00000	-0.00513	0.00000	0.00185	0.00463	0.00172	0.00025	-0.00036
40	a _{so,mo} (px-)	0.00214	0.00403	0.00270	0.02795	0.03800	-0.00352	0.01261	-0.00080	-0.03782	0.29493
	e.s.d.	0.00000	0.00000	0.00000	0.00574	0.00667	0.00379	0.01071	0.01752	0.00987	0.00929
	shift	0.00000	0.00000	0.00000	-0.00436	0.00064	0.00000	-0.00063	0.00000	0.00562	0.00080
41	a _{mo,so} (py-)	0.01356	0.00213	0.01047	0.21377	0.05048	-0.03010	-0.22214	-0.03659	-0.05921	-0.23569
	e.s.d.	0.00000	0.00000	0.00000	0.01513	0.01013	0.00692	0.00954	0.01058	0.00946	0.01227

	shift	0.00000	0.00000	0.00000	-0.00864	0.00536	0.00693	0.00315	0.00480	-0.00408	0.00225
so	H(N) _{soS+}										
43	a _{mo,so}	-0.00234	0.00426	0.00245	0.00856	-0.02267	-0.02371	-0.04998	-0.00647	0.02104	-0.06908
	e.s.d.	0.00000	0.00000	0.00000	0.00790	0.00797	0.04064	0.00267	0.01741	0.00477	0.02860
	shift	0.00000	0.00000	0.00000	-0.00041	-0.00084	-0.00095	0.00184	0.00000	-0.00213	0.00456
44	a _{mo,so}	-0.00395	0.01038	0.01126	0.10192	-0.05378	0.01723	-0.21882	0.01831	0.05708	0.00508
	e.s.d.	0.00000	0.00000	0.00000	0.00993	0.00699	0.01737	0.00347	0.01438	0.00597	0.01500
	shift	0.00000	0.00000	0.00000	-0.01287	0.00257	0.00317	0.00301	-0.01095	-0.00287	0.00000
45	a _{mo,so}	-0.00298	-0.00196	0.01437	0.03186	0.03074	0.04904	-0.24419	-0.01084	0.03400	0.00546
	e.s.d.	0.00000	0.00000	0.00000	0.01526	0.00775	0.00945	0.00396	0.00749	0.00930	0.00652
	shift	0.00000	0.00000	0.00000	-0.00866	0.00588	-0.00392	0.00259	-0.00464	0.00028	0.00000
46	a _{mo,so}	0.00045	-0.00294	-0.00024	-0.00343	0.00855	0.01985	0.00339	-0.03021	0.01220	0.00082
	e.s.d.	0.00000	0.00000	0.00000	0.00603	0.00408	0.01054	0.00497	0.00684	0.01091	0.00581
	shift	0.00000	0.00000	0.00000	0.00000	0.00266	0.00376	0.00000	-0.00395	-0.01452	0.00000
so	C _{soS+}										
51	a _{mo,so}	0.00231	0.00166	-0.99373	0.03989	0.00186	0.04977	-0.00098	0.01048	0.00580	0.01682
	e.s.d.	0.00000	0.00000	0.00000	0.03206	0.01056	0.01345	0.00908	0.00907	0.00768	0.01477
	shift	0.00000	0.00000	0.00000	-0.00841	-0.00148	0.00112	-0.00069	-0.00042	-0.00305	-0.00830
52	a _{mo,so}	-0.00052	-0.00713	0.02172	-0.01925	0.03779	-0.04483	-0.01496	-0.01187	-0.00709	0.00123
	e.s.d.	0.00000	0.00000	0.00000	0.01409	0.01025	0.01307	0.01034	0.00937	0.00939	0.00972
	shift	0.00000	0.00000	0.00000	0.00027	-0.00322	-0.00386	0.00068	-0.00231	-0.00170	-0.00243
53	a _{mo,so}	-0.00298	-0.00386	-0.01963	-0.05668	-0.02029	-0.01083	0.00944	-0.00745	-0.00909	-0.04667

	e.s.d.	0.00000	0.00000	0.00000	0.01036	0.00952	0.00426	0.00921	0.00508	0.00545	0.01336
	shift	0.00000	0.00000	0.00000	-0.00429	-0.00809	0.00343	0.00073	0.00216	-0.00415	-0.00393
54	a _{mo,so}	-0.00217	-0.00849	0.07289	-0.12563	0.10584	-0.43937	-0.11810	-0.14967	-0.09380	-0.00520
	e.s.d.	0.00000	0.00000	0.00000	0.00807	0.00859	0.00394	0.01029	0.00430	0.00575	0.01453
	shift	0.00000	0.00000	0.00000	-0.00589	-0.00308	0.00057	-0.00500	-0.00079	-0.00234	0.00000
55	a _{mo,so}	-0.00633	-0.01353	0.02612	-0.16299	-0.01177	-0.13622	-0.04513	0.00888	0.03086	-0.28601
	e.s.d.	0.00000	0.00000	0.00000	0.01559	0.00949	0.00656	0.01064	0.00644	0.00716	0.01044
	shift	0.00000	0.00000	0.00000	0.00691	0.00075	-0.00046	-0.00689	0.00192	-0.00166	0.00527
56	a _{mo,so}	0.00422	-0.00474	-0.00713	0.01793	-0.02509	-0.04955	-0.04014	0.04570	-0.02343	-0.37630
	e.s.d.	0.00000	0.00000	0.00000	0.01584	0.00599	0.00396	0.01090	0.00686	0.00767	0.00810
	shift	0.00000	0.00000	0.00000	0.01675	-0.00330	0.00099	-0.00567	0.00406	-0.00045	0.00278
so	C _{so} px-,py-										
78	a _{so,mo} (px-)	0.00442	-0.00036	-0.00190	-0.00096	0.06075	0.02776	-0.04817	0.05832	-0.04580	0.00688
	e.s.d.	0.00000	0.00000	0.00000	0.00539	0.00731	0.00401	0.00795	0.00584	0.00653	0.00351
	shift	0.00000	0.00000	0.00000	0.00000	0.00054	0.00031	-0.00139	0.00350	0.00064	0.00097
79	a _{mo,so} (py-)	-0.00278	0.00209	0.00121	0.00733	-0.02972	0.00953	-0.00760	-0.01973	-0.03740	-0.00921
	e.s.d.	0.00000	0.00000	0.00000	0.01265	0.00735	0.00351	0.00952	0.00883	0.00542	0.00950
	shift	0.00000	0.00000	0.00000	0.00368	0.00180	-0.00004	0.00304	-0.00258	0.00106	-0.00048
81	a _{so,mo} (px-)	-0.00153	-0.00018	0.00115	-0.03537	0.02399	0.06835	-0.10169	0.06694	-0.04970	0.10830
	e.s.d.	0.00000	0.00000	0.00000	0.00924	0.01540	0.00387	0.00593	0.00396	0.00584	0.00557
	shift	0.00000	0.00000	0.00000	0.00672	0.00254	0.00640	0.00072	-0.00089	-0.00345	-0.00159
82	a _{mo,so} (py-)	-0.00823	0.00450	0.00325	0.01384	-0.10054	0.03586	-0.04336	-0.02870	-0.15859	-0.01221
	e.s.d.	0.00000	0.00000	0.00000	0.00494	0.00370	0.00637	0.00788	0.00568	0.00245	0.01029

	shift	0.00000	0.00000	0.00000	0.00592	0.00317	0.00064	0.00624	-0.00026	0.00203	0.00037
84	a _{so,mo} (px-)	-0.00420	-0.00531	-0.00758	-0.17341	-0.00463	0.08760	0.10741	0.29253	-0.17904	0.07100
	e.s.d.	0.00000	0.00000	0.00000	0.00814	0.00543	0.00480	0.00639	0.00401	0.00644	0.01270
	shift	0.00000	0.00000	0.00000	0.00287	0.00266	0.00253	-0.00048	0.00176	-0.00212	-0.00266
85	a _{mo,so} (py-)	-0.01015	0.00827	0.00574	0.04138	-0.05669	0.05959	-0.00034	-0.19403	-0.20683	0.03706
	e.s.d.	0.00000	0.00000	0.00000	0.00690	0.00349	0.00532	0.00885	0.00699	0.00569	0.00870
	shift	0.00000	0.00000	0.00000	0.01136	0.00321	0.00058	0.00000	0.00198	0.00682	-0.00418
87	a _{so,mo} (px-)	0.00388	-0.00341	-0.00546	0.00577	0.02068	0.04917	-0.01443	0.12744	-0.11588	-0.13026
	e.s.d.	0.00000	0.00000	0.00000	0.00573	0.00520	0.00438	0.00968	0.00395	0.01086	0.00932
	shift	0.00000	0.00000	0.00000	0.00020	-0.00048	0.00388	0.00503	0.00298	-0.00056	-0.00708
88	a _{mo,so} (py-)	0.00841	0.00881	-0.00489	0.15431	0.04914	0.03912	0.02056	-0.13984	-0.09085	0.24772
	e.s.d.	0.00000	0.00000	0.00000	0.01093	0.00711	0.00642	0.00492	0.00792	0.00828	0.00920
	shift	0.00000	0.00000	0.00000	0.00031	0.00452	0.00125	0.00200	0.00199	0.01554	0.00316
90	a _{so,mo} (px-)	0.00620	0.00463	0.00423	0.11000	0.01451	-0.01765	-0.01308	-0.00845	-0.07331	0.03598
	e.s.d.	0.00000	0.00000	0.00000	0.01311	0.00762	0.00771	0.00973	0.00575	0.01481	0.01002
	shift	0.00000	0.00000	0.00000	-0.00270	0.00320	0.00084	0.01285	0.00024	-0.00760	0.00233
91	a _{mo,so} (py-)	-0.00105	0.00012	-0.00863	-0.09018	0.01857	-0.05634	0.14195	-0.01119	-0.02143	0.02522
	e.s.d.	0.00000	0.00000	0.00000	0.01237	0.00776	0.00693	0.01173	0.01287	0.01138	0.00978
	shift	0.00000	0.00000	0.00000	-0.00996	-0.00709	0.00175	-0.00381	-0.00369	0.01035	0.00533
so	H(C) _{so} S ⁺										
93	H ₉₃ S ⁺	-0.00009	0.00190	-0.00872	0.00425	0.01879	0.10061	-0.04863	0.05835	-0.00288	0.05331
	e.s.d.	0.00000	0.00000	0.00000	0.01813	0.03011	0.00514	0.02107	0.00892	0.01242	0.00980
	shift	0.00000	0.00000	0.00000	0.00116	-0.00082	-0.00027	0.00032	-0.00757	0.00000	-0.00044

94	H _{94S} ⁺	-0.01515	-0.00109	-0.01725	-0.15800	-0.10503	0.19027	0.03308	0.09887	-0.00187	0.10479
	e.s.d.	0.00000	0.00000	0.00000	0.03101	0.02396	0.00284	0.01358	0.00411	0.00720	0.00736
	shift	0.00000	0.00000	0.00000	-0.00856	0.01449	-0.00268	-0.00665	-0.00011	0.00000	-0.00231
95	H _{95S} ⁺	0.00275	0.01025	-0.00525	0.21035	0.01848	0.13514	-0.02487	0.01059	-0.09035	0.34168
	e.s.d.	0.00000	0.00000	0.00000	0.01356	0.02287	0.00444	0.01095	0.00488	0.00496	0.00791
	shift	0.00000	0.00000	0.00000	0.01327	0.00182	0.00074	0.00330	-0.00191	-0.00187	-0.00057
96	H _{96S} ⁺	0.00311	-0.00235	-0.00204	-0.01596	0.02122	-0.02264	-0.01523	0.00026	-0.00428	-0.12757
	e.s.d.	0.00000	0.00000	0.00000	0.02283	0.01431	0.00450	0.02063	0.00329	0.00433	0.00636
	shift	0.00000	0.00000	0.00000	-0.00039	-0.00758	-0.00353	-0.00550	0.00000	0.00000	0.00012
so	O _{soS} ⁺										
101	O _{101S} ⁺	-0.99089	0.00490	0.00056	0.01567	0.02722	-0.07480	-0.02490	-0.05544	-0.04906	0.00664
	e.s.d.	0.00000	0.00000	0.00000	0.00961	0.02433	0.01672	0.01166	0.00861	0.00948	0.00702
	shift	0.00000	0.00000	0.00000	0.00715	0.01168	-0.00325	-0.00494	-0.00299	-0.00778	-0.00032
102	O _{102S} ⁺	-0.01557	-0.01419	0.00522	-0.22144	-0.20361	0.08860	0.09000	0.10490	0.12500	-0.04621
	e.s.d.	0.00000	0.00000	0.00000	0.01257	0.01373	0.01273	0.00833	0.01357	0.00724	0.00703
	shift	0.00000	0.00000	0.00000	0.00131	0.00365	0.00403	-0.00241	-0.00269	-0.00102	-0.00007
103	O _{103S} ⁺	0.00919	-0.00038	-0.00414	-0.02777	-0.07354	0.01431	0.01340	0.01465	0.04807	-0.00329
	e.s.d.	0.00000	0.00000	0.00000	0.00360	0.00450	0.00860	0.00286	0.00604	0.00310	0.00280
	shift	0.00000	0.00000	0.00000	-0.00107	0.00035	-0.00838	-0.00096	-0.00138	-0.00205	0.00015
104	O _{104S} ⁺	-0.02531	-0.01602	0.02479	-0.54018	-0.40617	-0.00256	0.10598	0.01195	0.16727	-0.08532
	e.s.d.	0.00000	0.00000	0.00000	0.00295	0.00310	0.01150	0.00340	0.00339	0.00342	0.00266
	shift	0.00000	0.00000	0.00000	-0.00191	-0.00179	0.00000	-0.00306	-0.00244	-0.00240	0.00265
105	O _{105S} ⁺	-0.01806	0.01015	-0.00266	-0.07690	-0.21165	0.08180	0.01926	0.11589	0.03967	-0.00193

	e.s.d.	0.00000	0.00000	0.00000	0.00542	0.00573	0.01341	0.00563	0.00383	0.00421	0.00285
	shift	0.00000	0.00000	0.00000	-0.00123	0.00029	-0.00361	-0.00288	-0.00328	-0.00373	0.00000
106	O _{106S+}	-0.01584	-0.00595	-0.00264	-0.08117	-0.09799	0.09934	-0.12409	0.02242	0.14907	-0.06030
	e.s.d.	0.00000	0.00000	0.00000	0.00898	0.00840	0.01677	0.00411	0.00581	0.00637	0.00387
	shift	0.00000	0.00000	0.00000	0.00565	-0.00525	-0.00441	-0.03093	-0.00039	-0.00376	0.00093
so	O _{so} px-,py-										
128	a _{so,mo} (px-)	0.00048	-0.00268	-0.00421	-0.00148	-0.01786	0.00178	0.02273	0.07248	0.03426	-0.09226
	e.s.d.	0.00000	0.00000	0.00000	0.00424	0.00530	0.01745	0.00741	0.00311	0.00660	0.00261
	shift	0.00000	0.00000	0.00000	-0.00215	0.00042	-0.00814	-0.00488	-0.00143	-0.00412	0.00093
129	a _{mo,so} (py-)	-0.00546	-0.00114	-0.00979	-0.02590	-0.01056	0.07388	0.06065	0.01205	0.06525	0.07050
	e.s.d.	0.00000	0.00000	0.00000	0.00489	0.00605	0.00864	0.00370	0.01040	0.00396	0.00451
	shift	0.00000	0.00000	0.00000	-0.00454	-0.00135	-0.00379	-0.00029	-0.00559	0.00046	-0.00232
131	a _{so,mo} (px-)	0.00715	-0.00054	-0.01045	0.04987	-0.00061	0.01591	0.02794	0.19720	0.01743	-0.12306
	e.s.d.	0.00000	0.00000	0.00000	0.00410	0.00268	0.01222	0.00582	0.00440	0.00547	0.00306
	shift	0.00000	0.00000	0.00000	-0.00082	-0.00151	-0.00642	-0.00411	-0.00245	-0.00536	0.00146
132	a _{mo,so} (py-)	0.00479	0.00182	-0.01166	0.10985	0.01848	0.04984	0.07609	-0.00252	0.07585	0.06026
	e.s.d.	0.00000	0.00000	0.00000	0.00332	0.00338	0.00715	0.00246	0.00581	0.00310	0.00435
	shift	0.00000	0.00000	0.00000	-0.00401	-0.00213	-0.00255	-0.00140	-0.00467	-0.00018	0.00315
134	a _{so,mo} (px-)	0.00968	-0.00524	-0.01302	0.02659	0.05898	-0.00636	0.04816	0.14408	0.07208	-0.25684
	e.s.d.	0.00000	0.00000	0.00000	0.00527	0.00310	0.01278	0.00548	0.00241	0.00641	0.00189
	shift	0.00000	0.00000	0.00000	0.00034	-0.00246	-0.00478	-0.00696	-0.00239	-0.00585	0.00181
135	a _{mo,so} (py-)	0.00031	-0.00180	-0.02615	0.05501	0.02636	0.11886	0.29351	-0.01214	0.27040	0.12098
	e.s.d.	0.00000	0.00000	0.00000	0.00252	0.00272	0.00551	0.00547	0.00721	0.00396	0.00551

	shift	0.00000	0.00000	0.00000	-0.00350	-0.00210	-0.00339	-0.00780	-0.00281	-0.00058	0.00131
137	a _{so,mo} (px-)	0.00497	-0.00502	-0.00513	-0.03540	-0.02368	-0.09641	0.05595	0.09432	0.04493	-0.30073
	e.s.d.	0.00000	0.00000	0.00000	0.00759	0.00647	0.01643	0.00980	0.00694	0.00819	0.00474
	shift	0.00000	0.00000	0.00000	-0.00307	-0.00112	0.01523	-0.00563	-0.00364	-0.00824	0.00438
138	a _{mo,so} (py-)	0.00031	0.00336	-0.00916	-0.02222	-0.01213	-0.04133	0.08223	-0.04375	0.13190	0.13071
	e.s.d.	0.00000	0.00000	0.00000	0.00444	0.00565	0.01307	0.00769	0.00888	0.00456	0.00677
	shift	0.00000	0.00000	0.00000	-0.00397	-0.00568	-0.00707	-0.00403	-0.00373	-0.00496	-0.00011
140	a _{so,mo} (px-)	0.00241	-0.00140	-0.00042	0.01247	0.00004	-0.01036	-0.03003	0.04693	0.00179	-0.06523
	e.s.d.	0.00000	0.00000	0.00000	0.01196	0.00882	0.00703	0.01795	0.00881	0.01568	0.00917
	shift	0.00000	0.00000	0.00000	-0.00698	0.00000	0.00537	0.00552	-0.00387	0.00000	0.00107
141	a _{mo,so} (py-)	0.00006	-0.00001	-0.01136	-0.03722	-0.02179	-0.02745	0.10261	-0.00302	0.04213	-0.02367
	e.s.d.	0.00000	0.00000	0.00000	0.00840	0.01486	0.00619	0.01229	0.00592	0.00770	0.01195
	shift	0.00000	0.00000	0.00000	-0.00358	-0.00445	0.00461	0.00197	-0.00014	-0.00393	-0.00142
a _{mo,so} -max		0.99089	0.99337	0.99373	0.54018	0.40617	0.43937	0.29351	0.29253	0.27040	0.67723
so-max		101	1	51	104	104	54	135	84	135	6

Table S2 (b) Coefficients($a_{\text{mo,so}}$), e.s.d.'s and shifts of a_u XMO-MOs

a_u	mo	16	20
	E(RHF)	-0.66999	-0.48689
	E(XMO)	-0.35825	-0.32543
	E(diag.)	-0.51916	-0.32670
so	$N_{\text{so}}\text{pz}^+$		
9	$a_{\text{mo,so}}$	0.16977	-0.10372
	e.s.d.	0.00114	0.00404
	shift	-0.00077	0.00306
12	$a_{\text{mo,so}}$	0.16648	-0.08382
	e.s.d.	0.00260	0.00515
	shift	-0.00070	0.00241
15	$a_{\text{mo,so}}$	0.29111	-0.05252
	e.s.d.	0.00176	0.00273
	shift	-0.00153	0.00123
18	$a_{\text{mo,so}}$	0.24012	-0.58470
	e.s.d.	0.00446	0.00360
	shift	-0.00334	0.00330
21	$a_{\text{mo,so}}$	-0.02342	0.11318
	e.s.d.	0.01259	0.00792
	shift	-0.00190	0.00589
so	$C_{\text{so}}\text{pz}^+$		
59	$a_{\text{mo,so}}$	-0.10008	-0.07310
	e.s.d.	0.00428	0.00707
	shift	0.00424	0.00381
62	$a_{\text{mo,so}}$	-0.13235	-0.00306
	e.s.d.	0.00501	0.00520
	shift	0.00356	-0.00155
65	$a_{\text{mo,so}}$	-0.04097	-0.07032
	e.s.d.	0.00558	0.00870
	shift	-0.00203	0.00594
68	$a_{\text{mo,so}}$	-0.46378	-0.20586
	e.s.d.	0.00732	0.00770
	shift	-0.00113	0.00199
71	$a_{\text{mo,so}}$	0.12938	-0.08057

	e.s.d.	0.01211	0.01215
	shift	-0.00092	0.00183
so	O _{so} pz ⁺		
109	a _{mo,so}	-0.00343	-0.15811
	e.s.d.	0.00388	0.00161
	shift	-0.00148	-0.00057
112	a _{mo,so}	-0.13168	-0.18803
	e.s.d.	0.00288	0.00155
	shift	0.00011	-0.00020
115	a _{mo,so}	-0.18647	-0.13363
	e.s.d.	0.00464	0.00185
	shift	0.00007	-0.00071
118	a _{mo,so}	-0.13662	-0.36976
	e.s.d.	0.00806	0.00383
	shift	0.00512	0.00197
121	a _{mo,so}	0.31389	-0.05333
	e.s.d.	0.01087	0.00438
	shift	-0.01300	0.00209
a _{mo,so} -max		0.46378	0.58470
so-max		68	18

Table S2 (c) Coefficients($a_{\text{mo,so}}$), e.s.d.'s and shifts of b_g XMO-MOs

b_g	mo	19	23
	E(RHF)	-0.577	-0.377
	E(XMO)	-0.44193	-0.10304
	E(diag.)	-0.34427	-0.21921
so	$N_{\text{so}}\text{pz-}$		
30	$a_{\text{mo,so}}$	0.03440	0.19844
	e.s.d.	0.00476	0.00195
	shift	0.00398	0.00053
33	$a_{\text{mo,so}}$	0.07388	0.19732
	e.s.d.	0.00288	0.00137
	shift	0.00144	0.00077
36	$a_{\text{mo,so}}$	0.18463	0.17926
	e.s.d.	0.00312	0.00172
	shift	0.00285	0.00102
39	$a_{\text{mo,so}}$	0.16178	0.37656
	e.s.d.	0.00433	0.00263
	shift	0.00394	0.00119
42	$a_{\text{mo,so}}$	-0.08014	0.12441
	e.s.d.	0.01356	0.01087
	shift	0.00389	0.00565
so	$C_{\text{so}}\text{pz-}$		
80	$a_{\text{mo,so}}$	-0.12312	-0.01289
	e.s.d.	0.00276	0.02699
	shift	0.00001	-0.00730
83	$a_{\text{mo,so}}$	-0.12569	-0.07113
	e.s.d.	0.00467	0.02084
	shift	-0.00187	-0.00649
86	$a_{\text{mo,so}}$	-0.21426	0.05031
	e.s.d.	0.00586	0.00769
	shift	0.00208	0.00104
89	$a_{\text{mo,so}}$	-0.24437	0.01971
	e.s.d.	0.00555	0.00956
	shift	-0.00222	0.00032
92	$a_{\text{mo,so}}$	0.14912	-0.03327

	e.s.d.	0.01196	0.01201
	shift	-0.01094	-0.00151
so	O _{so} pz-		
130	a _{mo,so}	-0.13293	0.17216
	e.s.d.	0.00246	0.00157
	shift	-0.00207	0.00025
133	a _{mo,so}	-0.15150	0.23611
	e.s.d.	0.00159	0.00166
	shift	0.00019	0.00083
136	a _{mo,so}	-0.28300	0.11447
	e.s.d.	0.00191	0.00230
	shift	0.00102	0.00114
139	a _{mo,so}	-0.20635	0.18928
	e.s.d.	0.00520	0.00752
	shift	-0.00195	0.00381
142	a _{mo,so}	-0.00182	0.00410
	e.s.d.	0.00591	0.00809
	shift	0.00000	-0.00246
Max.	(a _{mo,so}) _{max}	-0.28300	0.37656
	so _{max}	136	39

Table S2 (d) Coefficients($a_{mo,so}$), e.s.d.'s and shifts of b_u XMO-MOs

b_u	mo	1	4	6	8	10	12	13	17	22
	E(RHF)	-20.55702	-15.66309	-11.39851	-1.42331	-1.17805	-0.89338	-0.78805	-0.63817	-0.46248
	E(XMO)	-20.16710	-14.99254	-11.16772	-1.19006	-0.52344	-0.24487	-0.05476	-0.50611	-0.24496
	E(diag.)	-20.37784	-15.03784	-11.22116	-1.27801	-0.93637	-0.63278	-0.58223	-0.50282	-0.22464
so	$N_{so,px+,py+}$									
7	$a_{mo,so}(px+)$	-0.00075	-0.00184	-0.00116	0.04311	-0.04150	-0.01703	-0.01515	-0.03107	0.00558
	e.s.d.	0.00000	0.00000	0.00000	0.00605	0.00418	0.00612	0.00902	0.02220	0.00420
	shift	0.00000	0.00000	0.00000	0.00202	0.00293	0.00123	0.00275	0.00585	0.00199
8	$a_{mo,so}(py+)$	0.00054	-0.00104	-0.00184	-0.03505	0.03728	-0.07025	-0.01784	0.02218	0.03607
	e.s.d.	0.00000	0.00000	0.00000	0.00964	0.00719	0.00269	0.01375	0.01089	0.00923
	shift	0.00000	0.00000	0.00000	-0.00257	0.00186	0.00088	-0.00553	-0.00155	-0.00528
10	$a_{mo,so}(px+)$	-0.00047	-0.00158	0.00151	0.06031	-0.05673	-0.00725	-0.03217	-0.01078	-0.00571
	e.s.d.	0.00000	0.00000	0.00000	0.00719	0.00335	0.00505	0.00751	0.01125	0.00538
	shift	0.00000	0.00000	0.00000	-0.00353	-0.00030	0.00182	0.00094	-0.00051	0.00310
11	$a_{mo,so}(py+)$	0.00151	-0.00224	-0.00620	-0.06037	0.03565	-0.19722	-0.04375	0.04241	0.02802
	e.s.d.	0.00000	0.00000	0.00000	0.00762	0.00387	0.00242	0.01342	0.01038	0.00905
	shift	0.00000	0.00000	0.00000	0.00304	0.00384	-0.00039	0.00965	0.00209	-0.00185
13	$a_{mo,so}(px+)$	-0.00256	-0.00302	0.00651	0.03473	-0.11392	-0.04493	-0.02472	0.11146	-0.02232
	e.s.d.	0.00000	0.00000	0.00000	0.00578	0.00382	0.00477	0.00773	0.01447	0.00675
	shift	0.00000	0.00000	0.00000	0.00067	-0.00210	0.00228	0.00227	0.00423	-0.00489
14	$a_{mo,so}(py+)$	0.00096	0.00069	-0.00896	-0.09311	0.03418	-0.27827	0.09797	0.10753	0.08402
	e.s.d.	0.00000	0.00000	0.00000	0.01074	0.00297	0.00384	0.01149	0.00865	0.00756

	shift	0.00000	0.00000	0.00000	0.00464	0.00239	-0.00211	0.00807	-0.00498	0.00340
16	$a_{\text{mo,so}}(\text{px}^+)$	0.00459	-0.01055	0.00645	0.03010	-0.01584	-0.02722	-0.21717	0.08548	0.01379
	e.s.d.	0.00000	0.00000	0.00000	0.01027	0.00465	0.00718	0.01224	0.01123	0.01231
	shift	0.00000	0.00000	0.00000	0.00655	-0.00003	0.00253	0.00209	0.01078	-0.00786
17	$a_{\text{mo,so}}(\text{py}^+)$	-0.00008	-0.00216	-0.00166	-0.02159	-0.01789	-0.19971	0.08446	0.02673	-0.03032
	e.s.d.	0.00000	0.00000	0.00000	0.01101	0.00669	0.00891	0.00838	0.01183	0.01162
	shift	0.00000	0.00000	0.00000	-0.00045	0.00454	0.00432	0.00316	-0.00835	0.00010
19	$a_{\text{mo,so}}(\text{px}^+)$	-0.00700	-0.00221	-0.00778	0.07079	-0.06463	-0.02138	0.00578	-0.02072	0.14629
	e.s.d.	0.00000	0.00000	0.00000	0.01552	0.00659	0.01037	0.00563	0.01616	0.01313
	shift	0.00000	0.00000	0.00000	0.00034	-0.00118	0.00941	-0.00215	0.00460	0.00546
20	$a_{\text{mo,so}}(\text{py}^+)$	-0.00117	-0.00416	-0.00606	-0.00345	-0.07997	-0.02666	0.01345	0.02678	0.12323
	e.s.d.	0.00000	0.00000	0.00000	0.01452	0.01137	0.00467	0.01212	0.00827	0.00910
	shift	0.00000	0.00000	0.00000	0.00000	0.00235	0.00689	0.00136	-0.00740	0.00798
so	$N_{\text{soS-}}$									
22	$a_{\text{mo,so}}$	0.00118	-0.98776	0.00194	0.01472	0.02056	0.00607	-0.08211	0.00412	-0.00130
	e.s.d.	0.00000	0.00000	0.00000	0.01192	0.00635	0.00665	0.01831	0.02205	0.01672
	shift	0.00000	0.00000	0.00000	-0.00152	-0.00328	0.00080	0.00089	0.00000	-0.00461
23	$a_{\text{mo,so}}$	-0.00738	-0.00256	-0.00231	0.05815	-0.24456	-0.07965	0.05843	0.00165	-0.04774
	e.s.d.	0.00000	0.00000	0.00000	0.01091	0.00700	0.01021	0.01444	0.01807	0.01958
	shift	0.00000	0.00000	0.00000	-0.00094	-0.00038	-0.00552	0.00144	0.00000	0.00741
24	$a_{\text{mo,so}}$	-0.00048	0.02159	0.00174	0.04150	-0.07147	-0.02091	-0.04635	0.00627	-0.03831
	e.s.d.	0.00000	0.00000	0.00000	0.00943	0.00672	0.00341	0.00937	0.01357	0.01313
	shift	0.00000	0.00000	0.00000	-0.00147	-0.00332	-0.00088	-0.00133	0.00536	0.00397

25	$a_{\text{mo,so}}$	-0.00727	-0.00989	0.00282	0.11634	-0.29306	-0.11636	-0.04824	0.03145	-0.04217
	e.s.d.	0.00000	0.00000	0.00000	0.00596	0.00459	0.00389	0.01136	0.01151	0.01285
	shift	0.00000	0.00000	0.00000	0.00459	-0.00062	-0.00327	0.00038	0.00823	0.00168
26	$a_{\text{mo,so}}$	-0.00088	0.00077	0.00028	0.06713	-0.11089	-0.15130	-0.00095	-0.04113	-0.12756
	e.s.d.	0.00000	0.00000	0.00000	0.00585	0.00430	0.00339	0.00453	0.01186	0.01849
	shift	0.00000	0.00000	0.00000	0.00123	-0.00103	-0.00201	-0.00203	0.00918	-0.00043
27	$a_{\text{mo,so}}$	0.00237	0.00136	0.00423	-0.00858	-0.00914	0.01972	-0.00357	0.01389	-0.11281
	e.s.d.	0.00000	0.00000	0.00000	0.00548	0.00474	0.00794	0.00362	0.01018	0.01140
	shift	0.00000	0.00000	0.00000	-0.00276	-0.00207	-0.00723	0.00000	0.00656	-0.00745
so	H(N) _{so} S-									
47	$a_{\text{mo,so}}$	0.00059	0.00157	0.00240	-0.01162	0.03961	0.06749	0.01552	0.01159	0.09049
	e.s.d.	0.00000	0.00000	0.00000	0.01852	0.00602	0.00309	0.01286	0.00753	0.02539
	shift	0.00000	0.00000	0.00000	-0.02081	0.00050	0.00149	0.01313	-0.00276	0.00393
48	$a_{\text{mo,so}}$	0.00015	0.00438	0.00603	0.05719	0.11788	0.28866	0.05820	-0.13630	0.01458
	e.s.d.	0.00000	0.00000	0.00000	0.02133	0.00680	0.00306	0.01979	0.01279	0.00991
	shift	0.00000	0.00000	0.00000	-0.01239	0.00232	0.00256	-0.00318	-0.00567	0.00352
49	$a_{\text{mo,so}}$	-0.00239	0.00755	-0.00318	-0.09695	-0.01743	-0.05126	-0.00215	-0.02998	-0.42237
	e.s.d.	0.00000	0.00000	0.00000	0.01759	0.00984	0.00394	0.00969	0.01229	0.01770
	shift	0.00000	0.00000	0.00000	0.01094	-0.00086	0.00183	0.00507	-0.00349	-0.00170
50	$a_{\text{mo,so}}$	-0.00157	0.00155	-0.00574	-0.02129	0.00746	0.00503	0.04219	-0.00324	0.08097
	e.s.d.	0.00000	0.00000	0.00000	0.01295	0.01888	0.01381	0.02622	0.03100	0.01326
	shift	0.00000	0.00000	0.00000	0.00416	0.00089	0.00000	-0.00026	0.00000	0.00333

so	C _{so} px+,py+									
57	$a_{\text{mo,so}}(\text{px}^+)$	0.00261	-0.00385	0.00311	0.04451	-0.02662	0.02548	-0.04793	0.02232	0.00522
	e.s.d.	0.00000	0.00000	0.00000	0.00707	0.00854	0.00973	0.00406	0.00413	0.00174
	shift	0.00000	0.00000	0.00000	0.00016	-0.00099	-0.00069	0.00269	0.00030	0.00130
58	$a_{\text{mo,so}}(\text{py}^+)$	0.00472	0.00016	0.00295	-0.01195	0.04078	-0.00359	0.01611	0.03681	0.00210
	e.s.d.	0.00000	0.00000	0.00000	0.00997	0.00540	0.00819	0.00915	0.00281	0.00732
	shift	0.00000	0.00000	0.00000	-0.00115	-0.00017	0.00000	0.00004	0.00131	0.00000
60	$a_{\text{mo,so}}(\text{px}^+)$	0.00692	-0.01076	0.00948	0.09116	0.01702	0.00673	-0.15878	0.04507	-0.02622
	e.s.d.	0.00000	0.00000	0.00000	0.00692	0.00777	0.01160	0.00367	0.00759	0.00439
	shift	0.00000	0.00000	0.00000	0.00397	-0.00288	0.01244	0.00262	-0.00058	-0.00173
61	$a_{\text{mo,so}}(\text{py}^+)$	0.00738	-0.00162	0.00663	-0.02282	0.03664	0.00476	0.03520	0.14546	0.00073
	e.s.d.	0.00000	0.00000	0.00000	0.00350	0.00505	0.00505	0.00594	0.00411	0.00584
	shift	0.00000	0.00000	0.00000	0.00627	0.00165	0.00000	0.00051	0.00287	-0.00470
63	$a_{\text{mo,so}}(\text{px}^+)$	0.00524	-0.01400	0.01158	0.01392	-0.08987	0.06227	-0.17152	0.15303	-0.04664
	e.s.d.	0.00000	0.00000	0.00000	0.00691	0.00905	0.00930	0.00246	0.00720	0.00665
	shift	0.00000	0.00000	0.00000	0.00858	-0.00406	0.00165	0.00221	0.00177	-0.00832
64	$a_{\text{mo,so}}(\text{py}^+)$	0.01861	0.00223	0.01498	-0.06338	0.33521	-0.10666	-0.00678	0.23792	0.08060
	e.s.d.	0.00000	0.00000	0.00000	0.00442	0.00260	0.00893	0.00610	0.00267	0.00594
	shift	0.00000	0.00000	0.00000	0.00416	0.00237	0.00372	0.00437	0.00493	-0.00396
66	$a_{\text{mo,so}}(\text{px}^+)$	-0.00145	-0.00450	0.00651	-0.03179	-0.00145	0.01587	-0.03908	0.08094	-0.00779
	e.s.d.	0.00000	0.00000	0.00000	0.01410	0.00537	0.00689	0.00560	0.00451	0.00523
	shift	0.00000	0.00000	0.00000	0.00166	-0.00020	0.00026	0.00915	0.00592	0.00306
67	$a_{\text{mo,so}}(\text{py}^+)$	-0.00948	-0.00723	0.00000	-0.01291	-0.36578	-0.05193	0.14354	0.11850	-0.01052

	e.s.d.	0.00000	0.00000	0.00000	0.00596	0.00721	0.01007	0.00773	0.00530	0.00714
	shift	0.00000	0.00000	0.00000	-0.00005	-0.00496	-0.00399	0.00589	0.00792	0.00095
69	$a_{mo,so}(px+)$	-0.00425	-0.00410	0.00040	-0.02724	-0.18199	-0.11622	0.05409	0.09107	-0.07632
	e.s.d.	0.00000	0.00000	0.00000	0.02458	0.02952	0.01956	0.01500	0.01803	0.01840
	shift	0.00000	0.00000	0.00000	0.00068	0.00334	-0.01003	0.00338	-0.00910	-0.00971
70	$a_{mo,so}(py+)$	0.00572	-0.00157	0.00121	0.00097	0.09337	-0.04157	-0.15559	0.01078	0.00738
	e.s.d.	0.00000	0.00000	0.00000	0.00414	0.01224	0.01317	0.00777	0.00897	0.00525
	shift	0.00000	0.00000	0.00000	0.00364	0.00183	-0.01436	-0.00193	0.01424	0.00080
so	C_{soS-}									
72	$a_{mo,so}$	-0.00019	-0.00076	-0.98945	0.02158	-0.03418	-0.01534	0.01608	-0.02818	0.02967
	e.s.d.	0.00000	0.00000	0.00000	0.01532	0.01143	0.02093	0.00703	0.01039	0.01578
	shift	0.00000	0.00000	0.00000	-0.00269	0.00313	0.00051	-0.00079	-0.00162	-0.00841
73	$a_{mo,so}$	0.00748	0.00149	0.00979	0.09633	-0.15919	0.04186	0.14982	0.00303	0.01601
	e.s.d.	0.00000	0.00000	0.00000	0.00676	0.00942	0.02644	0.00445	0.00551	0.01051
	shift	0.00000	0.00000	0.00000	0.00406	-0.00242	-0.00518	0.00173	0.00000	0.00115
74	$a_{mo,so}$	0.00141	0.00070	-0.02347	0.02039	-0.02068	-0.00901	0.03773	-0.00368	-0.00462
	e.s.d.	0.00000	0.00000	0.00000	0.00994	0.00678	0.00570	0.00313	0.00468	0.00582
	shift	0.00000	0.00000	0.00000	0.00300	0.00122	0.00199	0.00312	0.00000	0.00000
75	$a_{mo,so}$	0.00724	0.01147	0.03366	0.13911	-0.29592	0.19298	0.27444	0.19012	-0.15517
	e.s.d.	0.00000	0.00000	0.00000	0.00937	0.00798	0.00917	0.00341	0.00340	0.00649
	shift	0.00000	0.00000	0.00000	-0.00816	-0.00747	-0.00319	0.00004	-0.00386	0.00774
76	$a_{mo,so}$	-0.00283	0.00277	0.00990	-0.00447	-0.11035	0.03409	0.08066	0.09232	0.00333
	e.s.d.	0.00000	0.00000	0.00000	0.00403	0.00595	0.00962	0.00499	0.00780	0.00678

	shift	0.00000	0.00000	0.00000	0.00000	0.00373	0.00224	0.00083	-0.00751	0.00000
77	$a_{\text{mo,so}}$	-0.00561	-0.00573	0.00223	-0.01831	-0.22093	-0.06575	0.09013	0.06761	0.01618
	e.s.d.	0.00000	0.00000	0.00000	0.01191	0.01344	0.01621	0.00624	0.01104	0.01099
	shift	0.00000	0.00000	0.00000	-0.00017	0.01180	0.00455	0.00432	-0.00933	0.00712
so	H(C) _{so} S-									
97	H ₉₇ S-	0.00079	-0.00370	-0.00022	-0.02457	0.02130	0.01738	-0.08489	0.03001	0.00612
	e.s.d.	0.00000	0.00000	0.00000	0.01170	0.00557	0.04608	0.00476	0.01819	0.00551
	shift	0.00000	0.00000	0.00000	-0.00080	0.00201	-0.01484	-0.00080	-0.01163	-0.00371
98	H ₉₈ S-	0.00487	-0.01838	0.00237	-0.05429	0.12067	0.05247	-0.38645	0.06563	-0.02280
	e.s.d.	0.00000	0.00000	0.00000	0.02532	0.00988	0.03523	0.00280	0.00918	0.00475
	shift	0.00000	0.00000	0.00000	-0.00489	0.00153	-0.00465	-0.00253	0.00620	-0.00079
99	H ₉₉ S-	0.00121	0.00165	0.01049	-0.05447	-0.02742	-0.12003	0.02409	0.02892	-0.46283
	e.s.d.	0.00000	0.00000	0.00000	0.01986	0.01255	0.02802	0.00255	0.00753	0.00650
	shift	0.00000	0.00000	0.00000	-0.03239	0.01252	-0.01042	-0.00067	-0.00304	-0.00360
100	H ₁₀₀ S-	-0.00101	0.00096	0.00062	-0.02660	-0.01980	0.03094	0.00805	0.00272	0.00929
	e.s.d.	0.00000	0.00000	0.00000	0.02506	0.00682	0.02208	0.00493	0.00899	0.00744
	shift	0.00000	0.00000	0.00000	-0.00246	0.00872	-0.00493	-0.00039		-0.00370
so	O _{so} px ⁺ ,py ⁺									
107	$a_{\text{mo,so}}(\text{px}^+)$	-0.00068	-0.00515	-0.00326	-0.00662	0.02375	0.05100	-0.07250	-0.02066	0.13722
	e.s.d.	0.00000	0.00000	0.00000	0.00377	0.00572	0.00932	0.00364	0.00591	0.00215
	shift	0.00000	0.00000	0.00000	-0.00133	-0.00238	0.00469	0.00178	0.00105	0.00029
108	$a_{\text{mo,so}}(\text{py}^+)$	-0.00128	0.00269	-0.00612	0.01358	-0.00376	-0.05672	-0.02774	-0.07280	-0.08459

	e.s.d.	0.00000	0.00000	0.00000	0.00439	0.00424	0.00535	0.00755	0.00325	0.00416
	shift	0.00000	0.00000	0.00000	-0.00245	-0.00268	-0.00307	-0.00360	-0.00046	0.00016
110	$a_{\text{mo,so}}(\text{px}^+)$	-0.00164	-0.00798	-0.00399	-0.01406	0.02803	0.04352	-0.14054	-0.08427	0.17843
	e.s.d.	0.00000	0.00000	0.00000	0.00241	0.00367	0.00770	0.00527	0.00432	0.00222
	shift	0.00000	0.00000	0.00000	-0.00095	-0.00288	0.00579	-0.00125	-0.00294	0.00187
111	$a_{\text{mo,so}}(\text{py}^+)$	-0.00456	0.00339	-0.01112	-0.00883	-0.02087	-0.08912	-0.05844	-0.12696	-0.06705
	e.s.d.	0.00000	0.00000	0.00000	0.00350	0.00414	0.00481	0.00744	0.00171	0.00474
	shift	0.00000	0.00000	0.00000	-0.00185	-0.00325	0.00106	-0.00627	-0.00167	-0.00007
113	$a_{\text{mo,so}}(\text{px}^+)$	-0.00536	-0.00782	-0.00481	-0.02147	0.00984	0.04836	-0.12687	-0.11059	0.21201
	e.s.d.	0.00000	0.00000	0.00000	0.00160	0.00341	0.00964	0.00294	0.00301	0.00187
	shift	0.00000	0.00000	0.00000	-0.00133	-0.00337	0.00238	-0.00330	-0.00457	0.00182
114	$a_{\text{mo,so}}(\text{py}^+)$	-0.01071	0.00765	-0.02700	-0.08268	-0.04347	-0.13217	0.01040	-0.33031	-0.10057
	e.s.d.	0.00000	0.00000	0.00000	0.00221	0.00337	0.00793	0.00743	0.00340	0.00513
	shift	0.00000	0.00000	0.00000	-0.00209	-0.00381	0.00058	-0.00158	-0.00262	0.00086
116	$a_{\text{mo,so}}(\text{px}^+)$	-0.00102	-0.00680	-0.00844	0.00166	0.01079	0.06382	-0.06302	-0.03392	0.42701
	e.s.d.	0.00000	0.00000	0.00000	0.00914	0.00555	0.01746	0.00761	0.00656	0.00294
	shift	0.00000	0.00000	0.00000	0.00000	-0.00678	0.00257	-0.00351	-0.00660	0.00375
117	$a_{\text{mo,so}}(\text{py}^+)$	-0.00559	0.00261	-0.00455	0.03240	-0.16639	-0.08989	0.08075	-0.08449	-0.16632
	e.s.d.	0.00000	0.00000	0.00000	0.00405	0.00659	0.01097	0.00900	0.00590	0.00795
	shift	0.00000	0.00000	0.00000	-0.00560	-0.00927	0.00788	-0.00348	-0.00400	-0.00234
119	$a_{\text{mo,so}}(\text{px}^+)$	0.00194	-0.00607	0.00453	-0.03050	0.06562	-0.13610	-0.15323	0.00578	-0.04648
	e.s.d.	0.00000	0.00000	0.00000	0.01186	0.01684	0.01549	0.01079	0.01282	0.00961
	shift	0.00000	0.00000	0.00000	0.00578	0.00258	-0.00677	0.00272	-0.00087	-0.00575

120	$a_{\text{mo,so}}(\text{py}^+)$	-0.00269	0.00351	-0.00311	0.01134	-0.00640	0.08744	0.05622	-0.04845	-0.02290
	e.s.d.	0.00000	0.00000	0.00000	0.02785	0.00564	0.00954	0.01160	0.00605	0.00909
	shift	0.00000	0.00000	0.00000	0.00000	-0.00477	0.00008	0.00127	-0.00353	-0.00023
so	$O_{\text{soS-}}$									
122	$a_{\text{mo,so}}$	0.99467	-0.00029	0.00153	-0.00197	0.02145	0.01503	0.00865	0.00726	-0.00588
	e.s.d.	0.00000	0.00000	0.00000	0.00974	0.01625	0.01116	0.01095	0.00701	0.00586
	shift	0.00000	0.00000	0.00000	0.00646	-0.00546	0.00109	0.00299	-0.00101	-0.00103
123	$a_{\text{mo,so}}$	0.02704	-0.01368	-0.00215	0.21489	0.09216	-0.07290	-0.02802	-0.12082	-0.00422
	e.s.d.	0.00000	0.00000	0.00000	0.01037	0.01192	0.01222	0.01136	0.00796	0.00482
	shift	0.00000	0.00000	0.00000	0.00354	0.00304	0.00003	-0.00342	0.00038	-0.00021
124	$a_{\text{mo,so}}$	-0.00415	-0.00528	-0.00335	0.08155	0.05963	-0.04143	-0.02613	-0.06112	-0.00971
	e.s.d.	0.00000	0.00000	0.00000	0.00321	0.00385	0.00633	0.00593	0.00491	0.00404
	shift	0.00000	0.00000	0.00000	0.00061	-0.00097	-0.00142	0.00197	-0.00429	0.00165
125	$a_{\text{mo,so}}$	0.06397	-0.02980	0.01821	0.59063	0.28054	-0.05980	-0.01170	-0.15082	-0.01978
	e.s.d.	0.00000	0.00000	0.00000	0.00363	0.00235	0.00487	0.00438	0.00251	0.00362
	shift	0.00000	0.00000	0.00000	-0.00017	-0.00299	-0.00390	-0.00269	-0.00219	0.00065
126	$a_{\text{mo,so}}$	0.03069	-0.00657	-0.00889	0.18036	0.24158	-0.05438	-0.00392	-0.16269	-0.03093
	e.s.d.	0.00000	0.00000	0.00000	0.00358	0.00559	0.00453	0.00450	0.00325	0.00378
	shift	0.00000	0.00000	0.00000	-0.00053	-0.00012	-0.00028	-0.00317	-0.00539	0.00364
127	$a_{\text{mo,so}}$	0.01203	0.00115	-0.00499	0.05237	0.36828	-0.05202	-0.11611	-0.14249	0.00942
	e.s.d.	0.00000	0.00000	0.00000	0.00534	0.00828	0.01434	0.00881	0.00556	0.00378
	shift	0.00000	0.00000	0.00000	0.00626	-0.00202	0.00409	0.00097	-0.01038	0.00153
$a_{\text{mo,so}}\text{-max}$		0.99467	0.98776	0.98945	0.59063	0.36828	0.28866	0.38645	0.33031	0.46283

so-max	122	22	72	125	127	48	98	114	99
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Fig. S1 (deposited) Electron densities, (mo-1) $\rho_{m_o}^{XMO}(\mathbf{r})$, (mo-2) $\delta\rho_{m_o}(\mathbf{r})$ and (mo-3) $\rho_{m_o}^{RHF}(\mathbf{r})$ on the molecular plane for all MOs (mo=1 to 23). Contours are written in parentheses.

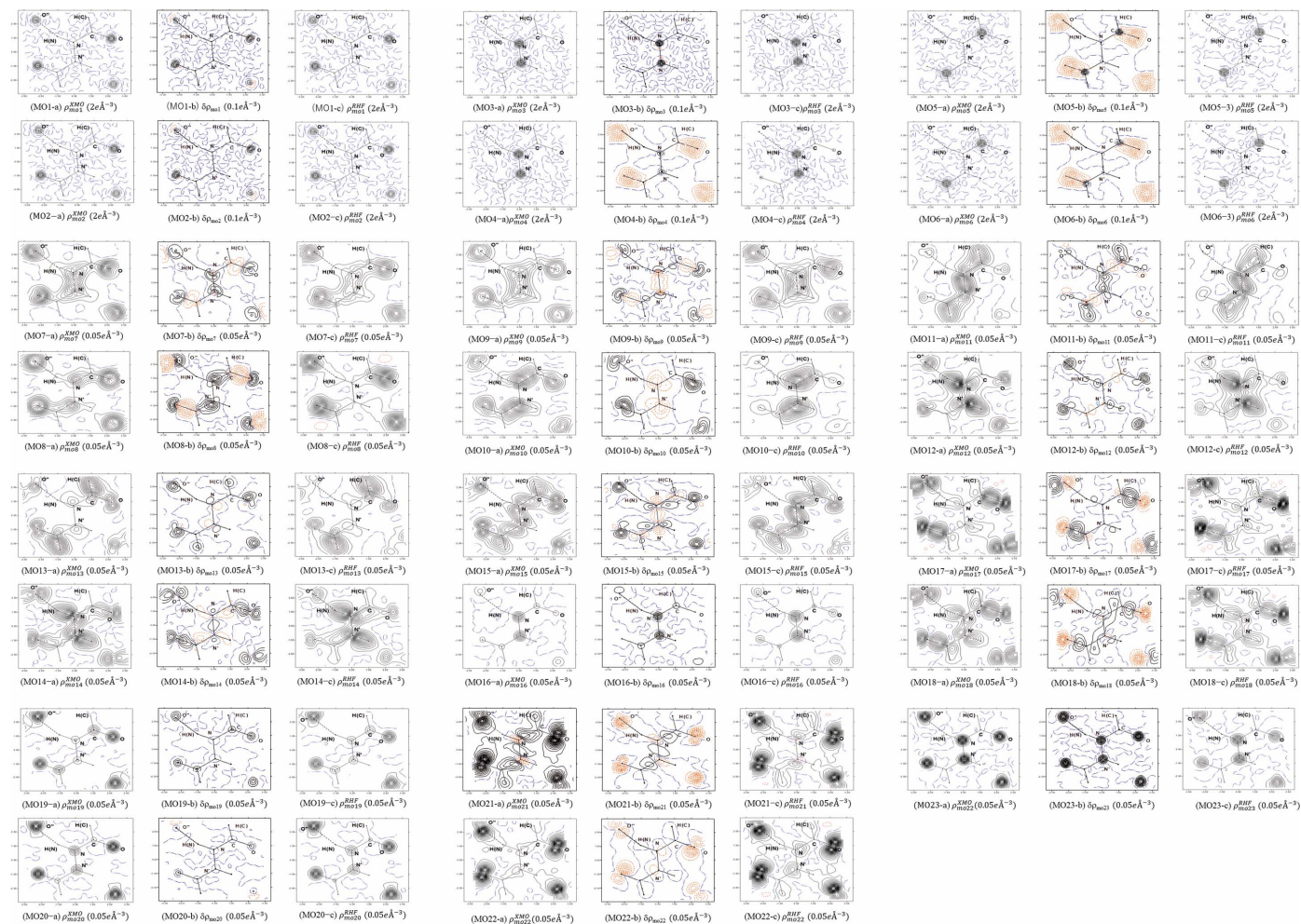


Fig. S2 (deposited) $\rho_{mo}^{XMO}(\mathbf{r})$ of MO7 to 23 are illustrated on the H-bond plane. Contours are the same as those in Fig. 1.

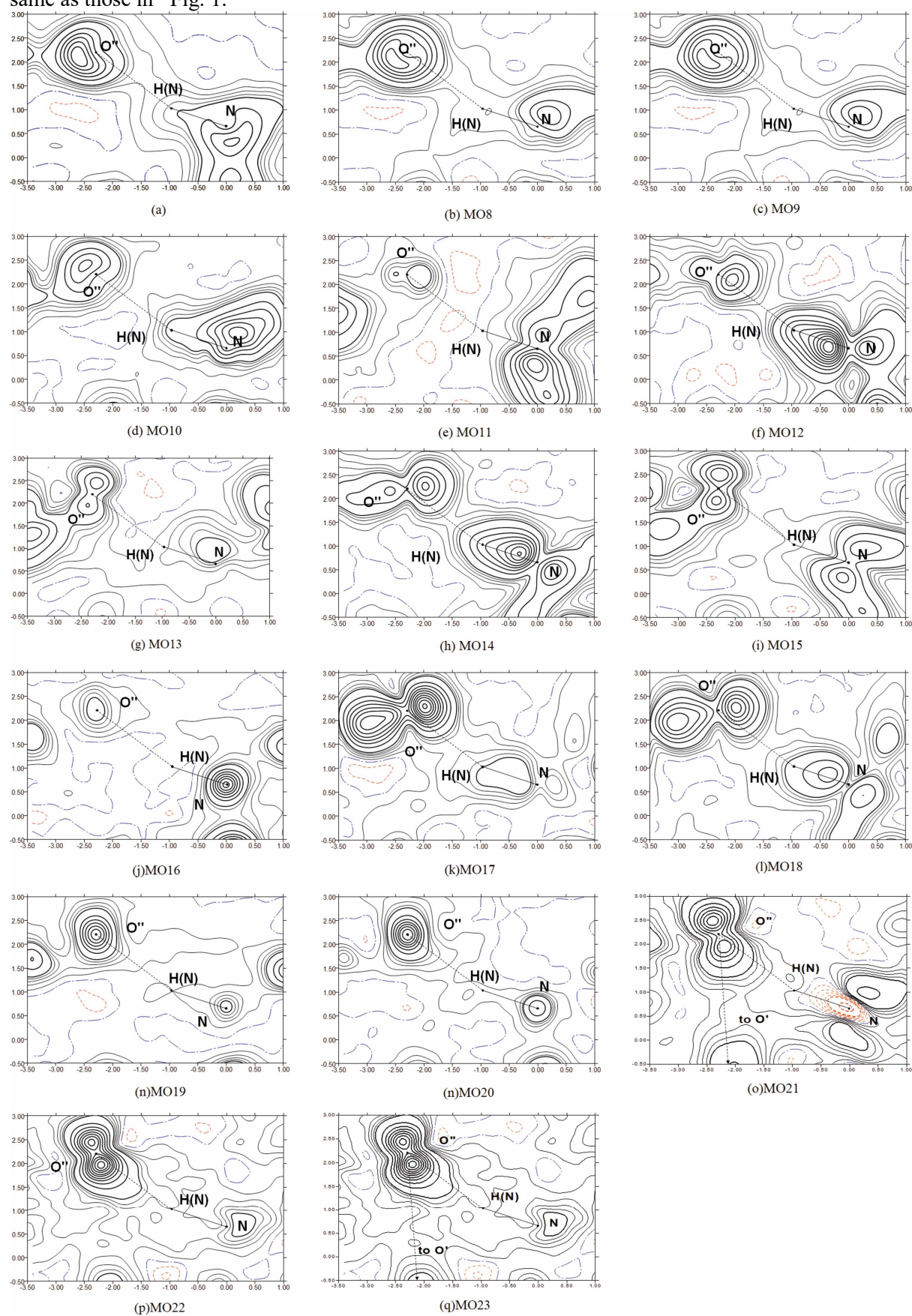


Fig. S3 (deposited) $\rho_{19}^{XMO}(\mathbf{r})$ (top) on the π -bond plane including (a) N'-N, (b) N-C and (c) C=O bonds and $dr_{\text{no}}(\mathbf{r})$ (bottom) including (d) N'-N, (e) N-C and (f) C=O bonds. Contours are the same as those in Fig.1.

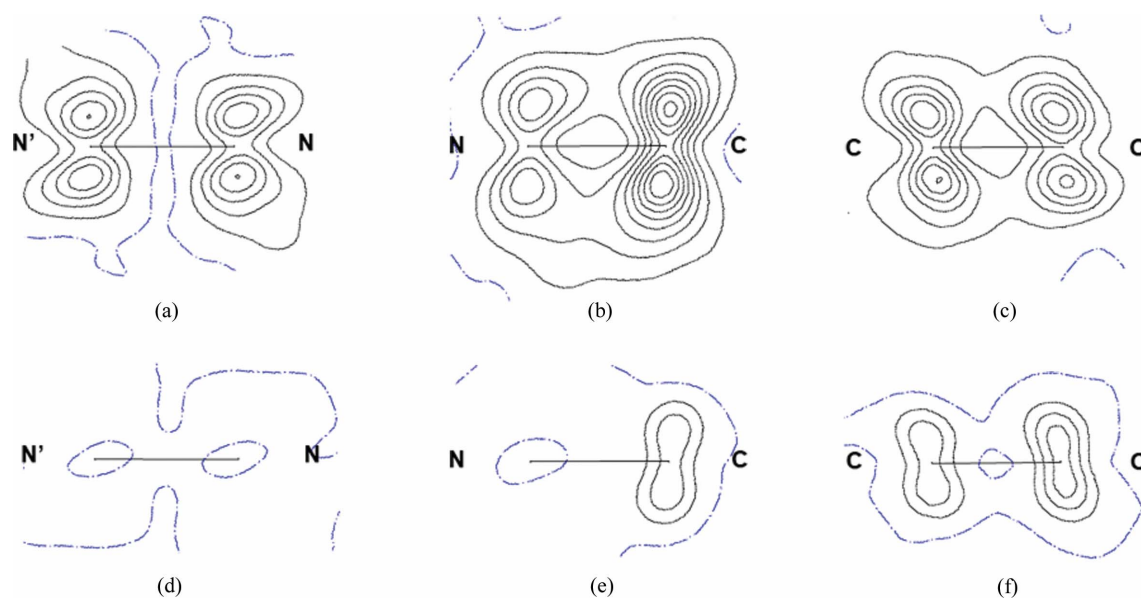


Fig. S4 (deposited) $\rho_{20}^{XMO}(\mathbf{r})$ (top) of on the π -bond plane including (a) N'-N, (b) N-C and (c) C=O bonds and $dr_{\text{no}}(\mathbf{r})$ (bottom) including (d) N'-N, (e) N-C and (f) C=O bonds. Contours are the same as those in Fig.1.

