

Molecule	molecule number	calculation	charge	spin	method	basis set	solvation (dielectric)	output file	input file
FeAB	01	FeAB cc C-fac OPT	-3	6	B3LYP-D3(BJ)	cc-pVDZ	cpcm (78.39)	C_FeABO_ccl_3sextet_SfS_b3lypD3bj_ccpVDZ_pcmH2O_opt.out	C_FeABO_ccl_3sextet_SfS_b3lypD3bj_ccpVDZ_pcmH2O_opt.in
FeAB	01	FeAB cc C-fac TDDFT	-3	6	B3LYP-D3(BJ)	cc-pVDZ	cpcm (78.39)	C_FeABO_ccl_3sextet_SfS_camb3lyp_augccpVDZ_pcmH2O_tddft100.out	C_FeABO_ccl_3sextet_SfS_camb3lyp_augccpVDZ_pcmH2O_tddft100.in
FeAB	02	FeAB cc N-fac OPT	-3	6	B3LYP-D3(BJ)	cc-pVDZ	cpcm (78.39)	C_FeABO_N_ccl_3sextet_SfS_b3lypD3bj_ccpVDZ_pcmH2O_opt_5.out	C_FeABO_N_ccl_3sextet_SfS_b3lypD3bj_ccpVDZ_pcmH2O_opt_5.in
FeAB	02	FeAB cc N-fac TDDFT	-3	6	B3LYP-D3(BJ)	cc-pVDZ	cpcm (78.39)	C_FeABO_N_ccl_3sextet_SfS_camb3lyp_augccpVDZ_pcmH2O_tddft100_2.out	C_FeABO_N_ccl_3sextet_SfS_camb3lyp_augccpVDZ_pcmH2O_tddft100_2.in
FeAB	03	FeAB ct C-mer OPT	-3	6	B3LYP-D3(BJ)	cc-pVDZ	cpcm (78.39)	C_FeABO_ctl_C_3sextet_SfS_b3lypD3bj_ccpVDZ_pcmH2O_opt_2.out	C_FeABO_ctl_C_3sextet_SfS_b3lypD3bj_ccpVDZ_pcmH2O_opt_2.in
FeAB	03	FeAB ct C-mer TDDFT	-3	6	B3LYP-D3(BJ)	cc-pVDZ	cpcm (78.39)	C_FeABO_ctl_C_3sextet_SfS_camb3lyp_augccpVDZ_pcmH2O_tddft100.out	C_FeABO_ctl_C_3sextet_SfS_camb3lyp_augccpVDZ_pcmH2O_tddft100.in
FeAB	04	FeAB ct N-mer OPT	-3	6	B3LYP-D3(BJ)	cc-pVDZ	cpcm (78.39)	C_FeABO_ctl_3sextet_SfS_b3lypD3bj_ccpVDZ_pcmH2O_opt_2.out	C_FeABO_ctl_3sextet_SfS_b3lypD3bj_ccpVDZ_pcmH2O_opt_2.in
FeAB	04	FeAB ct N-mer TDDFT	-3	6	B3LYP-D3(BJ)	cc-pVDZ	cpcm (78.39)	C_FeABO_ctl_3sextet_SfS_camb3lyp_augccpVDZ_pcmH2O_tddft100.out	C_FeABO_ctl_3sextet_SfS_camb3lyp_augccpVDZ_pcmH2O_tddft100.in
FeAB* enol	09	FeAB* enol cc C-fac OPT	-2	6	CAM-B3LYP	aug-ccpVDZ	cpcm (78.39)	C_FeABstar2_enol_ccl_2sextet_SkS_b3lypD3bj_ccpVDZ_pcmH2O_opt_2.out	C_FeABstar2_enol_ccl_2sextet_SkS_b3lypD3bj_ccpVDZ_pcmH2O_opt_2.in
FeAB* enol	09	FeAB* enol cc C-fac TDDFT	-2	6	CAM-B3LYP	aug-ccpVDZ	cpcm (78.39)	C_FeABstar2_enol_ccl_2sextet_SkS_camb3lyp_augccpVDZ_pcmH2O_tddft100.out	C_FeABstar2_enol_ccl_2sextet_SkS_camb3lyp_augccpVDZ_pcmH2O_tddft100.in
FeAB* enol	10	FeAB* enol cc N-fac OPT	-2	6	CAM-B3LYP	aug-ccpVDZ	cpcm (78.39)	C_FeABstar_enol_ccl_2sextet_SkS_b3lypD3bj_ccpVDZ_pcmH2O_opt.out	C_FeABstar_enol_ccl_2sextet_SkS_b3lypD3bj_ccpVDZ_pcmH2O_opt.in
FeAB* enol	10	FeAB* enol cc N-fac TDDFT	-2	6	CAM-B3LYP	aug-ccpVDZ	cpcm (78.39)	C_FeABstar_enol_ccl_2sextet_SkS_camb3lyp_augccpVDZ_pcmH2O_tddft100.out	C_FeABstar_enol_ccl_2sextet_SkS_camb3lyp_augccpVDZ_pcmH2O_tddft100.in
FeAB* enol	11	FeAB* enol cc C-mer OPT	-2	6	CAM-B3LYP	aug-ccpVDZ	cpcm (78.39)	C_FeABstar_enol_ctl_C_3sextet_SkS_b3lypD3bj_ccpVDZ_pcmH2O_opt.out	C_FeABstar_enol_ctl_C_3sextet_SkS_b3lypD3bj_ccpVDZ_pcmH2O_opt.in
FeAB* enol	11	FeAB* enol cc C-mer TDDFT	-2	6	CAM-B3LYP	aug-ccpVDZ	cpcm (78.39)	C_FeABstar_enol_ctl_C_3sextet_SkS_camb3lyp_augccpVDZ_pcmH2O_tddft100.out	C_FeABstar_enol_ctl_C_3sextet_SkS_camb3lyp_augccpVDZ_pcmH2O_tddft100.in
FeAB* enol	12	FeAB* enol cc N-mer OPT	-2	6	CAM-B3LYP	aug-ccpVDZ	cpcm (78.39)	C_FeABstar_enol_ctl_N_3sextet_SkS_b3lypD3bj_ccpVDZ_pcmH2O_opt.out	C_FeABstar_enol_ctl_N_3sextet_SkS_b3lypD3bj_ccpVDZ_pcmH2O_opt.in
FeAB* enol	12	FeAB* enol cc N-mer TDDFT	-2	6	CAM-B3LYP	aug-ccpVDZ	cpcm (78.39)	C_FeABstar_enol_ctl_N_3sextet_SkS_camb3lyp_augccpVDZ_pcmH2O_tddft100.out	C_FeABstar_enol_ctl_N_3sextet_SkS_camb3lyp_augccpVDZ_pcmH2O_tddft100.in
FePB	13	cc l-front -opt	-3	6	B3LYP-D3(BJ)	cc-pVDZ	cpcm (78.39)	C_FePB_ccl_3sextet_b3lypD3bj_ccpVDZ_pcmH2O_opt.out	C_FePB_ccl_3sextet_b3lypD3bj_ccpVDZ_pcmH2O_opt.in
FePB	13	cc l-front -tdfft	-3	6	B3LYP-D3(BJ)	cc-pVDZ	cpcm (78.39)	C_FePB_ccl_3sextet_camb3lyp_augccpVDZ_pcmH2O_tddft100.out	C_FePB_ccl_3sextet_camb3lyp_augccpVDZ_pcmH2O_tddft100.in
FePB	14	cc s-front -opt	-3	6	B3LYP-D3(BJ)	cc-pVDZ	cpcm (78.39)	C_FePB2_ccl_3sextet_b3lypD3bj_ccpVDZ_pcmH2O_opt_4.out	C_FePB2_ccl_3sextet_b3lypD3bj_ccpVDZ_pcmH2O_opt_4.in
FePB	14	cc s-front -tdfft	-3	6	B3LYP-D3(BJ)	cc-pVDZ	cpcm (78.39)	C_FePB2_ccl_3sextet_camb3lyp_augccpVDZ_pcmH2O_tddft100_4.out	C_FePB2_ccl_3sextet_camb3lyp_augccpVDZ_pcmH2O_tddft100_4.in
FePB	15	ct l-trans -opt	-3	6	B3LYP-D3(BJ)	cc-pVDZ	cpcm (78.39)	C_FePB_ctl2_3sextet_b3lypD3bj_ccpVDZ_pcmH2O_opt_2.out	C_FePB_ctl2_3sextet_b3lypD3bj_ccpVDZ_pcmH2O_opt_2.in
FePB	15	ct l-trans -tdfft	-3	6	B3LYP-D3(BJ)	cc-pVDZ	cpcm (78.39)	C_FePB_ctl2_3sextet_camb3lyp_augccpVDZ_pcmH2O_tddft100.out	C_FePB_ctl2_3sextet_camb3lyp_augccpVDZ_pcmH2O_tddft100.in
FePB	16	ct s-trans -opt	-3	6	B3LYP-D3(BJ)	cc-pVDZ	cpcm (78.39)	C_FePB_ctl_3sextet_b3lypD3bj_ccpVDZ_pcmH2O_opt.out	C_FePB_ctl_3sextet_b3lypD3bj_ccpVDZ_pcmH2O_opt.in
FePB	16	ct s-trans -tdfft	-3	6	B3LYP-D3(BJ)	cc-pVDZ	cpcm (78.39)	C_FePB_ctl_3sextet_camb3lyp_augccpVDZ_pcmH2O_tddft100.out	C_FePB_ctl_3sextet_camb3lyp_augccpVDZ_pcmH2O_tddft100.in
FePB* enol	21	R enol cc p-front -opt	-2	6	CAM-B3LYP	aug-ccpVDZ	cpcm (78.39)	C_FePBstar_enol_L_ccl_3sextet_b3lypD3bj_ccpVDZ_pcmH2O_opt.out	C_FePBstar_enol_L_ccl_3sextet_b3lypD3bj_ccpVDZ_pcmH2O_opt.in
FePB* enol	21	R enol cc p-front -tdfft	-2	6	CAM-B3LYP	aug-ccpVDZ	cpcm (78.39)	C_FePBstar_enol_L_ccl_3sextet_camb3lyp_augccpVDZ_pcmH2O_tddft100.out	C_FePBstar_enol_L_ccl_3sextet_camb3lyp_augccpVDZ_pcmH2O_tddft100.in
FePB* enol	22	R enol cc m-front -opt	-2	6	CAM-B3LYP	aug-ccpVDZ	cpcm (78.39)	C_FePBstar_enol_ccl_2pentet_b3lypD3bj_ccpVDZ_pcmH2O_opt_2.out	C_FePBstar_enol_ccl_2pentet_b3lypD3bj_ccpVDZ_pcmH2O_opt_2.in
FePB* enol	22	R enol cc m-front -tdfft	-2	6	CAM-B3LYP	aug-ccpVDZ	cpcm (78.39)	C_FePBstar_enol_ccl_2sextet_camb3lyp_augccpVDZ_pcmH2O_tddft100_2.out	C_FePBstar_enol_ccl_2sextet_camb3lyp_augccpVDZ_pcmH2O_tddft100_2.in
FePB* enol	23	R enol ct p-trans -opt	-2	6	CAM-B3LYP	aug-ccpVDZ	cpcm (78.39)	C_FePBstar_enol_L_ctl_3sextet_b3lypD3bj_ccpVDZ_pcmH2O_opt.out	C_FePBstar_enol_L_ctl_3sextet_b3lypD3bj_ccpVDZ_pcmH2O_opt.in
FePB* enol	23	R enol ct p-trans -tdfft	-2	6	CAM-B3LYP	aug-ccpVDZ	cpcm (78.39)	C_FePBstar_enol_L_ctl_3sextet_camb3lyp_augccpVDZ_pcmH2O_tddft100.out	C_FePBstar_enol_L_ctl_3sextet_camb3lyp_augccpVDZ_pcmH2O_tddft100.in
FePB* enol	24	R enol ct m-trans -opt	-2	6	CAM-B3LYP	aug-ccpVDZ	cpcm (78.39)	C_FePBstar_enol_ctl_2sextet_b3lypD3bj_ccpVDZ_pcmH2O_opt.out	C_FePBstar_enol_ctl_2sextet_b3lypD3bj_ccpVDZ_pcmH2O_opt.in
FePB* enol	24	R enol ct m-trans -tdfft	-2	6	CAM-B3LYP	aug-ccpVDZ	cpcm (78.39)	C_FePBstar_enol_ctl_S_2sextet_camb3lyp_augccpVDZ_pcmH2O_tddft100.out	C_FePBstar_enol_ctl_S_2sextet_camb3lyp_augccpVDZ_pcmH2O_tddft100.in